Chapter V

Implementation and Validation of GLEAMS-SF

DESCRIPTION OF GLEAMS

GLEAMS (Leonard et al., 1987; Knisel et al., 1992; Knisel, 1993) is a continuous, field-scale hydrology and chemical transport model like Opus, simulating the transport and transformations of nutrients and pesticides in the root zone and in surface runoff. It runs on a daily time step, using daily rainfall information. GLEAMS uses a modification of the SCS Curve Number method (William and La Seur, 1976) to predict runoff and a modification of the USLE (Onstad and Foster, 1975) to predict erosion. Potential ET is estimated in GLEAMS by either the Priestly-Taylor (1972) method, using daily temperature and radiation data interpolated from fitting mean monthly data (Kothandaraman and Evans, 1972), or the Penman-Montieth method (Jensen et al., 1990), which uses wind movement and dew point temperature fitted from monthly data (Kothandaraman and Evans, 1972) in addition to the temperature and radiation data. Actual soil evaporation and plant transpiration are simulated separately by the method developed by Ritchie (1972) for incomplete cover. Separate components of ET are needed to partition chemical movement upward in the soil and into the transpiration stream for plant uptake. Plant transpiration is extracted from the active root zone using an exponentially decreasing function.

The plant root zone effective for water uptake by crops is divided into a minimum of 3 and a maximum of 12 computational layers in GLEAMS depending on depth and thickness of soil horizons. A maximum of five soil horizons can be specified with varying soil properties. GLEAMS uses a capacity-based approach to simulate one-dimensional, vertical movement of water and solutes in the unsaturated zone. Water movement from one soil layer to the next is characterized by a system of linked linear storage utilizing three parameters – water content at field capacity (θ_{fc} or FC), water content at wilting point (θ_{wp} or BR15), and porosity (ϕ or POR). Saturated hydraulic conductivity (K_s or SATK) is also specified for each horizon in GLEAMS, and is used to calculate travel time. GLEAMS simulates the effect of restrictive soil layers or horizons that impede root growth and water movement (e.g., clay pan, plow pan, or a genetic layer such as plinthic or caliche material) by allowing the user to specify its saturated hydraulic conductivity (RC). The K_s for the horizon immediately below the effective root depth is used with a 30 cm thickness to calculate travel time in that horizon. If the K_s is the same or greater than that of the bottom horizon, the same values of θ_{fc}, θ_{wp}, and ϕ as that of the bottom horizon are used. If the K_s is less than that of the bottom horizon, characteristics of clay are assumed for θ_{fc}, θ_{wp}, and ϕ. Percolation is assumed to occur through the layer, but it is not allowed to move back up into the root zone since depth to water table is not known.

Although GLEAMS can simulate the transport and transformations of pesticides and plant nutrients, nitrogen and phosphorus, the description below is restricted to pesticides, which is the focus of this study. GLEAMS can simulate advective transport of pesticides in runoff, erosion, and with percolating water, considering foliar washoff, equilibrium adsorption, and first-order decay in foliage and soil. The model can simulate up to ten pesticides simultaneously. Chemical application can be partitioned between plant foliage and soil surface. Soil-applied chemicals can be surface-applied, incorporated to a certain depth, or applied by chemigation. The active surface layer for chemical extraction into runoff is set at a constant depth of 1 cm. Adsorption of pesticides is described by a linear isotherm (equilibrium adsorption), and is calculated from user specified values of K_{oc} and organic carbon content. Pesticide degradation in soil is calculated from soil half-life values, specified by the user, for each horizon, whereas pesticide degradation in plant foliage is calculated from the foliar half-life specified by the user. A plant uptake coefficient is used to vary the amount of dissolved solute transported to the plants during transpiration. GLEAMS allows the user to specify initial pesticide concentration levels in each soil horizon.

IMPLEMENTING GLEAMS IN THE STOCHASTIC FRAMEWORK

The spatially variable input parameters in GLEAMS were also generated by the LHS method, using @RISK software (Palisade Corporation, 1996), as the Opus parameters were generated. Truncated distributions were used for spatially variable parameters that result in physically impossible values. The values of water content at saturation, field capacity, and wilting point were, however, not truncated as truncation would lead to a very distorted (narrow) distribution than that described by the PDF. Instead, the samples which gave physically impossible values (i.e., a wilting point greater than field capacity), were truncated manually. Less than 1% of the trials led to physically impossible values, and these trials were excluded from the MCS. In the case of soil properties with statistically significant and physically meaningful trends, the trends were added back to the zero-mean random variates using the same method as with Opus. The input parameters generated by @RISK were output into Microsoft Excel (Microsoft, 1995a) spreadsheet, and the values of the spatially variable parameters for each trial were saved into a space-delimited text file. The number of trials was determined by considering the stability/convergence of the most variable output, pesticide leaching below the root zone.

Monte Carlo simulation of GLEAMS was performed using the batch procedure of Kumar and Thomson (1995), with minimal changes to the source code. Since GLEAMS had a separate output file for writing the output of selected variables, no modification was needed within the code for obtaining stochastic outputs. The batch procedure consists of a batch program (Appendix C) that uses several FORTRAN routines to provide control over repeated model execution, generate new input files and read output for each trial, and reset all flags once the required number of trials have been completed (Kumar and Thomson, 1995). Control over repeated model execution is provided by the routines MCCON and RSMCF. The MCCON routine always reads input from a file (mccon.dat), and initialization of a Monte Carlo run is achieved when a zero is read. This causes the routine to prompt for the number of trials which is written to another file (mcnrun.dat). The RSMCF routine simply reads the number in the mccon.dat file, increments it by one, writes this number to a new file with the same name, and displays the current trial number on screen. When MCCON reads a non-zero input from mccon.dat (at the start of a new trial), this number is compared with the required number of trials (from mcnrun.dat). If the number is greater than the required number of trials, MCCON creates a new file (endmc.dat) which signals the batch program to end the Monte Carlo run.

General purpose routines for generating new input parameter files and for writing the stochastic outputs were considered, but were found to be not feasible. This would include assigning identification numbers to all inputs that could potentially be treated as spatially variable, and initializing the linking routines. Instead, ad-hoc linking routines were used for generating new parameter files at the start of a trial (Kumar and Thomson, 1995). These ad-hoc routines were specific to the randomization of a particular set of input parameters, and had to be modified if a different set of input were to be randomized. In this study, the ad-hoc routines for hydrology and pesticide parameter files developed by Kumar and Thomson (1995) were modified and used. The linking routines read input from a base parameter file and the text file containing the values of the spatially variable parameters for each trial, and created a new parameter file by appropriate substitutions. The random inputs file contains vectors for each trial on a separate line, and the linking routines skip to the correct line by reading the current trial number (from mccon.dat). The model was executed, once the new input parameter files were generated for each trial. Input and output files were hard-wired, so that the model does not prompt for them each time it is executed. An output storage routine (RASOUT) was used to extract the desired output (water balance, soil water content, pesticide mass, and pesticide leaching) from the model output file for every trial, and write it to another file in abbreviated form. A listing of the output storage routine is given in Appendix C. The batch program then appends the abbreviated output to a file which contains the complete output for all trials at the end of the Monte Carlo run. Another routine (FINALMC) was used to reset all the flags at the end of the run. This involves deleting the file (endmc.dat) which signals the end of the Monte Carlo run, and rewriting mccon.dat with a zero, which insures that a new Monte Carlo run will be initiated the next time the batch program is used.

The execution of GLEAMS-SF for a 3-year simulation using 25 spatially variable parameters and 1400 trials takes approximately one hour on a Pentium Pro-200 MHz personal computer with 64 Mb memory. Version 2.10 of the GLEAMS model (Knisel, 1993) was used in this study. A unit conversion error with soil water content in the selected output algorithm was the only error encountered in the source code during the course of this study.

VERIFICATION AND VALIDATION OF GLEAMS-SF

The main objective of this part of this study was to 'partially' validate the performance of GLEAMS-SF for predicting spatial variations in subsurface soil water content and pesticide mass under field conditions. Since the deterministic model had already been verified extensively (Knisel, 1980; Knisel, 1993), an extensive verification of the code was not performed here. A sensitivity analysis of the model was performed to reveal any anomalies or unexpected effects using short, medium, and/or extreme perturbations of input parameters. The internal consistency of the model was verified by numerical testing using mass-balance checks of the output variables.

The performance of GLEAMS-SF in predicting subsurface water and pesticide transport in the root zone under field conditions was assessed using data from the two field studies: (i) a 3.9-ha agricultural field in the Dougherty Plain region of Georgia; and (ii) an 18x27 m (0.0486 ha) field plot in the Nomini Creek watershed in Virginia. The first step in the validation process consisted of a review and evaluation of data, where the spatially variable input parameters were tested for spatial correlation across the field and cross-correlation among them. This ensured that the assumptions in the stochastic framework regarding input data were met. The conceptual approach used to represent spatial variability in the stochastic framework, i.e., the field consisting of non-interacting, vertical one-dimensional stream tubes, could not be tested directly due to inadequate data. Finally, the results obtained from model predictions were then compared with field-measured data. The following output variables from GLEAMS-SF on the field sampling dates were considered for comparison with observed data: depth-averaged soil water content, depth-wise soil water content distribution, bromide mass, pesticide mass, and depth-wise pesticide mass distribution in the root zone.

Sensitivity Analysis of GLEAMS

Sensitivity analysis of GLEAMS, like that of Opus, was conducted by computing relative sensitivities of output variables, percolation loss, soil water content, and pesticide leaching below the root zone to parameters capable of affecting subsurface water flow and chemical transport from the Dougherty Plain field site. The model was used to simulate water flow and metolachlor mass in the 3.9-ha peanut field using actual rainfall, temperature, and radiation records from April 1 to September 30, 1985. The 1.2 m root zone was divided into the four horizons delineated in the field. The plinthite layer (1.2-1.5 m) was not physically added as another layer in GLEAMS; instead the K_s of the plinthite layer was specified as the K_s of the layer below the root depth that restricted water flow. A listing of the input parameters used in the sensitivity analysis and their base values are given in Table 29. The base values of the input parameters represent average values calculated from field-measured soil physical, biological, and pesticide properties at the Dougherty Plain field site (Hook, 1987; Smith et al., 1987; Smith and Parrish, 1993).

Results of Sensitivity Analysis

Relative sensitivity of total percolation loss below the root zone for the six month period, average soil water content over the six month period, and resident metolachlor mass remaining in the root zone at the end of the six month period to soil parameters and root depth are shown in Figures 25, 26, and 27, respectively. Relative sensitivity of resident metolachlor mass to pesticide-related parameters is shown in Figure 28. As with Opus, GLEAMS did not predict any metolachlor leaching losses at the Dougherty Plain site, and hence, that output was not used for the sensitivity analysis. The maximum relative sensitivity values obtained for GLEAMS were lower than those obtained for Opus.

Percolation loss was sensitive to water content at field capacity (FC) in all layers and wilting point (BR15) in the bottom two layers with an absolute S_R over 0.05. Soil water content was sensitive to saturated conductivity of the restricting plinthite layer (RC), initial plant-available water parameter (BST), and FC and BR15 in all layers, with an absolute S_R of over 0.05. The relative sensitivity of resident metolachlor mass in the 1.2 m profile to soil evaporation parameter (CONA), porosity (POR) and FC in all layers, and BR15 in the bottom two layers was over 0.05. Resident metolachlor mass in the 1.2 m profile was sensitive to the pesticide parameters, half-life (SOLLIF) and adsorption coefficient (KOC) with absolute S_R of 1.0, whereas absolute S_R of metolachlor mass to soil organic matter content (OM) in all layers was over 0.05.

The sensitivity analysis, therefore, shows that the parameters controlling water flow, POR, FC, and BR15, are important to movement of water and pesticides in all four horizons of the root zone. Movement and fate of pesticides in the root zone was sensitive to pesticide degradation half-life and adsorption coefficient. Water flow and/or pesticide movement were also sensitive to saturated hydraulic conductivity of the plinthite layer, initial plant-available water parameter, soil evaporation parameter, soil organic matter content, and crop rooting depth. Water flow or pesticide movement at the Dougherty Plain site did not exhibit any sensitivity to saturated hydraulic conductivity and clay content in the four horizons.

MODELING FLOW AND TRANSPORT AT THE DOUGHERTY PLAIN SITE

Development of Base Parameters

The simulation period consisted of three cropping seasons, from April 1, 1985 to September 10, 1987. Weather data used in the simulation consisted of daily values of rainfall and average daily temperature, and monthly values of minimum and maximum temperature and solar radiation for each year. The rainfall and temperature data were from the Dougherty Plain site, and solar radiation data from Albany airport (EarthInfo, 1995), 16 kilometers from the site. The runoff and erosion parameters were set so that there was no simulated runoff or sediment loss from the field. The soil profile was divided into four horizons, 0-0.3, 0.3-0.45, 0.45-0.75, and 0.75-1.2 m, with the rooting depth for peanuts set at 1.0 m. The initial plant-available water parameter (BST) was set to the value measured in the field on April 1, 1985. Soil hydraulic and retention properties and organic matter content, measured or estimated from field data, were used to describe each soil horizon. In order to represent the effect of a plinthite layer present in the field below the fourth horizon, K_s of the plinthite layer was specified as K_s of the restrictive soil horizon below the root zone.

Initial concentrations of the pesticides were set to zero based on analysis of background concentrations in the field. The planting and harvest dates of the peanuts for the three study years were set according to field observations. Laboratory values of pesticide half-lives in each horizon (Smith et al., 1987), and an average value of K_{oc} for each horizon, calculated from adsorption distribution coefficients (K_D) and organic matter content (Rao et al., 1986; Smith et al., 1987), were used in the simulations. Bromide was simulated as a conservative, non-reactive tracer with a zero degradation rate and a zero adsorption coefficient. Values for other parameters for which field data were not available were selected based on information and recommendations in the GLEAMS User Manual (Knisel et al., 1992); values for these parameters were described in detail in the corresponding section for Opus in the previous chapter.

Selection of Spatially Variable Parameters

Selection of the spatially-variable parameters to be used in the simulations was based on the sensitivity of the model to the parameter, physical considerations and availability of data. Among the soil parameters, water retention parameters (POR, FC, and BR15) in the four horizons were automatic choices to be described as spatially variable parameters due to their sensitivity and impact on water flow and solute transport. Initial plant-available water parameter (BST) and saturated hydraulic conductivity of the restricting plinthite layer (RC) were also sensitive and treated as spatially variable. Even though the soil evaporation parameter (CONA) was found to be a sensitive parameter, there were no data available to describe its spatial variability and therefore it was treated as a fixed parameter. Among the pesticide parameters, the pesticide degradation rate (SOLLIF) and the soil organic matter content (OM) in the four horizons, and the pesticide application rate(s) (APRATE) were selected to be spatially variable.

Statistical/Geostatistical Analysis of Spatially Variable Parameters

The spatial variability of the GLEAMS parameters were described using probability density functions (PDFs) fitted to measured field data. The soil physical parameters were also analyzed for spatial trends. The spatial variability analysis was conducted the same way as for the Opus parameters from the Dougherty Plain site. Truncated distributions were used when necessary so that all parameter values would be physically meaningful. Cross-correlation between soil physical parameters within a horizon were computed from the observed data and considered in the generation of input parameters. Statistical characteristics of the spatially variable soil properties and the cross-correlation coefficients among soil physical properties are given in Tables 30 and 31, respectively.

The spatially variable pesticide parameters in GLEAMS (half-life, application rate) were the same as in Opus, with the only exception that GLEAMS uses half-life instead of degradation rate, to describe pesticide degradation in soil. Soil half-life values for each horizon were generated separately assuming a lognormal distribution and using the mean and standard deviation obtained from laboratory measurements (Table 32). Correlation between half-life in one horizon and the remaining horizons, computed from the laboratory measurements (Table 33), were used in the generation of half-lives for the four horizons. Spatial variability in pesticide sorption was represented by spatial variations in organic matter content.

Number of Trials

The median, 10th and 90th percentiles of percolation loss predicted by GLEAMS-SF at the end of the 1985, 1986, and 1987 cropping seasons as a function of the number of trials are given in Figure 29a, and corresponding values for aldicarb leaching as a function of the number of trials are given in Figure 29b. The median, 10th and 90th percentiles of percolation loss in all three years converged by 500 trials. With the exception of the 90th percentile of aldicarb leaching loss in 1986 and 1987 which fluctuated close to 1400 trials, all other values of aldicarb leaching had converged by 1000 trials. It was decided to run GLEAMS for 1400 trials, the same number of trials as Opus. The execution of GLEAMS-SF for a 3-year simulation for 1400 trials using 25 spatially variable parameters took approximately an hour on a Pentium Pro-200 MHz personal computer with 64 Mb memory.

Generation of Spatially Variable Parameters

Spatially variable parameters were generated as for Opus-SF, for which the details were given in the previous chapter. Input parameters that exhibited spatial trends were generated using the PDF and distribution parameters estimated from the detrended residuals (Table 30), while the other parameters were generated using the PDF and distribution parameters estimated from the measured data (Table 30, Table 32). Correlated variates of soil physical properties in each horizon were generated using the correlation matrix in Table 31a. Correlated variates of soil organic matter content in the different horizons were generated using the correlation matrix in Table 3b. Soil half-life of aldicarb and metolachlor for the four horizons were generated using correlation coefficients (Table 31b,c) computed from laboratory measurements. All other spatially variable parameters were generated assuming no correlation.

Truncation limits for the soil properties were set to physically reasonable values, by considering the minimum and maximum values observed in the field. Minimum values for BST, BR15, OM were set to zero so as to avoid negative values. Minimum values for other properties were set lower than the minimum value measured in the field. Maximum values for all spatially variable soil properties were set greater than the field-measured maximum for the property. Truncation limits for detrended residuals were computed by inserting the minimum and maximum values into the trend equation.

Even though water content at field capacity should always fall between water content at wilting point and porosity, truncation was not used as it led to a very distorted distribution of field capacity. Instead, the few trials that had field capacity greater than porosity or less than BR15 in any of the soil layers were removed from analysis. A total of 17 trials were thus removed. There were no run-time errors for the GLEAMS-SF simulation. Therefore, analysis of output variables from GLEAMS-SF was based on 1393 trials.

Comparison with Observed Data

Water Balance

Mean monthly ET and percolation predicted by GLEAMS-SF over the simulation period are given in Table 34, along with monthly rainfall measured at the site, and ET and percolation amounts predicted by the deterministic version of GLEAMS. ET, as expected, was high in the summer months and low in the winter months. Percolation, on the other hand, was almost zero in the summer months and high in the winter when there was a lot of precipitation. From the ET and percolation values, it is obvious that there were soil water deficits in the root zone in some months, particularly in summer. In line with the field observation, parameters were selected so that no runoff was predicted.

The monthly ET predicted by a deterministic simulation of GLEAMS, using average values of the stochastic input parameters, were not much different from the mean monthly ET and percolation values predicted by GLEAMS-SF. There was almost no difference between monthly ET predicted by GLEAMS-SF (mean) and GLEAMS for eight months from October 1985 and for nearly a year from July 1986. The highest difference in monthly ET predictions by Opus-SF (mean) and Opus was about 3 mm in September 1985. The net difference between monthly ET predicted by deterministic GLEAMS and GLEAMS-SF (mean) over the entire simulation period was about 8 mm, with the deterministic version predicting more ET. Monthly percolation predicted by the deterministic version was sometimes greater than the mean predicted by GLEAMS-SF, while the opposite was true in most other months. The largest difference between the two was about 12 mm in November 1985. Over the entire simulation period, GLEAMS-SF (mean) predicted about 23 mm of percolation more than deterministic GLEAMS.

Soil Water Content

Depth-averaged soil water contents predicted by GLEAMS-SF on the field measurement dates and at the end of every month are shown in Figure 30, along with corresponding depth-averaged soil water content predicted by deterministic GLEAMS and daily rainfall measured at the site. The observed data on sampling dates where soil water content was measured from at least the upper 0.9 m are shown in Figure 30. The mean, minimum, and maximum values of depth-averaged soil water content varied seasonally, with values decreasing in summer and increasing in winter.

GLEAMS-SF predicted the mean of depth-averaged soil water content well on three of the five sampling dates, excluding the simulation start date (Fig. 30). The Mann-Whitney test showed that the observed medians were significantly different ($\alpha = 0.01$) from the simulated medians on all dates except in late-June/July of each year (Table 35). The simulated standard deviations were less than the observed standard deviations, except for the drought period in 1986 and June 12, 1985. The simulated range, however, was always greater than the observed range, and remained almost constant throughout the study period. The range statistics indicated that a majority (more than 85%) of the depth-averaged soil water content observations fell within the simulated range (Table 35). The observed mean was within the simulated range on all sampling dates, and the simulated mean was within the observed range on all dates (Fig. 30). The KS test showed that the distribution of observed and simulated depth-averaged soil water content were not significantly different ($\alpha = 0.05$) on July 22, 1985, July 8, 1986, and June 28, 1987 (Table 35). On July 27, 1987, the differences between the distribution of observed and simulated depth-averaged soil water content were not significantly different at the 0.01 level.

Depth-wise distributions of soil water content simulated by GLEAMS-SF are compared with observed data on the same four dates as with Opus-SF (Fig. 31). As expected, GLEAMS-SF, with the capacity-based water flow routing, was not able to predict the shape of the observed soil water profile as well. GLEAMS-SF showed a trend of underpredicting the observed soil water content in the upper horizons and overpredicting soil water content in the lower horizons.

GLEAMS-SF overpredicted the observed ranges of soil water content mainly in the lower depths on the four dates (Fig. 31). However, the overprediction was not too large, considering the fact that the simulated minimum was well below the observed minimum on the simulation start date (Fig. 30).

Since the observed range derived from 20 observations may not describe the entire range of soil water content present in the field, one cannot conclude that the model was doing a poor job of predicting the spatial variability of soil water content in the field. Range statistics calculated on soil water content from the different depths on the four dates (data not shown) showed that almost all observations on these four dates fell within the simulated range.

Comparison between soil water content simulated by the deterministic version of GLEAMS and the mean value obtained from GLEAMS-SF indicated that the differences between the two were very small. The depth-averaged values (Fig. 30) show that there were some differences initially and in December 1985, when there was significant rainfall. Depth-wise distribution of soil water content (Fig. 31) showed noticeable differences between the two model versions on July 22, 1985, especially in the lower depths. As discussed earlier, such differences are caused by the spatial characterization of the parameters as well as nonlinearity in model response.

Bromide Mass

The observed mean and range of bromide mass in the field on 14 sampling dates over the two and a half year simulation period are shown along with mean and range predicted by GLEAMS-SF in Figure 32. Bromide mass continued to decrease with time. By February of 1986 (approximately 300 days after application), mean bromide mass in the 1.2 m profile had gone below 0.1 kg ha^{-1} and the maximum value had gone below 1 kg ha^{-1}. Like Opus-SF, bromide loss predicted by GLEAMS-SF early in the simulation period was mainly due to plant uptake. Leaching below the root zone did not take place in substantial amounts until the large rainfall events in October, November, and December of 1985. The observed data, however, showed bromide to remain in the profile in appreciable amounts throughout the study period. Less than 20 kg ha^{-1} of bromide was detected on the first three dates (until Aug. 26, 1985), after which the bromide mass detected increased to nearly 40 kg ha^{-1} and then gradually decreased.

As explained in the previous chapter, the difference in observed and simulated bromide leaching may be due to more than one reason. Retention of bromide in field soils for prolonged time could not be adequately explained. Plant uptake of bromide was perhaps higher than what occurred in the field, and GLEAMS, like Opus, does not simulate dispersion in soil which may affect predicted leaching rate.

The Mann-Whitney test showed that the observed and simulated medians of total bromide mass in the root zone were significantly different on all dates except Aug. 26, 1985 at $\alpha = 0.05$ and June 12, 1985 at $\alpha = 0.01$ (Table 36). The KS test showed that the EDFs of observed and simulated bromide mass were significantly different ($\alpha = 0.01$) on all dates except Aug. 26, 1985 (Table 36). The simulated standard deviations were much less than the observed standard deviations. Range statistics showed that more than 45% of the observations on the first three dates was inside the simulated range (Table 36). As described in the last chapter, the observed data from the first three dates seemed to reflect incomplete recovery of bromide, and therefore, the range statistics and the statistical test results from these dates may not be reliable. After Aug. 26, 1985, none of the bromide mass observations were within the simulated range, with the exception of May 18, 1987 when two of the observations were zero.

Aldicarb Mass

The simulated mean and range of aldicarb mass are shown in Figure 33 with observed data on the field sampling dates. Summary statistics and results from statistical tests between observed and simulated data are given in Table 37. The mean values of aldicarb mass were generally overpredicted by GLEAMS-SF, with the differences between observed and simulated mean increasing as the cropping season progressed. The Mann-Whitney test showed that there were significant differences ($\alpha = 0.05$) between observed and simulated medians of aldicarb mass on all field sampling dates, except June 12, 1985 and April 30, 1986 (Table 37).

The observed standard deviation and maximum values of aldicarb mass were also overpredicted on most dates (Table 37, Fig. 33). However, since the simulated maximum values were much more than the observed maximum and because the observed sample size was small for such a large field, the larger maximum value on some of the earlier post-application dates may be expected. The range statistics showed that almost all of the observations were within the simulated range, except on July 27, 1987 when 30% (6/20) of the observations were outside the simulated range (Table 37). The observed mean was within the simulated range, and simulated mean was within the observed range on all field sampling dates. The KS test showed that there were no significant differences ($\alpha = 0.05$) between observed and simulated EDFs of aldicarb mass on all the field sampling dates, except June 12, 1985 and Apr. 30, 1986 (Table 37).

The reasonable performance of GLEAMS-SF in predicting aldicarb mass is also evident from Figure 34, where the observed and simulated depth-wise distribution of aldicarb mass on four dates are plotted. GLEAMS-SF predicted higher aldicarb mass than what was observed in the field in the top horizon, with the exception of April 30, 1986. At all other depths, GLEAMS-SF predictions were generally lower but comparable to what was observed in the field. It is hard to say whether the higher mass in the top horizon was the result of inaccurate degradation and/or adsorption parameters, as postulated in the previous chapter. On the two 1987 dates, GLEAMS-SF overpredicted the observed range considerably.

There were some differences between deterministic predictions and mean values of aldicarb mass predicted by GLEAMS-SF. The depth-wise aldicarb mass distribution predicted by the two model versions on June 28 and July 27, 1987 (Fig. 34c,d), show clearly the differences between the two model versions, with deterministic GLEAMS predicting more aldicarb mass in the 0-0.30 m layer than mean value predicted by GLEAMS-SF.

Metolachlor Mass

The mean and range of observed and simulated metolachlor mass in the 1.2 m profile over the entire simulation period are shown in Figure 35, while the summary statistics and statistical test results are given in Table 38. GLEAMS-SF underpredicted mean total metolachlor mass in the root zone in 1985 and 1986, and overpredicted mean metolachlor mass in 1987. The Mann Whitney test showed that the observed and simulated medians were significantly different ($\alpha = 0.01$) on all the sampling dates, except June 12 and July 22, 1985 (Table 38).

The simulated standard deviations were considerably less than the observed standard deviations in 1985 and 1986, and were comparable to the observed standard deviations in 1987. Likewise, the simulated range was much less than the observed range in 1985 and 1986 (except for the application date), while the simulated range was greater than observed range on the application date and the two sampling dates in 1987. The reduced variation in the 1986 (and possibly 1985) sampling dates may be because of low rainfall soon after pesticide application, causing GLEAMS-SF to predict very little metolachlor to move by leaching. Observed data, however, shows that there was movement of metolachlor in the field (Fig. 36). The observed mean was not within the simulated range, and the simulated mean was not within the observed range on June 17 and July 8, 1986. Range statistics showed that none of the observations were within the simulated range on June 17, 1986, and only 4 of the observations (20%) were within the simulated range on July 8, 1986 (Table 38). The KS test showed that the EDFs of metolachlor mass were significantly different (α = 0.05) on all sampling dates (Table 38).

The depth-wise distribution of metolachlor mass (Fig. 36) showed that mean metolachlor mass was predicted close to the observed data on July 22, 1985, slightly underpredicted on April 30, 1986, and overpredicted on the two 1987 dates. Most of the pesticide remained in the upper 0.3 m, as metolachlor is a strongly adsorbed and highly degradable herbicide. On the two 1987 dates, GLEAMS-SF overpredicted the observed range considerably.

There were some differences between predictions of metolachlor by the deterministic version of GLEAMS and the mean predicted by GLEAMS-SF (Fig. 36). As with the aldicarb predictions, the deterministic version of GLEAMS on the two 1987 dates overpredicted and was farther away from the observed metolachlor mass in the upper 0.3 m than the mean predicted by GLEAMS-SF (Fig. 36c,d).

Comparison with Traditional Monte-Carlo Simulation

Statistical tests were performed to determine if the output variables (depth-averaged soil water content, bromide, aldicarb, and metolachlor mass) predicted by the two approaches were the same, and to compare the GLEAMS-MC predictions with observed data. The two sample KS test was used to test for significant differences between EDFs predicted by GLEAMS-SF and GLEAMS-MC, and the observed EDF and the EDF predicted by GLEAMS-MC. The Mann-Whitney test was used to test for significant differences between medians predicted by GLEAMS-SF and GLEAMS-MC, and the observed median and the median predicted by GLEAMS-MC. Comparisons between outputs from the two models were made considering the entire 1.2 m profile, whereas comparisons with observed data on the field sampling dates were made using model output from the depths at which field measurements were taken.

Water Balance and Soil Water Content

There was very little difference in the monthly ET and percolation amounts predicted by GLEAMS-MC and GLEAMS-SF (Table 39). In the months which showed the differences, GLEAMS-MC predicted more ET and less percolation than GLEAMS-SF. It is interesting to note that the opposite trend was seen with Opus, showing that the addition of the deterministic trend component had different effects on results from the two models. Over the entire simulation period, GLEAMS-MC predicted approximately 5 mm of ET more than GLEAMS-SF, with the maximum difference in one month (Aug. 1987) being approximately 0.9 mm. GLEAMS-MC predicted approximately 4 mm of percolation less than GLEAMS-SF over the simulation period, with the maximum difference in one month (Aug. 1987) being approximately 1.4 mm.

The two sample KS test on the depth-averaged soil water content EDFs predicted by GLEAMS-MC and GLEAMS-SF showed that the distributions were not significantly different ($\alpha = 0.05$) on all sampling dates (Table 40). The Mann-Whitney test also showed that the depth-averaged soil water content medians predicted by GLEAMS-MC and GLEAMS-SF were not significantly different ($\alpha = 0.05$) on all dates (Table 40). These results were in spite of the fact that the EDFs and medians of soil water content predicted by GLEAMS-MC and GLEAMS-SF were significantly different on the simulation start date. Thus, including spatial trends of the soil retention properties in the second soil horizons (Table 30) had no impact on soil water results from the stochastic simulation of GLEAMS.

The p-values obtained from KS and Mann-Whitney tests by comparing GLEAMS-MC predictions and observed data were not much different than the p-values obtained by comparing GLEAMS-SF predictions and observed data (Table 35). At $\alpha = 0.05$, GLEAMS-MC showed that there were no significant differences between the observed and the simulated EDFs and medians on the same dates as GLEAMS-SF. At $\alpha = 0.01$, GLEAMS-MC resulted in one less rejection of the null hypothesis (on Mar. 24, 1986) than GLEAMS-SF; but even on that date, the p-values were close to one another (0.0105 and 0.0091).

Bromide Mass

There were some differences between bromide leaching losses predicted by the two models. There were some differences between model predictions in November-December of 1985 (about 0.1 kg ha^{-1}), when most of the leaching took place. The net difference in bromide leaching predicted by the two models was approximately 0.3 kg ha^{-1} (0.5% of applied amount), with GLEAMS-SF predicting more leaching than GLEAMS-MC.

The EDFs of bromide mass predicted by GLEAMS-MC and GLEAMS-SF were not significantly different ($\alpha = 0.05$) on the first sampling date, 56 days after application (Table 41). On the next four dates (until 236 days after application), the EDFs predicted by the two models were significantly different at the 0.05 level but were not significantly different at the 0.01 level (on three dates). These were the dates when GLEAMS-MC and GLEAMS-SF were predicting large bromide leaching losses. The EDFs were not significantly different on all subsequent dates. The Mann Whitney test also gave somewhat similar results for the medians predicted by GLEAMS-MC and GLEAMS-SF as the KS test (Table 41). Therefore, there were some differences in the EDFs and medians of solute mass predicted by GLEAMS-MC and GLEAMS-SF, especially during the time when considerable leaching was taking place.

The p-values obtained from the KS and the Mann-Whitney tests by comparing bromide mass predictions from GLEAMS-MC and observed data were not much different than the p-values obtained by comparing GLEAMS-SF predictions and observed data (Table 36). It was difficult to determine which was closer to observed data, as the GLEAMS-MC predictions were closer to observed data on some sampling dates, and the GLEAMS-SF predictions were closer to observed data on other dates. At $\alpha = 0.05$, GLEAMS-MC resulted in one less rejection of the null hypothesis (on July 22, 1985) than GLEAMS-SF; but even on that date, the p-values were close to one another (0.0582 and 0.0417).

Pesticide Mass

There was hardly any aldicarb or metolachlor leaching predicted by both GLEAMS-MC and GLEAMS-SF, so it was meaningless to compare predictions from the two models. The distributions as well as the medians of aldicarb mass predicted by GLEAMS-MC and GLEAMS-SF were not significantly different ($\alpha = 0.05$) on all post-application dates within the cropping season (Table 42). The only case that resulted in rejection of the null hypothesis was on Apr. 28, 1987 (386 days after application), when there was hardly any of the pesticide remaining in the profile. With metolachlor also, the statistical tests did not show any significant differences ($\alpha = 0.05$) between the distributions as well as the medians predicted by GLEAMS-MC and GLEAMS-SF (Table 43).

The p-values obtained from the KS and the Mann-Whitney tests by comparing aldicarb and metolachlor mass predictions from GLEAMS-MC and observed data were very close to the p-values obtained by comparing GLEAMS-SF predictions and observed data (Tables 37 and 38). At $\alpha = 0.05$ and 0.01, GLEAMS-MC resulted in rejection of the null hypothesis on the same dates as GLEAMS-SF for both aldicarb and metolachlor mass. Therefore, there were hardly any differences between pesticide mass predicted by GLEAMS-MC and GLEAMS-SF, although there were some differences between bromide mass predicted by the two models.

Summary

Soil water properties and organic matter content in the four horizons, saturated hydraulic conductivity of the plinthite layer, initial water storage parameter, pesticide degradation rate in the four horizons, and pesticide application rates in the three years were selected as the spatially variable input parameters for the stochastic simulation of water flow and pesticide transport at the Dougherty Plain site using GLEAMS-SF. In the stochastic simulation of bromide, all of the above parameters except organic carbon content and degradation rates were considered spatially variable. Bromide was also applied only once in 1985. The spatially variable parameters were described by their PDFs, after analyzing them for spatial trends. For the variables with physically meaningful and statistically significant trends, the trends were removed before PDF analysis and later reinstated after generation of random variates. Correlation between the soil properties within a horizon was also considered in the input parameter generation.

GLEAMS-SF simulated seasonal variations in the water balance by predicting high ET during the summer and low ET in the winter months. Percolation was almost zero in the summer months and high in the high rainfall months in the fall and winter. High ET demands during the summer months led to soil water deficits in the root zone.

GLEAMS-SF overpredicted the mean of depth-averaged soil water content on most of the field sampling dates except two dates during the drought period in 1986. The observed and simulated soil water contents were not significantly different ($\alpha = 0.01$) in late June-July of each year. Spatial variations in simulated soil water content were less than the observed variation on all except the three sampling dates in the drought period of 1986. More than 85% of the depth-averaged soil water content observations on all sampling dates fell within the simulated range. GLEAMS-SF, with the capacity-based water flow routing, was not able to predict the shape of the observed soil water profile well.

GLEAMS-SF, like Opus-SF, was not able to predict the field-scale movement of bromide well. GLEAMS-SF overpredicted bromide mass in the field for the first two months after application, after which it predicted extensive loss of bromide from the root zone due to plant uptake and leaching. The simulated maximum was less than the observed minimum after about 225 days of application. The mean bromide mass simulated by GLEAMS-SF was less than 1 kg ha^{-1} after approximately 270 days after application, whereas mean bromide mass observed in the field was never below 10 kg ha^{-1} for over 700 days after application. Plant uptake and leaching of bromide was overpredicted by GLEAMS-SF. A general conclusion regarding bromide transport could not be reached due to the inconsistency of the observed data and lack of explanation for bromide retention in soil.

The mean of the total aldicarb mass in the root zone was overpredicted by GLEAMS-SF, with the differences between observed and simulated mean increasing with time. The observed and simulated medians and EDFs of aldicarb mass were not significantly different ($\alpha = 0.01$) on the first sampling date in 1985 and 1986. Simulated standard deviation of aldicarb mass was greater than observed standard deviation on all dates except the first sampling date in 1985 and 1986, and the simulated maximum was greater than the observed maximum on all dates except the first sampling date in 1986. Thus, the spatial variability of aldicarb mass simulated by GLEAMS-SF was greater than the observed variability, except in the early stages of the 1985 and 1986 crop years. Over 90% of the observations were contained in the simulated range on all sampling dates except the last sampling date in 1987. GLEAMS-SF, however, could not predict the depthwise distribution of aldicarb mass well on most sampling dates, as it overpredicted mass in the first horizon and underpredicted mass in the lower horizons.

GLEAMS-SF underpredicted the mean metolachlor mass in 1985 and in 1986, but overpredicted it in 1987. Observed and simulated medians were not significantly different ($\alpha = 0.01$) on the first two sampling dates in 1985. Like Opus-SF, spatial variations in metolachlor mass predicted by GLEAMS-

SF were less than the observed variations on all dates except the last date in 1987. The observed and simulated EDFs of total metolachlor mass in the root zone was significantly different (α = 0.01) on all sampling dates. Range statistics of total metolachlor mass were greater than 50% in one sampling date in 1985 and 1986, and all dates in 1987. The depth-wise distribution of metolachlor mass was predicted well on some dates, whereas mean and range of metolachlor mass in the top horizon was overpredicted on other dates (mainly in 1987). In the two 1987 dates, GLEAMS-SF overpredicted the observed mean and range considerably in the upper 0.3 m. Like Opus-SF, GLEAMS-SF was able to predict total pesticide mass in the root zone much better than total bromide mass.

The deterministic version of GLEAMS predicted soil water content, bromide and pesticide mass similar to the mean values obtained from the stochastic simulation of GLEAMS. There were some differences in the water balance: the deterministic GLEAMS predicted about 8 mm more of ET than GLEAMS-SF (mean), and predicted about 23 mm more of percolation than GLEAMS-SF, over the entire simulation period. This difference resulted in some differences in soil water content and in the solute mass predicted by the two versions. Such differences were influenced by the characterization of the spatially variable parameters and the non-linear response of GLEAMS.

A comparison of stochastic outputs from GLEAMS-SF and GLEAMS-MC, in which spatial trends are not considered in the description of the spatially variable parameters, showed that there was very little difference between the two. The only noticeable difference between the two models was in their bromide mass predictions. GLEAMS-SF predicted more bromide leaching losses than GLEAMS-MC in November-December 1985, when most of the leaching took place. This difference was corroborated by statistically significant differences in bromide mass in the profile during that time period. In comparison to observed data, it was hard to distinguish which model predicted bromide mass better than the other. A better judgment could have been made if there were additional sampling dates in one cropping season and if the trend was better characterized using more sampling points. Overall, spatial trends in only two of the soil retention parameters (POR and B15) in the second horizon were not enough to cause a change in the prediction of GLEAMS-SF as compared to GLEAMS-MC.

MODELING FLOW AND TRANSPORT AT THE NOMINI CREEK SITE

Development of Base Parameters

The simulation period started on the day before corn planting, April 22, 1990 (day 112), and ended on the harvest date, September 30, 1990 (day 273). Weather data used in the simulation consisted of daily values of rainfall, monthly values of minimum and maximum air temperature, and solar radiation. Runoff was not simulated in the model; instead, the measured runoff was subtracted from rainfall on runoff-producing days. This assumption was considered reasonable for the runoff volume observed from the plot (total runoff observed over the 6-month study period was approximately 55 mm). Runoff cannot be accurately simulated using the stochastic stream tube approach without considering routing from one tube to the other. Because average initial water content in the plot was slightly above field capacity, BST was set to its maximum value of 1.0.

The soil profile was characterized into five depth layers, 0-0.15, 0.15-0.3, 0.3-0.45, 0.45-0.6, and 0.6-0.9 m, with an effective corn rooting depth of 0.9 m. Because the last horizon in GLEAMS must end at the rooting depth, only the top 0.9 m of the plot could be simulated. Soil water properties (POR, FC, BR15) for the stochastic simulation were estimated, as for Opus parameters, using texture data. Porosity was computed from field-measured bulk density. Field capacity was assumed to be water content at 20 kPa (0.2 bar), and was computed from sand, clay, porosity, and organic matter content values using the regression equation provided by Rawls et al. (1982). Residual water content was computed from sand, clay, and porosity values using the regression equation provided by Rawls and Brakensiek (1985). Soil properties used to estimate soil hydraulic and retention properties are summarized in Table 15.

Initial concentrations of bromide, atrazine and metolachlor were set to zero, as there were no residues left from previous applications. Pesticide and bromide application rates measured in the NT plot using filter papers (Heatwole et al., 1997) were used in the simulation. Sources of all pesticide properties used in GLEAMS were the same as in Opus, and are described in detail in the previous chapter. As described there, atrazine half-life of 60 days and metolachlor half-life of 18 days was used in the surface soil layer (0-0.15 m). Since there were no data available for atrazine half-life in the subsurface horizon, it was decided to use the method used in Opus (reducing the degradation rate by the ratio of organic carbon in the subsurface and surface layer) to compute half-life in the subsurface soil layers.

The simulation domain consisted of the top 0.9 m of the NT plot area (Fig. 16). The simulation was performed with the entire domain (18x27x0.9 m) as no-till, and simulated data were compared with observed data from the 0.9 m profile in the no-till plot.

Selection of Spatially Variable Parameters

Selection of the spatially-variable parameters to be used in the simulations was based on the sensitivity of the model to the parameter, physical considerations and availability of data. The soil water properties (POR, FC, BR15) were treated as spatially variable parameters as they were sensitive to water flow and solute transport. However, these properties were considered spatially variable only in the upper 0.6 m, as they were not expected to be sensitive in the coarser-textured soil lying beneath the argillic horizon. For the same reason, saturated hydraulic conductivity of the layer below rooting depth (RC) was also not sensitive. Even though the initial water parameter, BST, was a sensitive parameter, there were not enough data to specify its distribution. The soil evaporation parameter (CONA) was once again treated as a fixed parameter, due to unavailability of data. Among the pesticide parameters, soil half-life and soil organic carbon content in the upper 0.6 m, and the pesticide application rate(s) were selected to be spatially-variable. Spatial variability of pesticide sorption was represented by spatial variations in organic carbon content.

Statistical/Geostatistical Analysis of Spatially Variable Parameters

The method used to estimate soil water properties (FC, BR15) at the Nomini Creek site, using the regression equations of Rawls et al. (1982) and Rawls and Brakensiek (1985) consisted of: (i) generating the required number of trials (1350 trials) of sand, clay, porosity, and organic matter content from the field-measured data; and (ii) calculating the soil water parameters for each trial from the generated sand, clay, porosity, and organic matter content values using the regression equations.

The results from PDF, correlation, and trend analysis of sand and clay content, porosity, and organic matter content are described in the previous chapter, and are summarized in Tables 15 and 16. Soil water parameters computed from the regression equations are summarized in Table 44. Among pesticide parameters, soil half-life in each soil layer was assumed to follow a lognormal distribution. Statistical characteristics of the soil half-life values, along with pesticide application rates and other important fixed pesticide parameters at the Nomini Creek site, are given in Table 45.

Generation of Spatially Variable Parameters

Sand, clay, and porosity values were generated with @RISK software (Palisade Corporation, 1996) using the LHS method, details of which are given in the previous chapter. Sand and clay content that exhibited spatial trends were generated using the PDF and distribution parameters estimated from the detrended residuals (Table 15), while the other parameters were generated using the PDF and distribution parameters estimated from the measured data (Table 15, Table 45). The spatial trends were added back to each of the zero mean (detrended) random variates, by using a 0.6x0.6 m grid (which resulted in a total of 1350 grids covering the field area). Correlated variates of soil physical properties in each horizon were generated using the correlation matrix in Table 16a.

Truncation limits for sand and clay content were set such that their total did not exceed 100, which is physically impossible. Truncation limits for detrended residuals were computed by inserting the minimum and maximum values into the trend equation. There were also five other trials where the saturated water content was low and less than field capacity. These six trials were not considered in the stochastic simulation.

Simulation of GLEAMS-SF did not result in any run-time errors. Therefore, a total of 1344 trials were available for analysis of soil water, bromide, and pesticide outputs.

Comparison with Observed Data

Water Balance

Mean monthly ET and percolation predicted by GLEAMS-SF and deterministic version of GLEAMS over the simulation period are given in Table 46, along with monthly rainfall and runoff measured at the plot. [As described earlier, rainfall excess, obtained by subtracting field-measured runoff from rainfall, was provided in the rainfall file. Over 90% of the total runoff from the NT plot was produced during the very large rainfall events on day 146 (104 mm), day 149 (105 mm), and day 235 (91 mm)].

The high rainfall in May resulted in approximately 200 mm of water percolating below 0.9 m. Monthly ET was close to or higher than 100 mm from July through September. There was not much percolation from the root zone during these months, with the exception of some percolation due to rainfall in August. As with Opus-SF, the total runoff, ET, and percolation values indicated that there was a net loss of soil water storage over the simulation period.

Monthly ET predicted by the deterministic version of GLEAMS was lower than the mean values predicted by GLEAMS-SF in the months of July through September, whereas monthly percolation predicted by deterministic GLEAMS was higher than GLEAMS-SF mean in August. The differences, however, were small. The total difference in monthly ET predictions by GLEAMS-SF (mean) and GLEAMS was 6 mm, with the maximum difference of approximately 5 mm in July. The total difference in monthly percolation was approximately 3 mm (Table 46). These results showed either that spatial characterization of soil parameters and non-linearities in the model did not have a strong influence on monthly water balance, or that their effects were averaged out during the six-month period.

Soil Water Content

The mean, minimum and maximum values of depth-averaged soil water content predicted by GLEAMS-SF are shown in Figure 37, along with corresponding deterministic values and the observed mean and range on the field sampling dates and daily rainfall measured at the site. Results from the statistical comparison of observed and simulated (GLEAMS-SF) depth-averaged soil water content are given in Table 47. The summary statistics, p-values from the Mann-Whitney test for equality of medians and Kolmogorov-Smirnov (KS) test for equality of EDFs, as well as the range statistic (the percentage of observations in simulated range), are given in Table 47. Depthwise distributions of soil water content in the root zone on two of the sampling dates (days 118 and 209) are shown in Figure 38.

GLEAMS-SF predicted depth-averaged soil water content (mean and to some extent, the range) fairly well except on day 118 and 272, when it underpredicted soil water content measured in the field (Fig. 37). The underprediction on day 118 was partly due to the fairly high water content in the field at the start of the simulation. The BST parameter, used in GLEAMS to specify initial water condition, can only set the water content in the field to be between field capacity and wilting point; the depth-averaged soil water content in the field on day 112 was, however, about 0.04 mm mm^{-1} more than the average field capacity. The mean and median of depth-averaged soil water content on all field sampling dates were almost identical (Table 47), implying that their distributions were symmetrical. Soil water content medians predicted by GLEAMS-SF were significantly different than the observed medians on all dates except day 128 at the 0.05 level of significance and on all dates except days 128 and 145 at the 0.01 level of significance.

The simulated range was almost the same throughout the study period, except for the dry period in July-August. The smaller standard deviation (Table 47) and range (Fig. 38) predicted by GLEAMS-SF on all six sampling dates showed that simulated variation of depth-averaged soil water content was much less than what was observed in the field. The smaller variation in depth-averaged soil water content in the root zone is attributed to two reasons: (a) soil physical properties derived from texture data are less variable than their field-measured values; and (b) there was no variation in the 0.6-0.9 m depth (Fig. 38), as spatial variability of soil physical properties were considered only up to 0.6 m. Simulated range and standard deviation of depth-averaged soil water content from the upper 0.6 m was still lower than the corresponding observed range and standard deviation (data not shown), indicating that point (a) was the dominant cause for the reduced simulated variation. The above statement can also be substantiated by the fact that the simulated range was lower than the observed range of soil water content in the first four soil layers (0-0.6 m) on days 118 (Fig. 38a).

The KS test showed that the observed and simulated EDFs of depth-averaged soil water content were significantly different on all dates at $\alpha = 0.05$ and on all dates except day 128 at $\alpha = 0.01$ (Table 47). The range statistic indicated that except for days 128 and 145, less than 50% of the observations were within the simulated range. The observed mean was within the simulated range on all dates except days 118 and 272, whereas the simulated mean was within the observed range on all six dates.

Depth-wise distribution of observed and simulated soil water content (Fig. 38) showed that GLEAMS-SF was not able to predict the depth-wise variation in soil water very well. There was no variation in soil water content in the 0.6-0.9 m, as variation in soil water properties was considered only up to 0.6 m. The simulated range was less than observed range on all depths on day 118, and on all except 0.15-0.3 m and 0.45-0.6 m depths on day 209. On both dates, the observed mean was within the simulated range on all depths except 0-0.15 m and 0.6-0.9 m, whereas the simulated mean was within the observed range on all depths except 0-0.15 m.

Comparison of the mean depth-averaged soil water content predicted by GLEAMS-SF and corresponding predictions by deterministic GLEAMS showed that there were some differences, especially in the first two months and last two months of the simulation period (Fig. 37). The differences can be more clearly seen in Figure 38. On days 118 and 209, GLEAMS predicted lower soil water content in the root zone than GLEAMS-SF mean except for 0-0.15 m. These differences were influenced by the characterization of the spatially variable parameters and nonlinear nature of some of the model components.

Bromide Mass

GLEAMS-SF, like Opus-SF, does not simulate the effect of preferential flow that could have been responsible for the loss of approximately 10 kg ha^{-1} of bromide from the field, soon after application (Fig. 39, Table 48). As in the case of bromide simulations at the Dougherty Plain site, GLEAMS-SF predicted the mean bromide mass fairly well early in the cropping season but consistently underpredicted bromide mass 50 days after application (Fig. 39). Both observed and simulated bromide mean in the root zone, and to some extent, its standard deviation and range, remained steady on the last three sampling dates, days 167, 209, and 272.

The difference in observed and simulated bromide leaching may be because GLEAMS simulates all of the bromide to move with downward movement of water, whereas substantial amounts of bromide are retained in the soil matrix.

Mean and median of bromide mass simulated by GLEAMS-SF differed by less than 4% (Table 48). Such differences were also found between observed mean and median, and indicate that the bromide mass distribution in soil was slightly skewed. The Mann-Whitney test showed that observed and simulated medians of total bromide mass in the root zone were significantly different ($\alpha = 0.05$) on all dates (Table 48).

Simulated standard deviation of total bromide mass in the root zone (Table 48) was comparable to observed standard deviation, but lower on all field sampling dates. Thus, bromide variability was underpredicted even though maximum bromide mass was higher than the observed maximum values on the application date and the first three sampling dates. As with soil water variability, the underprediction may be caused by the reduced variation in soil physical properties derived from texture data. The KS test showed that the observed and simulated EDFs of total bromide mass in the root zone were significantly different on all dates at $\alpha = 0.05$, and on all dates except days 128 and 145 at $\alpha = 0.01$ (Table 48). The range statistic showed that over 80% of the observations were contained within the simulated range on the first four sampling dates, whereas less than 10% of the observations were contained within the simulated range on day 272 (Table 48).

There were some differences between predictions of total bromide mass in the root zone by deterministic GLEAMS and the mean predicted by GLEAMS-SF, after June 1 (Fig. 39). These differences were, however, small, as in the case of depth-averaged soil water content.

Atrazine Mass

GLEAMS-SF predicted the mean atrazine mass to constantly decrease with time, whereas mean atrazine mass observed in the field reduced by approximately 0.46 kg ha^{-1}, between days 128 and 145 (Fig. 40, Table 49). As discussed in the previous chapter, this rapid decrease in mean atrazine mass may be attributed to losses in leaching (57 mm rainfall during the period) and degradation, and perhaps, incomplete recovery of atrazine from the soil and crop residue. The simulated mean leaching loss below the root zone (0.9 m) by day 145 was approximately 0.068 kg ha^{-1}, whereas degradation losses was over 0.2 kg ha^{-1}. By the end of the simulation period, GLEAMS-SF predicted 0.21 kg ha^{-1} of atrazine mass (mean) to remain in the field as compared to a mean atrazine mass of 0.3 kg ha^{-1} observed in the field (Table 49). Mean atrazine leaching losses predicted by GLEAMS-SF was approximately 0.085 kg ha^{-1}, and degradation and plant uptake accounted for the remaining 89% of atrazine losses.

Mean and median of atrazine mass simulated by GLEAMS-SF differed by less than 8% (Table 49). Such differences were also found between observed mean and median, and indicate that the atrazine mass distribution in soil was skewed. The Mann-Whitney test showed that observed and simulated medians of total atrazine mass in the root zone were not significantly different on days 118 and 128 at

$\alpha = 0.05$ and also on day 209 at $\alpha = 0.01$ (Table 49). Observed data from day 167 were excluded from analysis, due to anomalous data (Heatwole et al., 1997, pg.1273).

Simulated standard deviation of total atrazine mass in the root zone (Table 49) was comparable to observed standard deviation, but lower on all five sampling dates. Thus, atrazine variability was underpredicted even though maximum atrazine mass was higher than observed maximum values on all dates except day 209. The simulated minimum atrazine mass coincided with the observed minimum on almost all dates. The KS test showed that the observed and simulated EDFs of total atrazine mass in the root zone were not significantly different on days 118 and 128 at $\alpha = 0.05$ (Table 49). Range statistic showed that over 80% of the observations were contained within the simulated range on all sampling dates (Table 49).

Depth-wise distribution of observed and simulated atrazine mass on day 118 (Fig. 41a) showed that GLEAMS-SF overpredicted atrazine mass in the 0-0.15 m and underpredicted atrazine mass in the remaining depths. Depth-wise distribution of observed and simulated atrazine mass on day 209 (Fig. 41b) showed that while atrazine distribution was even throughout the 0.9 m profile, GLEAMS-SF predicted more herbicide in the 0.15-0.3 m depths. The simulated means, however, were still within the observed range at all depths.

Metolachlor Mass

GLEAMS-SF predicted a gradual decrease in total metolachlor mass in the root zone, and was close to the observed mean on all dates except day 118 (Fig. 42, Table 50). Observed metolachlor mass on the application date (day 115) and day 118 (Table 44, Fig. 42, Table 50) showed that there was a difference of 0.44 kg ha^{-1}. As discussed in the previous chapter, even though part of this difference may have been due to incomplete recovery of herbicide from the soil and crop residue, the difference could reflect the loss of the herbicide as a result of leaching below 0.9 m, degradation, and volatilization. As in the case of bromide and atrazine, leaching below the root zone by preferential movement may have been one of the loss pathways following the rainfall simulator application on day 118. Total metolachlor loss in runoff was less than 1% of the herbicide applied (0.006 kg ha^{-1}).

Leaching losses of metolachlor were lower than that of atrazine because it has a higher adsorption rate and a higher degradation rate (Table 44). By the end of the simulation period, GLEAMS-SF predicted a mean metolachlor mass of 0.022 kg ha^{-1} remaining in the root zone on day 272 (157 days after application) as compared to 0.070 kg ha^{-1} observed in the field. Degradation and plant uptake accounted for more than 99% of metolachlor losses predicted by GLEAMS-SF, whereas leaching loss was approximately 0.008 kg ha^{-1}.

With the exception of day 118 and day 272, GLEAMS-SF was able to predict the mean and median of total metolachlor mass in the root zone well (Table 50). The Mann-Whitney test showed that observed and simulated medians of total metolachlor mass were not significantly different ($\alpha = 0.05$) on days 128, 145, and 209 (Table 50). Observed data from day 167 were excluded from analysis, due to anomalous data (Heatwole et al., 1997, pg.1273).

Simulated standard deviation of total metolachlor mass in the root zone (Table 50) was comparable to observed standard deviation, but lower on all sampling dates except day 118. Thus, metolachlor variability was underpredicted even though maximum metolachlor mass was higher than the observed maximum values on all sampling dates. The KS test showed that the observed and simulated EDFs of total metolachlor mass in the root zone were not significantly different ($\alpha = 0.05$) on days 128 and 145 (Table 50). Range statistics indicated that over 95% of the observations were contained within the simulated range on all sampling dates (Table 50).

Depth-wise distribution of observed and simulated metolachlor mass on day 118 (Fig. 43a) showed that GLEAMS-SF overpredicted metolachlor mass in the 0-0.15 m and underpredicted metolachlor mass in the remaining depths. Depth-wise distribution of observed and simulated metolachlor mass on day 209 (Fig. 43b) showed that GLEAMS-SF predicted more of the herbicide in the 0.15-0.3 m depth. The simulated mean of metolachlor mass was always within the observed range on most depths, and the observed mean was always within the simulated range.

Overall, GLEAMS-SF predicted pesticide mass in the root zone better than bromide mass in the root zone over the entire simulation period. As with the results from the Dougherty Plain study, this once again shows that even though the model could not do a good job of predicting bromide transport, it could predict fate and transport of pesticides (solutes that adsorb and degrade) reasonably well [provided reasonably good estimates of adsorption and degradation parameters were available, as in this study].

Comparison with Traditional Monte-Carlo Simulation

GLEAMS-SF was compared with the traditional Monte-Carlo simulation of GLEAMS (GLEAMS-MC). The difference between the two approaches is that GLEAMS-SF describes spatially variable input parameters that exhibit spatial trends as a sum of the deterministic trend and the random variations, whereas GLEAMS-MC treats all spatially input parameters to be random, and describes the parameters by their PDFs.

Water Balance and Soil Water Content

Overall, the water balance predicted by GLEAMS-MC was comparable to that of GLEAMS-SF (Table 51), with seasonal variations in mean ET and percolation amounts predicted by both models in a similar fashion. GLEAMS-SF predicted 6 mm of total ET more than GLEAMS-MC over the simulation period, with all of the differences occurring in the months of July, August, and September. The difference in total percolation losses over the simulation period was 2.2 mm, with all of the differences occurring in the month of August. These small differences in ET and percolation resulted from the differences in the soil parameters used in the two models.

The difference in mean and median of depth-averaged soil water content predicted by GLEAMS-SF and GLEAMS-MC on the simulation start date, day 118, was less than 2% (Table 52). This difference increased by a maximum of 1% in the subsequent dates. The standard deviations predicted by GLEAMS-SF and GLEAMS-MC were equal, except on day 209 when the GLEAMS-SF standard deviation was slightly greater than the GLEAMS-MC standard deviation. The Mann-Whitney and KS tests, however, showed that the depth-averaged soil water content medians and EDFs predicted by GLEAMS-MC and GLEAMS-SF were significantly different ($\alpha = 0.05$) on all dates (Table 52). As discussed in the previous chapter, tests are likely to detect statistically significant differences for small departures from the null hypothesis that might be quite unimportant in practice, in the case of large samples (Snedecor and Cochran, 1980, pg.67). However, it can be said that calculating soil hydraulic and retention properties by including spatial trends of sand and clay content in some of the soil layers (Table 15) in the upper 0.6 m profile had some impact on soil water predictions from the stochastic simulation of GLEAMS (Table 52).

GLEAMS-SF predicted observed mean and median better than GLEAMS-MC on days 118, 128, and 272. On day 128, the Mann Whitney test comparing depth-averaged soil water content predicted by GLEAMS-MC and observed data gave a p-value of 0.152 as compared to a p-value of 0.506 obtained for the corresponding test involving GLEAMS-SF (Table 47). The opposite result was obtained on days 145, 167, and 209, when observed depth-averaged soil water content was lower than the simulated values. On these dates, GLEAMS-MC predicted observed mean and median better than GLEAMS-SF. On day 145, the Mann Whitney test comparing depth-averaged soil water content predicted by GLEAMS-MC and observed data gave a p-value of 0.413 as compared to a p-value of 0.036 obtained for the corresponding test involving GLEAMS-SF (Table 47).

The KS tests showed a similar trend to the Mann-Whitney test when comparing observed EDFs with EDFs obtained from GLEAMS-SF and GLEAMS-MC. On day 128, the KS test comparing EDF of depth-averaged soil water content predicted by GLEAMS-MC and observed data gave a p-value of 0-0.01 as compared to a p-value of 0.01-0.02 obtained for the corresponding test involving GLEAMS-SF (Table 47). On day 145, the KS test comparing EDF of depth-averaged soil water content predicted by GLEAMS-MC and observed data gave a p-value of 0.05-0.1 as compared to a p-value of 0-0.01 obtained for the corresponding test involving GLEAMS-SF (Table 47). The test statistics showed that EDF predicted by GLEAMS-SF was closer to observed EDF on days 128 and 272, whereas EDF predicted by GLEAMS-MC was closer to observed EDF on days 145, 167, and 209. The test statistics obtained from observed vs. GLEAMS-SF and observed vs. GLEAMS-MC were the same on day 118. Therefore, it is difficult to say whether GLEAMS-MC or GLEAMS-SF did a better job of predicting observed data.

Bromide Mass

The mean and median of bromide mass predicted by GLEAMS-MC on all sampling dates were lower than the mean and median predicted by GLEAMS-SF, even though the opposite was true on the application date, day 115 (Table 53). However, the Mann-Whitney test did not show any significant differences (α = 0.05) between the two medians until day 167 (Table 53). The standard deviation predicted by GLEAMS-SF was greater than that predicted by GLEAMS-MC on all dates. The KS test for the EDFs predicted by GLEAMS-SF and GLEAMS-MC also did not show any significant differences (α = 0.05) until day 167 (Table 53). The EDFs on day 209 were also not significantly different at $\alpha = 0.01$. The above results showed that there were differences between the models only after substantial amounts of bromide had leached out of the root zone.

Comparison between observed median and medians predicted by GLEAMS-MC and GLEAMS-SF gave the same results at $\alpha = 0.05$. It was difficult to determine which model predicted observed data better, as the GLEAMS-MC medians were closer to observed data on days 128 and 145 and the GLEAMS-SF predictions were closer to observed data on the last three dates. Comparison between observed EDF and EDFs from GLEAMS-MC and GLEAMS-SF also gave the same results at $\alpha = 0.05$. The test statistics indicated that the GLEAMS-MC EDFs were closer to observed EDFs on all dates except day 272 as compared to GLEAMS-SF, although the difference was very small. On day 272, the test statistics for both models were exactly the same.

Pesticide Mass

There were very little differences between mean, median, and standard deviation of total atrazine mass in the root zone predicted by GLEAMS-MC and GLEAMS-SF, on all sampling dates (Table 54). In the case of total metolachlor mass also, there was very little difference between the mean, median, and standard deviation predicted by GLEAMS-MC and GLEAMS-SF (Table 55). The medians as well as the EDFs of atrazine and metolachlor mass predicted by GLEAMS-MC and GLEAMS-SF were not significantly different ($\alpha = 0.05$) on all sampling dates (Tables 54 and 55).

The p-values obtained from Mann-Whitney and KS tests for comparing atrazine and metolachlor mass predictions from GLEAMS-MC and observed data were very close to the p-values obtained by comparing GLEAMS-SF predictions and observed data (Tables 49 and 50). Atrazine medians predicted by GLEAMS-SF were closer to observed data on days 118 and 272, whereas those predicted by GLEAMS-MC were closer to observed data on days 128 and 167. The medians predicted by the two models were equal on days 145 and 209. The test statistics from the KS tests indicated that atrazine mass EDFs from GLEAMS-SF were closer to observed EDFs than GLEAMS-MC on all sampling dates. With metolachlor mass, the medians predicted by GLEAMS-SF were closer to observed medians on days 118, 167, 209, and 272 than the medians predicted by GLEAMS-MC. Metolachlor mass EDFs predicted by GLEAMS-SF were closer to observed EDFs on days 145, 167, 209, and 272, whereas the opposite was true on day 118; the test statistics were equal on day 128.

Overall, GLEAMS-SF predicted field-measured herbicide mass in the root zone slightly better than GLEAMS-MC. However, these differences were small and did not change the results from the statistical tests conducted for comparing simulated data with observed data.

Summary

Soil water properties and organic matter content in the upper 0.6 m of the soil profile (four soil layers), pesticide degradation rate in the four layers, and chemical application rates were selected as the spatially variable input parameters for the stochastic simulation of water flow and pesticide transport at the Nomini Creek site using GLEAMS-SF. The soil water properties were derived from texture, porosity, and organic matter data measured at the site. Spatial variability of sand and clay content were described by their PDFs, after analyzing them for spatial trends. Soil hydraulic and retention properties for the four layers were computed from correlated random variates of sand and clay content and independent random variates of porosity and organic matter content, using the regression equations of Rawls et al. (1982) and Rawls and Brakensiek (1985).

GLEAMS-SF predicted high ET during the summer months and high percolation during the high rainfall events in April and May. Soil water content was underpredicted for the first 10-15 days of the simulation, because of limitations of the initial plant available water parameter in GLEAMS. This parameter cannot describe the initial soil water profile in the plot, which was above field capacity. GLEAMS-SF overpredicted the soil water content for most of the remaining crop growing season, including the dry period in July and August. The simulated medians were not significantly different ($\alpha = 0.01$) from the observed medians on days 128 and 145, whereas simulated EDFs were not significantly different on only day 128. Spatial variability of simulated soil water content was much lower than the observed variability on all sampling dates, and there were only two of the six sampling dates where at least 50% of the observations fell within the simulated range. As with Opus-SF, the reduced variation of simulated soil water content was primarily due to the reduced variability in soil water properties computed using the regression equation. GLEAMS-SF did not predict any variation in soil water content in the layers beyond 0.6 m, as spatial variability of soil water properties were not considered beyond that depth.

As with the Dougherty Plain simulation, GLEAMS-SF was not able to predict the field-scale movement of bromide well. Before bromide predictions by the model can be fully evaluated, the retention of the tracer in field soils for prolonged time will have to be better explained. GLEAMS-SF overpredicted bromide mass in the field in the first month after application and underpredicted bromide mass for the remainder of the simulation period. GLEAMS-SF could not simulate preferential movement of chemicals, which had resulted in considerable amount of bromide loss from the field soon after application. Two large rainfall events of approximately105 mm each at the end of May caused extensive movement of bromide from the root zone, which resulted in the underprediction of the tracer thereafter. Spatial variations in bromide mass predicted by GLEAMS-SF were comparable but less than the observed variation until the majority of the bromide leached out of the root zone. More than 80% of the observations were contained in the simulated range in the first 52 days of application (until day 167).

The mean and median of total atrazine mass in the root zone was predicted well in the first two weeks of application, after which it was overpredicted, and then underpredicted in the latter stages of the cropping season. The observed and simulated medians were not significantly different ($\alpha = 0.01$) on days 118, 128, and 209, where the EDFs were not significantly different ($\alpha = 0.01$) on days 118 and 128. Spatial variations in atrazine mass were comparable, but lower than the spatial variations in the field. More than 80% of the atrazine mass observations on all field sampling dates were within the simulated range.

GLEAMS-SF predicted the mean and median of total metolachlor mass in the root zone well during the cropping season, except for the first sampling date when metolachlor mass in the field was low because of incomplete recovery or preferential movement and the last sampling date when it underpredicted the observed metolachlor mass. The observed and simulated medians were not significantly different ($\alpha = 0.01$) on days 128, 145, and 209, and the EDFs were not significantly different ($\alpha = 0.01$) on days 128 and 145. Spatial variations in metolachlor mass were comparable, but greater than the observed spatial variation on days 118 and 145 and lower than the observed spatial variation on three other sampling dates. More than 95% of the metolachlor mass observations on all field sampling dates were within the simulated range. Unlike atrazine, GLEAMS-SF was able to predict the depth-wise distribution of metolachlor mass well.

The water balance, soil water content, bromide and pesticide mass predicted by the deterministic version of GLEAMS were similar, but not equal to the mean values predicted by GLEAMS-SF. Monthly ET predicted by the deterministic version of GLEAMS was lower than the mean values predicted by GLEAMS-SF in the months of July through September, whereas monthly percolation predicted by deterministic GLEAMS was higher than GLEAMS-SF mean in August. The deterministic GLEAMS predicted lower soil water content than GLEAMS-SF (mean) throughout the simulation period, with the differences greatest in the beginning and in the end. These differences reflect the differences in characterization of the spatially variable parameters as well as the effect of nonlinear components in the model. The differences between pesticide mass predictions by the two versions were less distinct than the differences in soil water content and bromide mass predictions.

A comparison of stochastic outputs from GLEAMS-SF and GLEAMS-MC showed that soil water content predicted by the two models were significantly different ($\alpha = 0.01$) on all dates in the 5-month period. It was difficult to determine which model performed better, as soil water predictions by Opus-SF were closer to observed data on some dates while the opposite was true on other dates. The difference between bromide mass predictions from the two models was significant only after most of the solute had moved out of the root zone. There were no significant differences ($\alpha = 0.01$) between pesticide mass predictions by GLEAMS-SF and GLEAMS-MC. The small differences between bromide and pesticide mass predicted by GLEAMS-MC and GLEAMS-SF did not change the results from the statistical tests used for comparing simulated data with observed data.

Table 29. Model parameters and base values used in the sensitivity analysis of GLEAMS.

Parameter description	Identifier	Base values†
Soil parameters		
Sat. conductivity of restricting layer (cm/hr)	RC	1.41
Fraction of initial plant available water	BST	0.6
Soil evaporation parameter	CONA	3.5
Porosity	POR()	0.404,0.374,0.374,0.374
Soil water content at field capacity (cm/cm)	FC()	0.167,0.181,0.213,0.233
Soil water content at wilting point (cm/cm)	BR15()	0.034,0.069,0.117,0.132
Saturated hydraulic conductivity (cm/hr)	SATK()	21.35,36.49,28.89,7.05
Clay content	CLAY()	0.04,0.11,0.17,0.20
Rooting depth (cm)	CCRD	100.0
Pesticide (Metolachlor) parameters		
Degradation half-life in soil (1/days)	SOLLIF	27.3
Adsorption coefficient (mL/g)	KOC	200
Organic matter content of soil (%)	OM()	1.28,0.47,0.45,0.45
Water solubility	H2OSOL	530
Plant uptake coefficient	COFUP	0.8

† Base values listed are for the four horizons in the Dougherty Plain field site.

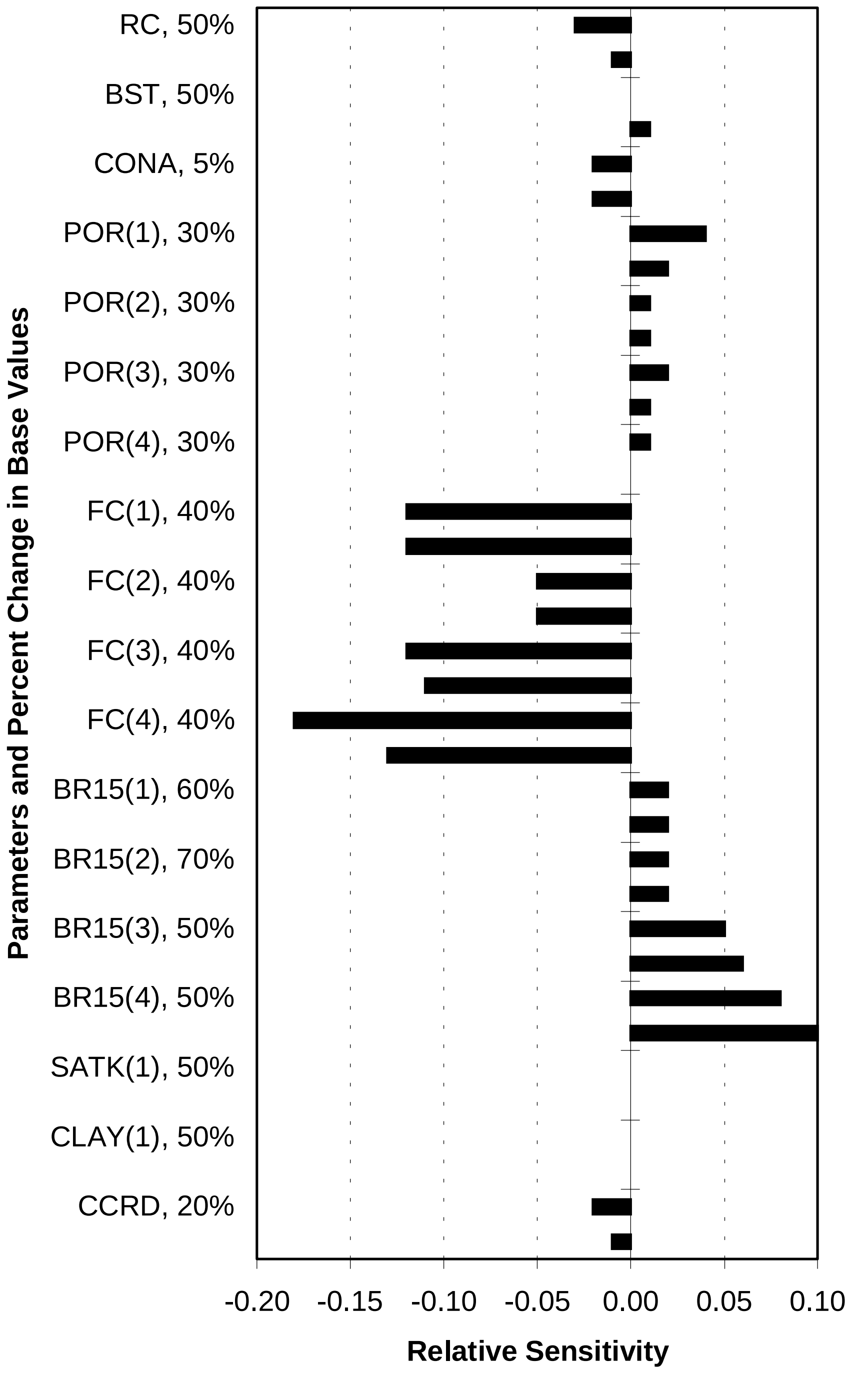

Figure 25. Relative sensitivity of total percolation below the top 1.2 m profile of the Dougherty Plain field predicted by GLEAMS to soil parameters (The two bars for each parameter denote sensitivity to negative and positive change in base values).

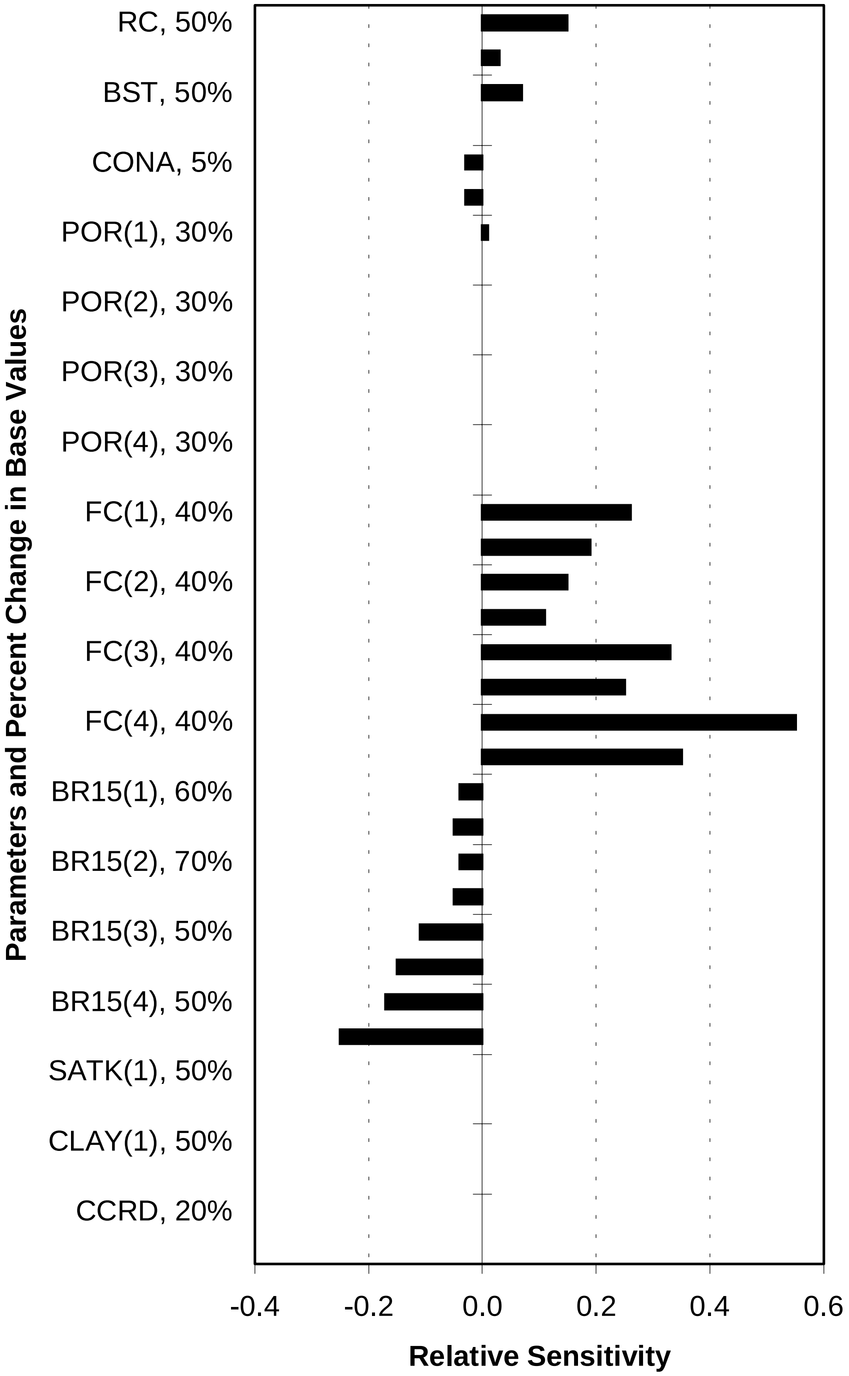

Figure 26. Relative sensitivity of average soil water content in the top 1.2 m profile of the Dougherty Plain field predicted by GLEAMS to soil parameters (The two bars for each parameter denote sensitivity to negative and positive change in base values).

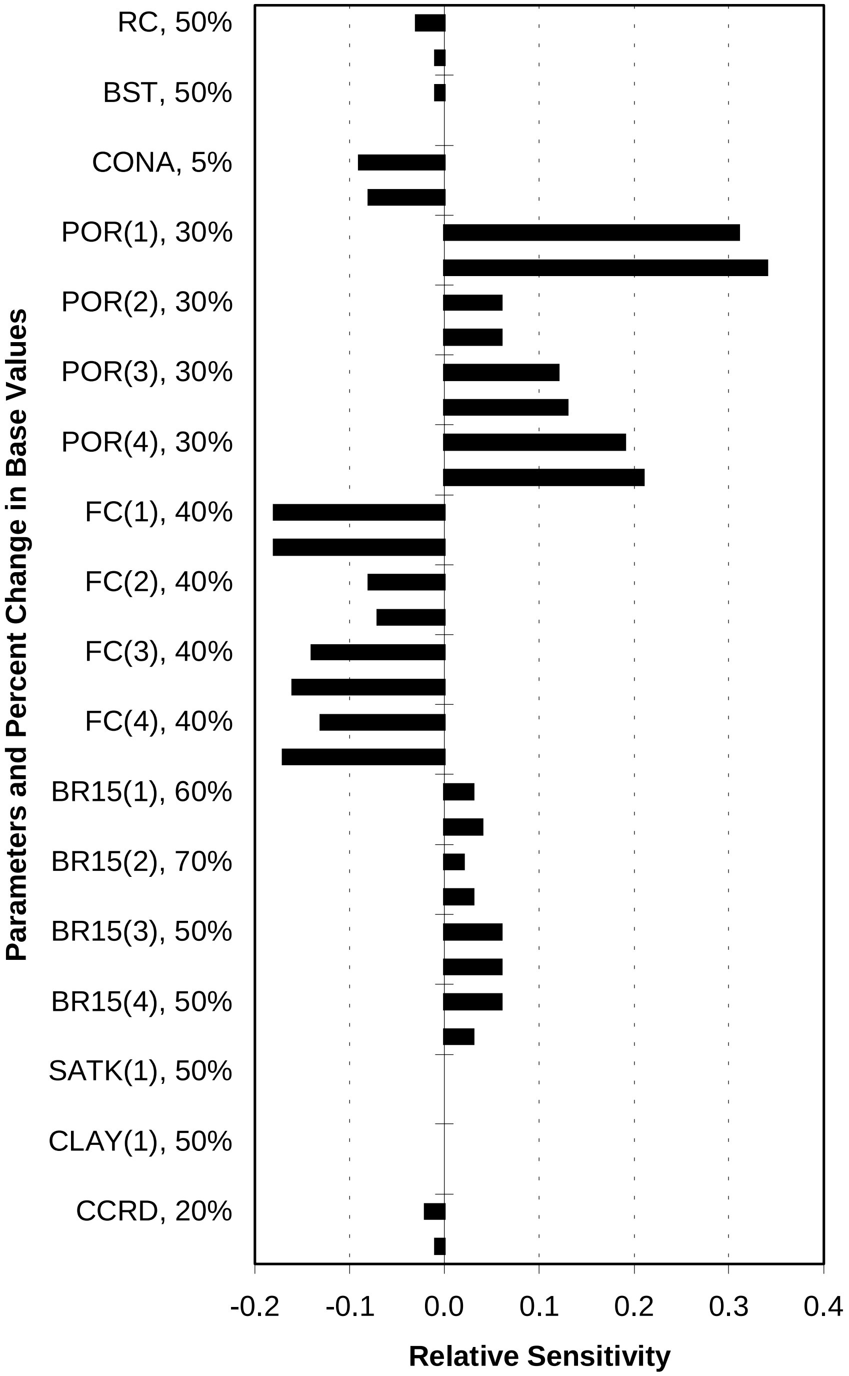

Figure 27. Relative sensitivity of resident metolachlor mass in the top 1.2 m profile of the Dougherty Plain field predicted by GLEAMS to soil parameters (The two bars for each parameter denote sensitivity to negative and positive change in base values).

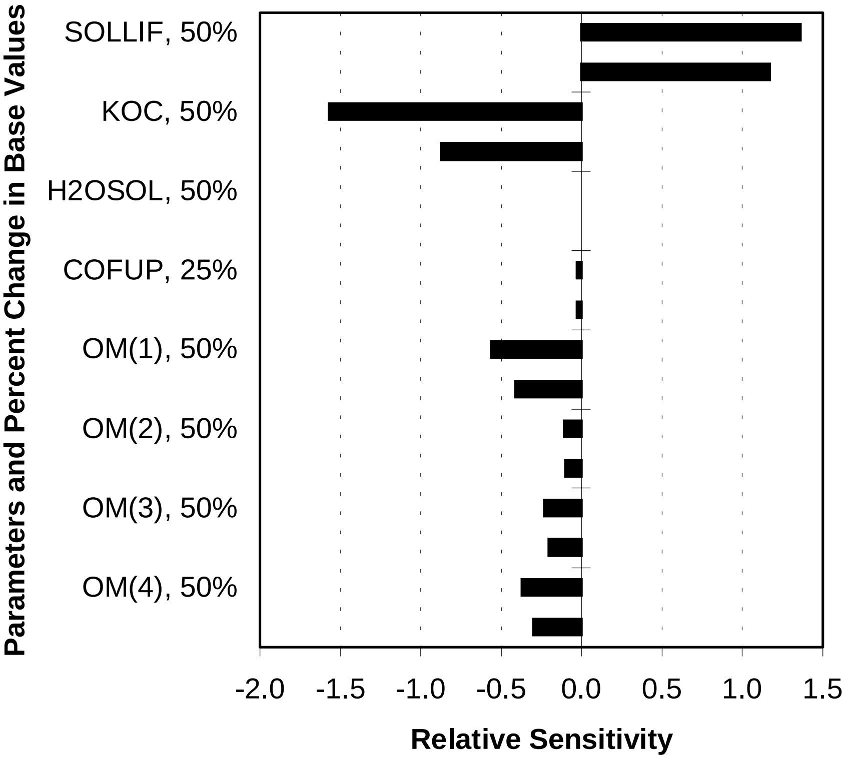

Figure 28. Relative sensitivity of resident metolachlor mass in the top 1.2 m profile of the Dougherty Plain field predicted by GLEAMS to pesticide parameters (The two bars for each parameter denote sensitivity to negative and positive change in base values).

Table 30. Statistical characteristics of spatially variable soil properties at the Dougherty Plain site used in GLEAMS-SF.

Soil property	Measured data			Order of	Detrended data†		
	Mean	St.dev.	PDF	Trend Surface†	Mean	St.dev.	PDF
Init. plant available water (BST)	0.67	0.14	Normal				
Porosity (ϕ or POR)							
Horizon 1 (0-0.3 m)	0.404	0.03	Normal				
Horizon 2 (0.3-0.45 m)	0.374	0.026	Normal	First[1]	0	0.021	Normal
Horizon 3 (0.45-0.75 m)	0.374	0.029	Normal				
Horizon 4 (0.75-1.2 m)	0.374	0.026	Normal				
Water content at field capacity (θ_{fc} or FC), mm/mm							
Horizon 1 (0-0.3 m)	0.167	0.03	LogNormal				
Horizon 2 (0.3-0.45 m)	0.181	0.032	Normal				
Horizon 3 (0.45-0.75 m)	0.213	0.032	Normal				
Horizon 4 (0.75-1.2 m)	0.233	0.039	Normal				
Water content at wilting point (θ_{wp} or BR15), mm/mm							
Horizon 1 (0-0.3 m)	0.031	0.009	LogNormal				
Horizon 2 (0.3-0.45 m)	0.069	0.033	LogNormal	First[2]	0	0.420	Normal
Horizon 3 (0.45-0.75 m)	0.117	0.036	Normal				
Horizon 4 (0.75-1.2 m)	0.132	0.039	Normal				
Organic matter content (OM), %							
Horizon 1 (0-0.3 m)	0.94	0.4	Normal				
Horizon 2 (0.3-0.45 m)	0.31	0.14	Normal				
Horizon 3 (0.45-0.75 m)	0.25	0.1	Normal				
Horizon 4 (0.75-1.2 m)	0.15	0.12	Normal				

† Only for properties that exhibited spatial trend

[1] Trend coefficients of θ_s: $\beta_0=0.347$, $\beta_1=-0.0002$, $\beta_2=0.0002$

[2] Trend coefficients of $\ln(\theta_{wp})$: $\beta_0=-1.868$, $\beta_1=-0.003$, $\beta_2=-0.003$

Table 31. Correlation between soil water properties in each horizon at the Dougherty Plain site.

Horizon	Property	ϕ	θ_{fc}	θ_{wp}
1	ϕ	1.00		
	θ_{fc}	0.35	1.00	
	θ_{wp}	0.38	0.57	1.00
2	ϕ	1.00		
	θ_{fc}	-0.37	1.00	
	θ_{wp}	0.00	0.73	1.00
3	ϕ	1.00		
	θ_{fc}	0.00	1.00	
	θ_{wp}	0.51	0.18	1.00
4	ϕ	1.00		
	θ_{fc}	0.11	1.00	
	θ_{wp}	0.32	0.55	1.00

† Correlation coefficients were calculated on log-transformations for log-normally distributed variables, and on detrended residuals for variables that exhibited spatial trends.

Table 32. Estimates of important pesticide parameters used in GLEAMS-SF simulation of the Dougherty Plain site.

Property	**Aldicarb**			**Metolachlor**		
	Mean	**St.dev.†**	**PDF†**	**Mean**	**St.dev.†**	**PDF†**
Solubility in water (H2OSOL), mg L^{-1}	6000			530		
Adsorption coefficient (KOC), cm^3 g^{-1}	24.4			153.0		
Washoff fraction (WASHFRC)	0.5			0.6		
Foliar degradation rate (HAFLIF), days	5			5		
Soil half-life ($t_{1/2}$ or SOLLIF), days						
Horizon 1 (0-0.3 m)	42.0	8.8	LogNormal	17.7	2.0	LogNormal
Horizon 2 (0.3-0.45 m)	42.0	16.0	LogNormal	27.3	9.1	LogNormal
Horizon 3 (0.45-0.75 m)	47.0	12.2	LogNormal	42.3	2.9	LogNormal
Horizon 4 (0.75-1.2 m)	62.0	13.0	LogNormal	43.0	16.3	LogNormal
Plant uptake coefficient (COFUP)	0.60			0.32		
Application rate (APRATE), kg ha^{-1}						
1985 (May 7)	2.96	1.05	Normal	2.49	0.48	LogNormal
1986 (April 7)	3.04	1.47	Normal	2.96	0.92	LogNormal
1986 (April 7) - High application rate‡	11.63	5.05	Normal			
1987 (June 1)	2.67	1.27	Normal	3.36	1.26	Normal
Bromide§ - 1985 (April 17)	58.83	14.94	Normal			

† Standard deviation and PDF's are given only for spatially variable parameters

‡ Aldicarb was applied at two target rates in 1986: a higher rate was applied to the easternmost 36 rows (22% of total area) and a lower (regular) rate to the rest of the field.

§ Other bromide properties used in the simulation are: H20SOL = 1000 mg L^{-1}; KOC = 0 cm^3 g^{-1}; WASHFRC = 0.75; HAFLIF = SOLLIF() = 99999 days; COFUP = 0.6.

Table 33. Correlation between pesticide half-lives in different horizons at the Dougherty Plain site.

Pesticide	Depth (m)	0-0.3	0.3-0.45	0.45-0.75	0.75-1.2
Aldicarb	0-0.3	1.00			
	0.3-0.45	0.73	1.00		
	0.45-0.75	0.78	0.81	1.00	
	0.75-1.2	0.33	0.03	0.27	0.00
Metolachlor	0-0.3	1.00			
	0.3-0.45	0.64	1.00		
	0.45-0.75	0.50	0.35	1.00	
	0.75-1.2	0.56	0.64	0.50	0.00

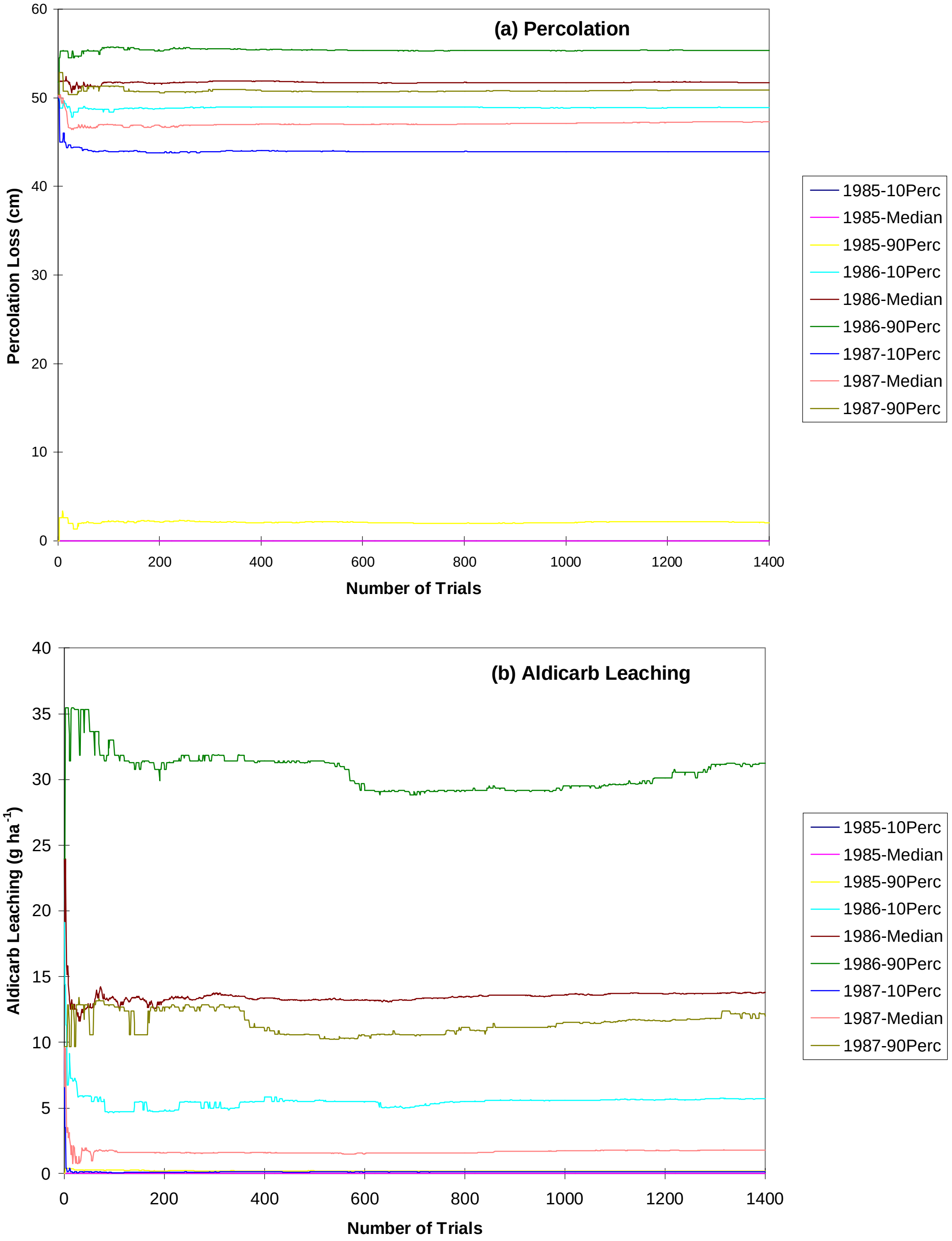

Figure 29. Simulated median, 10th and 90th percentile of (a) percolation and (b) aldicarb leaching predicted by GLEAMS-SF at the end of each cropping season at the Dougherty Plain site, as a function of the number of trials. (Note: Median and 10th percentile of percolation and aldicarb leaching losses in 1985 were zero or close to zero).

Table 34. Mean monthly evapotranspiration (ET) and percolation predicted by GLEAMS-SF at the Dougherty Plain site, along with ET and percolation predicted by deterministic GLEAMS.

Month-Year	Rainfall, mm	…..ET, mm…..		.....Percolation, mm…..	
		GLEAMS-SF	GLEAMS	GLEAMS-SF	GLEAMS
Apr-85	47.2	46.6	46.6	0.4	0.0
May-85	81.5	63.5	63.5	4.3	0.0
Jun-85	106.1	130.2	132.3	0.0	0.0
Jul-85	94.3	114.6	113.6	0.0	0.0
Aug-85	100.9	49.3	49.3	1.8	0.0
Sep-85	31.1	87.0	90.2	0.0	0.0
Oct-85	176.0	33.6	33.6	61.7	64.9
Nov-85	187.3	32.1	32.1	138.6	126.8
Dec-85	149.9	30.3	30.3	117.5	116.2
Total-85	974.3	587.1	591.4	324.4	307.9
Jan-86	76.3	30.7	30.7	53.9	51.1
Feb-86	133.7	38.5	38.5	92.0	92.0
Mar-86	89.8	39.2	39.2	52.1	52.1
Apr-86	14.9	20.5	20.5	0.0	0.0
May-86	4.4	23.8	23.8	0.0	0.0
Jun-86	65.4	96.7	97.2	0.0	0.0
Jul-86	63.3	56.9	56.9	0.0	0.0
Aug-86	108.6	80.0	79.9	0.0	0.0
Sep-86	57.5	93.1	93.3	0.0	0.0
Oct-86	77.8	40.0	40.1	0.0	0.0
Nov-86	150.1	33.8	33.8	82.4	82.1
Dec-86	110.8	30.5	30.5	80.7	80.3
Total-86	952.6	583.6	584.4	361.2	357.7
Jan-87	177.3	31.5	31.5	146.9	146.9
Feb-87	142.5	35.7	35.7	105.4	105.7
Mar-87	62.7	52.7	52.7	15.1	14.9
Apr-87	28.9	34.7	34.7	8.3	8.3
May-87	79.2	69.6	69.6	10.2	10.2
Jun-87	135.1	159.7	160.5	8.6	8.5
Jul-87	165.7	131.8	131.6	0.4	0.0
Aug-87	204.7	152.0	153.3	34.1	31.9
Sep-87†	12.7	54.6	55.3	0.0	0.0
Total-87	1008.8	722.4	725.0	329.1	326.4

† September 1-10 only

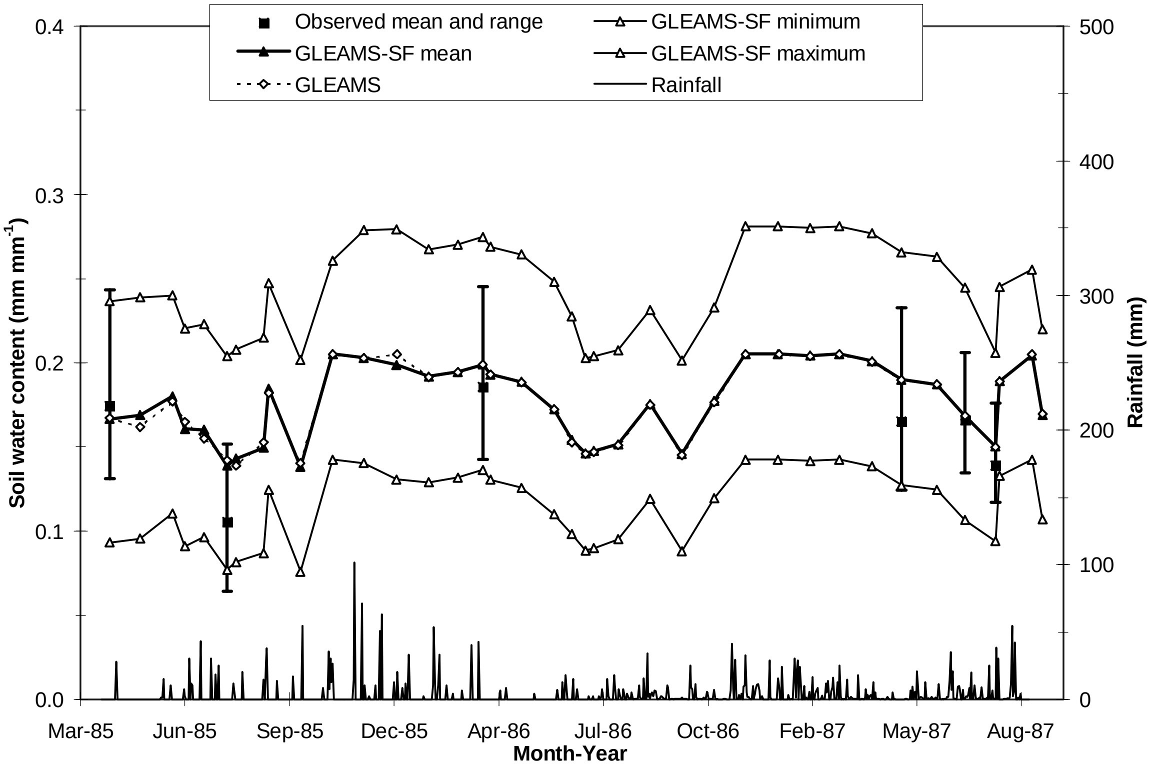

Figure 30. Observed and simulated (GLEAMS-SF) mean and range of depth-averaged soil water content in the 1.2 m soil profile at the Dougherty Plain site, along with depth-averaged soil water content predicted by deterministic GLEAMS.

Table 35. Statistical comparison of observed and simulated (GLEAMS-SF) depth-averaged soil water content at the Dougherty Plain site.

	Soil	Observed			GLEAMS-SF			p-value†		Range
Date	depth (m)	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test	Statistics‡
6/12/85	0-0.30	0.066	0.062	0.015	0.041	0.036	0.021	0-0.01	0.0000	100
7/22/85	0-0.90	0.105	0.108	0.026	0.115	0.116	0.014	0.05-0.10	0.0920	95
8/26/85	0-0.60	0.076	0.073	0.021	0.089	0.088	0.014	0-0.01	0.0005	85
3/24/86	0-1.20	0.186	0.181	0.033	0.199	0.199	0.019	0-0.01	0.0091	100
4/30/86	0-0.15	0.043	0.034	0.028	0.070	0.067	0.029	0-0.01	0.0000	100
6/17/86	0-0.30	0.048	0.048	0.009	0.034	0.031	0.015	0-0.01	0.0000	100
7/8/86	0-0.30	0.040	0.039	0.012	0.039	0.036	0.015	0.2-1.0	0.4085	100
4/28/87	0-1.20	0.165	0.152	0.032	0.190	0.190	0.019	0-0.01	0.0001	95
6/28/87	0-1.20	0.166	0.167	0.030	0.169	0.169	0.019	0.2-1.0	0.7266	95
7/27/87	0-1.20	0.139	0.135	0.029	0.150	0.151	0.017	0.01-0.02	0.0243	95

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

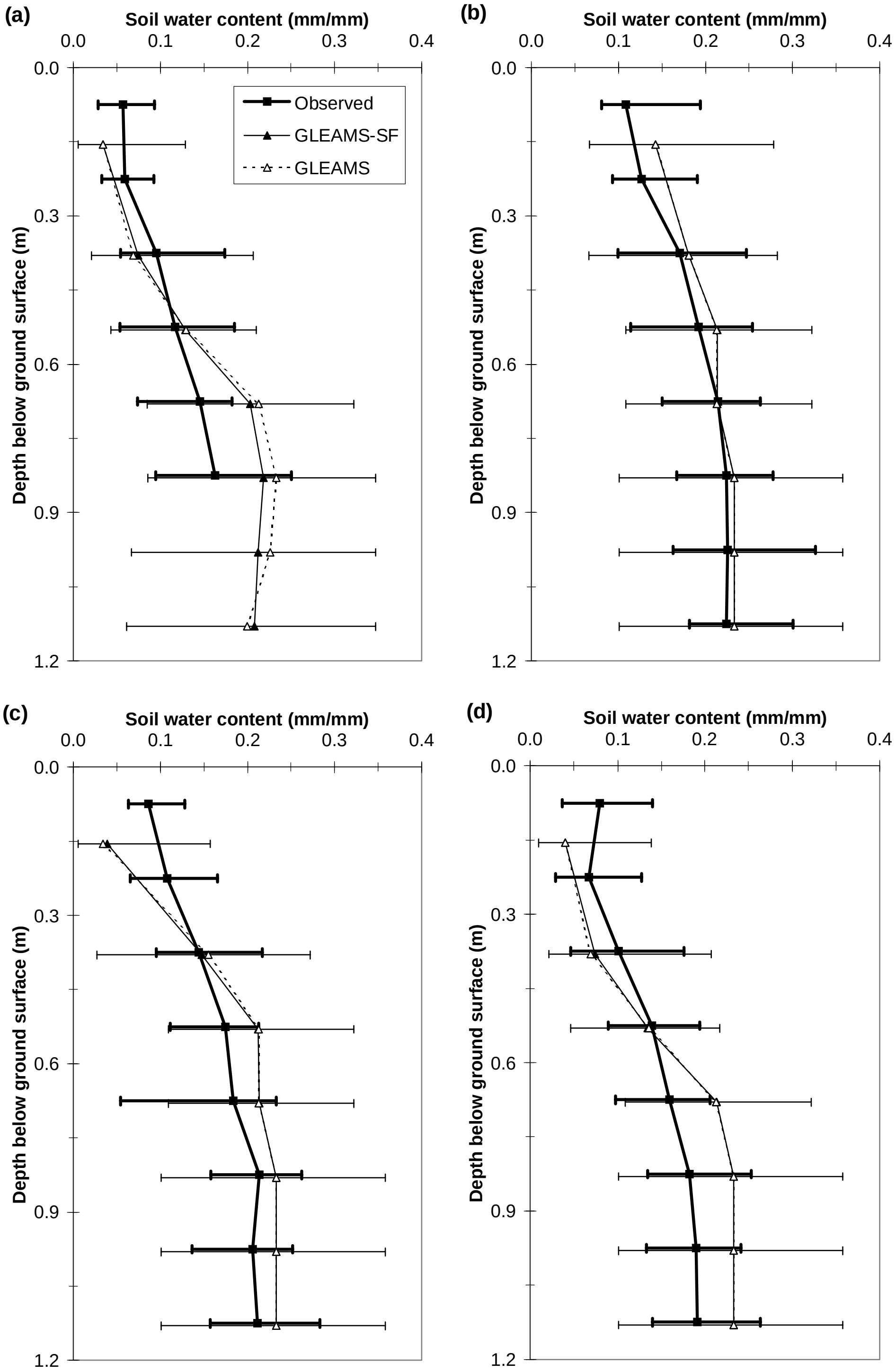

Figure 31. Observed and simulated (GLEAMS-SF) mean and range of soil water content in the 1.2 m soil profile at the Dougherty Plain site, along with soil water content predicted by deterministic GLEAMS, on: a) July 22, 1985, b) March 24, 1986, c) June 28, 1987, and d) July 27, 1987.

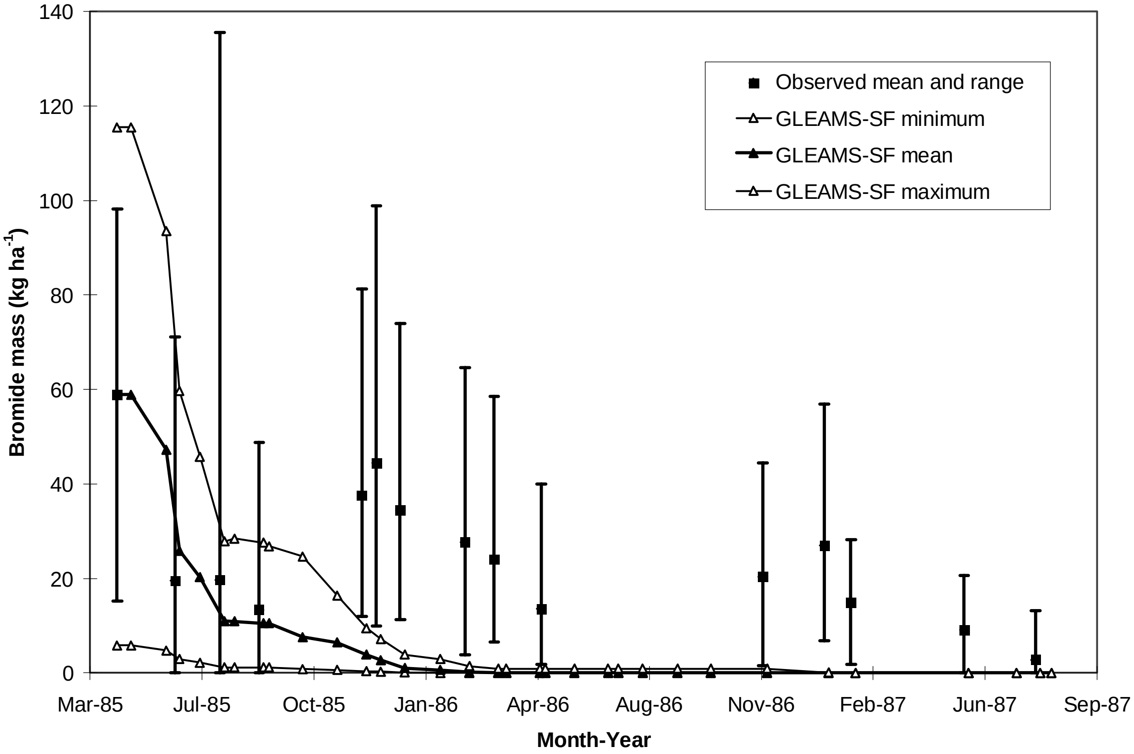

Figure 32. Observed and simulated (GLEAMS-SF) total bromide mass in the 1.2 m soil profile at the Dougherty Plain site.

Table 36. Statistical comparison of observed and simulated (GLEAMS-SF) bromide mass at the Dougherty Plain site.

	Soil	Observed			GLEAMS-SF			p-value†		Range
Date	depth (m)	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test	Statistics‡
6/12/85	0-0.30	19.57	11.29	23.68	25.84	25.08	7.67	0-0.01	0.0145	70
7/22/85	0-0.90	19.69	4.89	35.80	10.96	10.62	3.73	0-0.01	0.0017	45
8/26/85	0-1.20	13.36	10.05	12.68	10.50	10.12	3.66	0.01-0.02	0.9967	75
11/26/85	0-1.20	37.57	38.73	17.42	3.90	3.77	1.37	0-0.01	0.0000	0
12/9/85	0.30-1.20	44.47	40.77	23.99	2.73	2.59	1.04	0-0.01	0.0000	0
12/30/85	0.30-1.20	34.48	35.81	16.53	1.08	1.01	0.49	0-0.01	0.0000	0
2/26/86	0.15-1.20	27.69	27.92	15.74	0.20	0.17	0.13	0-0.01	0.0000	0
3/24/86	0-1.20	24.00	18.30	16.28	0.10	0.08	0.07	0-0.01	0.0000	0
5/5/86	0-1.20	13.59	13.07	8.70	0.10	0.08	0.07	0-0.01	0.0000	0
11/19/86	0-1.20	20.40	19.55	13.03	0.09	0.07	0.07	0-0.01	0.0000	0
1/13/87	0-1.20	26.94	26.54	13.89	0.01	0.00	0.01	0-0.01	0.0000	0
2/6/97	0-1.20	14.85	14.21	8.41	0.00	0.00	0.00	0-0.01	0.0000	0
5/18/97	0-1.20	9.04	9.12	6.55	0.00	0.00	0.00	0-0.01	0.0000	10
7/21/87	0-1.20	2.85	1.21	3.64	0.00	0.00	0.00	0-0.01	0.0000	0

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

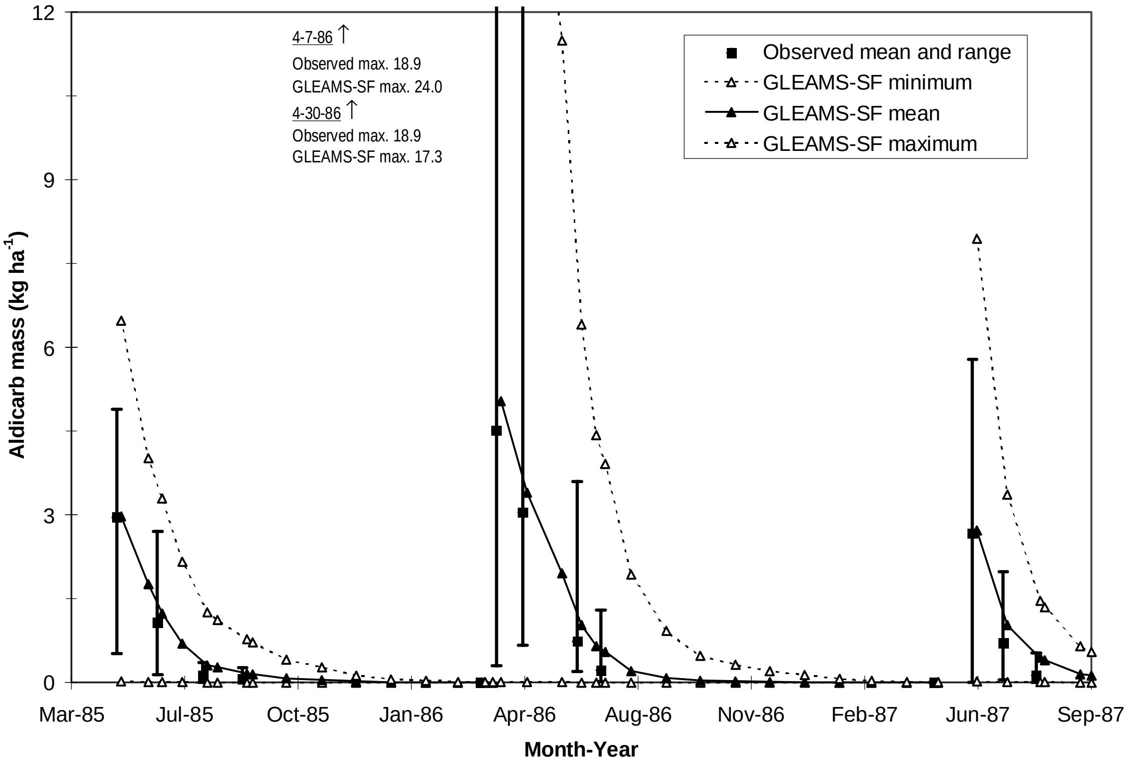

Figure 33. Observed and simulated (GLEAMS-SF) mean and range of aldicarb mass in the 1.2 m soil profile at the Dougherty Plain site.

Table 37. Statistical comparison of observed and simulated (GLEAMS-SF) aldicarb mass at the Dougherty Plain site.

	Soil	Observed			GLEAMS-SF			p-value†		Range
Date	**depth (m)**	**Mean**	**Median**	**St.dev.**	**Mean**	**Median**	**St.dev.**	**KS Test**	**MW Test**	**Statistics‡**
6/12/85	0-0.30	1.082	0.936	0.657	1.236	1.224	0.480	0.1-0.2	0.1596	100
7/22/85	0-0.60	0.124	0.098	0.102	0.316	0.295	0.159	0-0.01	0.0000	90
8/26/85	0-0.60	0.067	0.043	0.066	0.162	0.145	0.094	0-0.01	0.0000	90
3/24/86	0-1.20	0.000	0.000	0.000	0.000	0.000	0.001	—§	—	100
4/30/86	0-0.15	3.047	1.791	4.235	3.396	2.379	2.991	0.02-0.05	0.0500	95
6/17/86	0-0.30	0.737	0.405	0.883	1.025	0.718	0.963	0-0.01	0.0068	100
7/8/86	0-0.30	0.214	0.095	0.306	0.551	0.372	0.551	0-0.01	0.0000	100
4/28/87	0-1.20	0.000	0.000	0.000	0.000	0.000	0.001	—	—	100
6/28/87	0-1.20	0.707	0.715	0.459	1.030	1.003	0.500	0-0.01	0.0024	100
7/27/87	0-1.20	0.128	0.104	0.135	0.436	0.412	0.233	0-0.01	0.0000	70

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

§ The test could not be performed as all observed or simulated values were zero

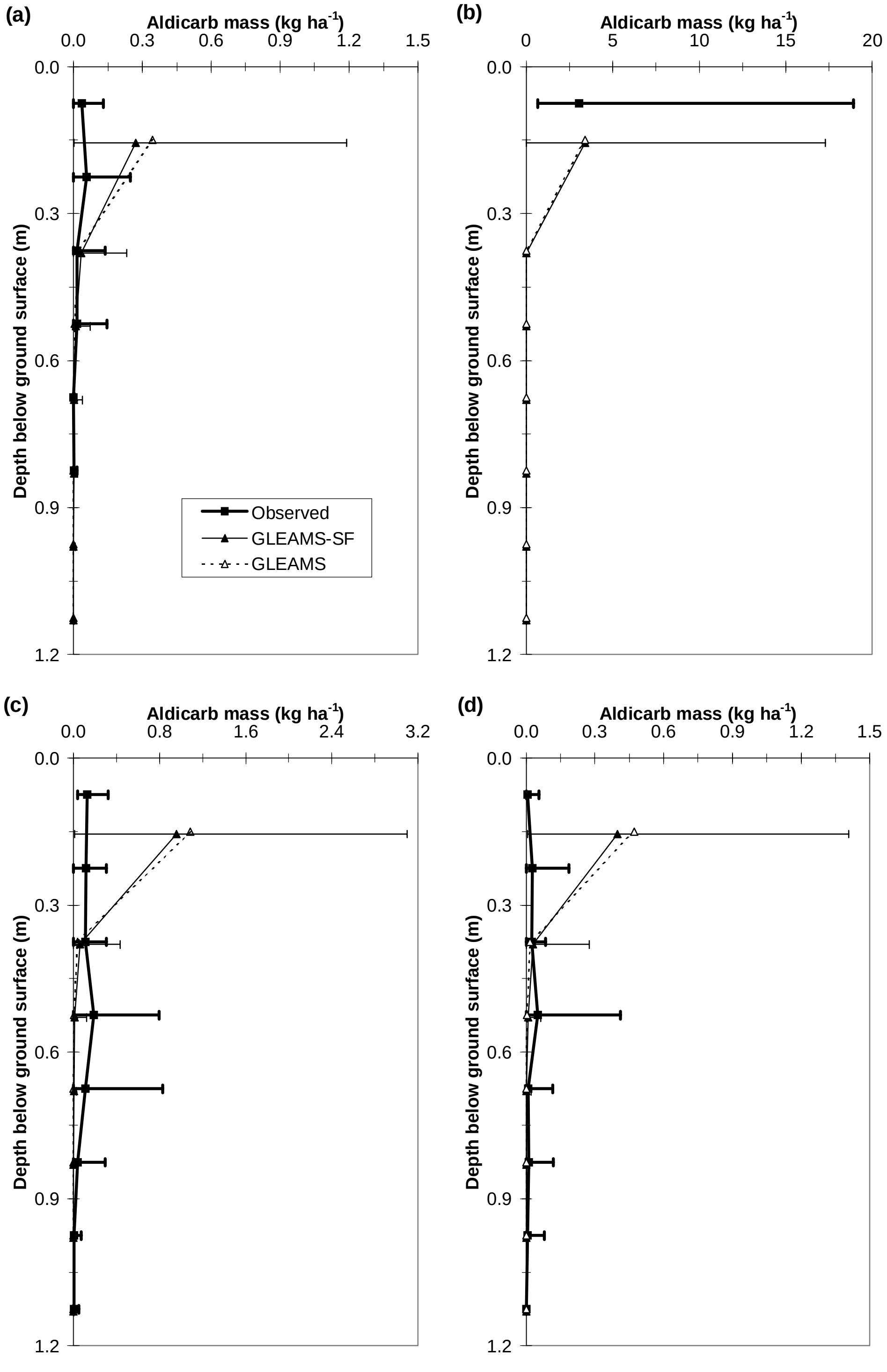

Figure 34. Observed and simulated (GLEAMS-SF) mean and range of aldicarb mass in the 1.2 m soil profile at the Dougherty Plain site, along with aldicarb mass predicted by deterministic GLEAMS, on: a) July 22, 1985, b) April 30, 1986, c) June 28, 1987, and d) July 27, 1987. (Note difference in scales).

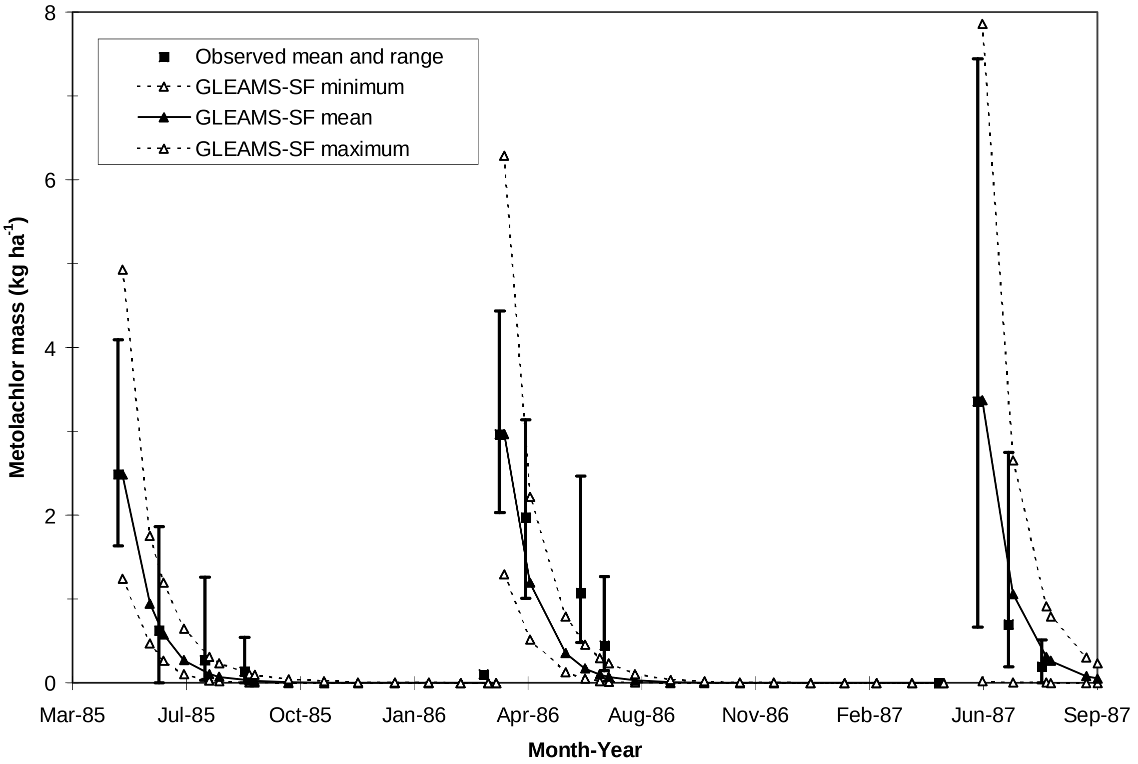

Figure 35. Observed and simulated (GLEAMS-SF) mean and range of metolachlor mass in the 1.2 m soil profile at the Dougherty Plain site.

Table 38. Statistical comparison of observed and simulated (GLEAMS-SF) metolachlor mass at the Dougherty Plain site.

Date	Soil depth (m)	Observed Mean	Observed Median	Observed St.dev.	GLEAMS-SF Mean	GLEAMS-SF Median	GLEAMS-SF St.dev.	p-value† KS Test	p-value† MW Test	Range Statistics‡
6/12/85	0-0.30	0.623	0.498	0.549	0.582	0.566	0.142	0-0.01	0.7405	40
7/22/85	0-0.60	0.272	0.149	0.342	0.108	0.102	0.041	0-0.01	0.0348	75
8/26/85	0-0.60	0.139	0.145	0.121	0.028	0.025	0.014	0-0.01	0.0000	40
3/24/86	0-1.20	0.106	0.045	0.291	0.000	0.000	0.000	—§	—	30
4/30/86	0-0.15	1.975	2.077	0.620	1.198	1.171	0.277	0-0.01	0.0000	75
6/17/86	0-0.30	1.074	0.860	0.539	0.175	0.166	0.065	0-0.01	0.0000	0
7/8/86	0-0.30	0.448	0.401	0.268	0.076	0.070	0.034	0-0.01	0.0000	20
4/28/87	0-1.20	0.000	0.000	0.000	0.000	0.000	0.000	—	—	100
6/28/87	0-1.20	0.701	0.590	0.532	1.059	1.044	0.414	0-0.01	0.0000	95
7/27/87	0-1.20	0.192	0.196	0.140	0.314	0.298	0.143	0-0.01	0.0002	80

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

§ The test could not be performed as all observed or simulated values were zero

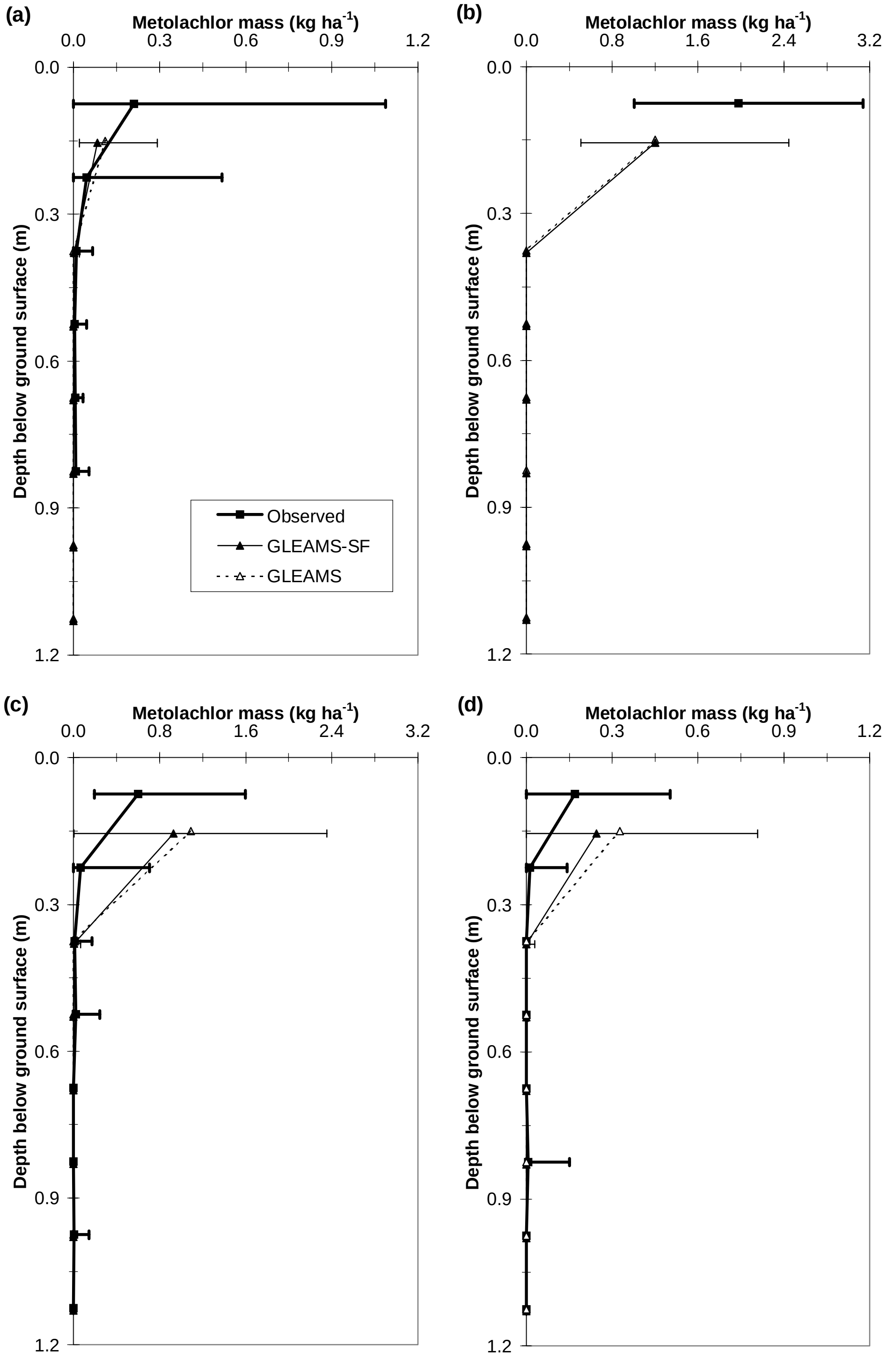

Figure 36. Observed and simulated (GLEAMS-SF) mean and range of metolachlor mass in the 1.2 m soil profile at the Dougherty Plain site, along with metolachlor mass predicted by deterministic GLEAMS, on: a) July 22, 1985, b) April 30, 1986, c) June 28, 1987, and d) July 27, 1987. (Note difference in scales).

Table 39. Mean monthly evapotranspiration (ET) and percolation predicted by GLEAMS-SF and GLEAMS-MC at the Dougherty Plain site.

Month-Year	Rainfall, mm	…..ET, mm….. GLEAMS-SF	GLEAMS-MC	.....Percolation, mm….. GLEAMS-SF	GLEAMS-MC
Apr-85	47.2	46.6	46.6	0.4	0.4
May-85	81.5	63.5	63.5	4.3	4.2
Jun-85	106.1	130.2	130.9	0.0	0.0
Jul-85	94.3	114.6	114.6	0.0	0.0
Aug-85	100.9	49.3	49.3	1.8	1.4
Sep-85	31.1	87.0	87.7	0.0	0.0
Oct-85	176.0	33.6	33.6	61.7	60.4
Nov-85	187.3	32.1	32.1	138.6	138.9
Dec-85	149.9	30.3	30.3	117.5	117.5
Total-85	974.3	587.1	588.7	324.4	322.9
Jan-86	76.3	30.7	30.7	53.9	54.0
Feb-86	133.7	38.5	38.5	92.0	92.0
Mar-86	89.8	39.2	39.2	52.1	52.1
Apr-86	14.9	20.5	20.5	0.0	0.0
May-86	4.4	23.8	23.8	0.0	0.0
Jun-86	65.4	96.7	97.5	0.0	0.0
Jul-86	63.3	56.9	56.8	0.0	0.0
Aug-86	108.6	80.0	80.0	0.0	0.0
Sep-86	57.5	93.1	93.3	0.0	0.0
Oct-86	77.8	40.0	40.1	0.0	0.0
Nov-86	150.1	33.8	33.8	82.4	81.6
Dec-86	110.8	30.5	30.5	80.7	80.7
Total-86	952.6	583.6	584.5	361.2	360.4
Jan-87	177.3	31.5	31.5	146.9	146.9
Feb-87	142.5	35.7	35.7	105.4	105.5
Mar-87	62.7	52.7	52.7	15.1	15.1
Apr-87	28.9	34.7	34.7	8.3	8.3
May-87	79.2	69.6	69.6	10.2	10.2
Jun-87	135.1	159.7	160.0	8.6	8.5
Jul-87	165.7	131.8	132.2	0.4	0.2
Aug-87	204.7	152.0	152.9	34.1	32.7
Sep-87†	12.7	54.6	55.1	0.0	0.0
Total-87	1008.8	722.4	724.5	329.1	327.4

† September 1-10 only

Table 40. Statistical comparison of depth-averaged soil water content predicted by GLEAMS-SF and GLEAMS-MC at the Dougherty Plain site.

Date	K-S Test p-value	M-W Test p-value
4/1/85	0-0.01	0.0000
6/12/85	0.2-1.0	0.5676
7/22/85	0.05-0.1	0.1434
8/26/85	0.05-0.1	0.1180
3/24/86	0.2-1.0	0.6161
4/30/86	0.2-1.0	0.6166
6/17/86	0.2-1.0	0.2510
7/8/86	0.05-0.1	0.1163
4/28/87	0.2-1.0	0.6166
6/28/87	0.2-1.0	0.5811
7/27/87	0.1-0.2	0.1598

Table 41. Statistical comparison of bromide mass predicted by GLEAMS-SF and GLEAMS-MC at the Dougherty Plain site.

Date	K-S Test p-value	M-W Test p-value
6/12/85	0.2-1.0	0.9395
7/22/85	0.02-0.05	0.0103
8/26/85	0.01-0.02	0.0086
11/26/85	0-0.01	0.0032
12/9/85	0.02-0.05	0.0079
12/30/85	0.1-0.2	0.0227
2/26/86	0.1-0.2	0.0866
3/24/86	0.2-1.0	0.1124
5/5/86	0.2-1.0	0.1127
11/19/86	0.2-1.0	0.3256
1/13/87	0.2-1.0	0.3673
2/6/87	0.2-1.0	0.3129
5/18/87	0.2-1.0	0.9517
7/21/87	0.2-1.0	0.9214

Table 42. Statistical comparison of aldicarb mass predicted by GLEAMS-SF and GLEAMS-MC at the Dougherty Plain site.

Date	K-S Test p-value	M-W Test p-value
6/12/85	0.2-1.0	0.7625
7/22/85	0.2-1.0	0.9901
8/26/85	0.2-1.0	0.8318
3/24/86	0.2-1.0	0.7405
4/30/86	0.2-1.0	0.9485
6/17/86	0.2-1.0	0.9949
7/8/86	0.2-1.0	0.9356
4/28/87	0-0.01	0.0443
6/28/87	0.2-1.0	0.5823
7/27/87	0.2-1.0	0.3486

Table 43. Statistical comparison of metolachlor mass predicted by GLEAMS-SF and GLEAMS-MC at the Dougherty Plain site.

Date	K-S Test p-value	M-W Test p-value
6/12/85	0.2-1.0	0.7454
7/22/85	0.2-1.0	0.7538
8/26/85	0.2-1.0	0.7270
3/24/86	—†	—
4/30/86	0.2-1.0	0.6780
6/17/86	0.2-1.0	0.6683
7/8/86	0.2-1.0	0.7111
4/28/87	—	—
6/28/87	0.2-1.0	0.9426
7/27/87	0.2-1.0	0.9397

† The test could not be performed as all simulated values were zero

Table 44. Important soil parameters used in the GLEAMS-SF simulation of the Nomini Creek site.

Soil parameter	**Mean**	**St.dev.†**
Hyd. conductivity of layer below root zone (RC), cm hr^{-1}	21.0	
Initial plant available water (BST)	1.0	
Porosity (ϕ or POR)		
Depth 1 (0-0.15 m)	0.387	0.049
Depth 2 (0.15-0.3 m)	0.370	0.035
Depth 3 (0.3-0.45 m)	0.369	0.028
Depth 4 (0.45-0.6 m)	0.402	0.034
Depth 5 (0-6-0.9 m)	0.410	
Water content at field capacity (θ_{fc} or FC), mm mm^{-1}		
Depth 1 (0-0.15 m)	0.192	0.008
Depth 2 (0.15-0.3 m)	0.224	0.016
Depth 3 (0.3-0.45 m)	0.241	0.028
Depth 4 (0.45-0.6 m)	0.197	0.032
Depth 5 (0-6-0.9 m)	0.127	
Water content at wilting point (θ_{wp} or BR15), mm mm^{-1}		
Depth 1 (0-0.15 m)	0.056	0.005
Depth 2 (0.15-0.3 m)	0.070	0.010
Depth 3 (0.3-0.45 m)	0.080	0.010
Depth 4 (0.45-0.6 m)	0.073	0.010
Depth 5 (0-6-0.9 m)	0.059	
Organic matter content (OM), %		
Depth 1 (0-0.15 m)	0.94	0.19
Depth 2 (0.15-0.3 m)	0.55	0.19
Depth 3 (0.3-0.45 m)	0.42	0.17
Depth 4 (0.45-0.6 m)	0.32	0.15
Depth 5 (0-6-0.9 m)	0.23	

† Standard deviation is given only for spatially variable parameters

Table 45. Estimates of important pesticide parameters used in GLEAMS-SF simulation of the Nomini Creek site.

Parameter	Atrazine			Metolachlor		
	Mean	**St.dev.†**	**PDF†**	**Mean**	**St.dev.†**	**PDF†**
Solubility in water (H2OSOL), mg L^{-1}	33			530		
Adsorption coefficient (KOC), $cm^3\ g^{-1}$	100			200		
Washoff fraction (WASHFRC)	0.5			0.6		
Foliar degradation rate (HAFLIF), days	5.0			5.0		
Soil half-life ($t_{1/2}$ or SOLLIF), days						
Depth 1 (0-0.15 m)	60.0	12.0	LogNormal	18.0	3.6	LogNormal
Depth 2 (0.15-0.3 m)	110.2	42.5	LogNormal	33.0	12.7	LogNormal
Depth 3 (0.3-0.45 m)	156.9	81.8	LogNormal	47.1	24.7	LogNormal
Depth 4 (0.45-0.6 m)	218.4	123.1	LogNormal	66.4	38.4	LogNormal
Depth 5 (0-6-0.9 m)	240.9			72.3		
Plant uptake coefficient (COFUP)	0.59			0.32		
Application rate (APRATE), kg ha^{-1}	0.97	0.34	LogNormal	1.05	0.48	LogNormal
Bromide‡ application rate, kg ha^{-1}	36.65	10.37	LogNormal			

† Standard deviation and PDF's are given only for spatially variable parameters

‡ Other bromide properties used in the simulation are: H20SOL = 1000 mg L^{-1}; KOC = 0 $cm^3\ g^{-1}$; WASHFRC = 0.75; HAFLIF = SOLLIF() = 99999 days; COFUP = 0.6.

Table 46. Mean monthly evapotranspiration (ET) and percolation predicted by GLEAMS-SF at the Nomini Creek site, along with ET and percolation predicted by the deterministic version of GLEAMS.

Month-Year	Rainfall (mm)	Runoff (mm)	ET (mm)		Percolation (mm)	
			GLEAMS-SF	GLEAMS	GLEAMS-SF	GLEAMS
Apr-90†	57.4	0.2	17.7	17.7	41.1	41.1
May-90	295.0	41.0	59.3	59.3	198.1	198.1
Jun-90	47.7	0.0	66.6	66.6	0.0	0.0
Jul-90	87.2	0.4	127.0	122.0	0.0	0.0
Aug-90	206.4	13.3	104.3	103.8	32.9	35.5
Sep-90	47.9	0.0	93.3	92.7	0.0	0.0
Total	741.6	54.8	468.1	462.0	272.1	274.8

† April 22-30 only

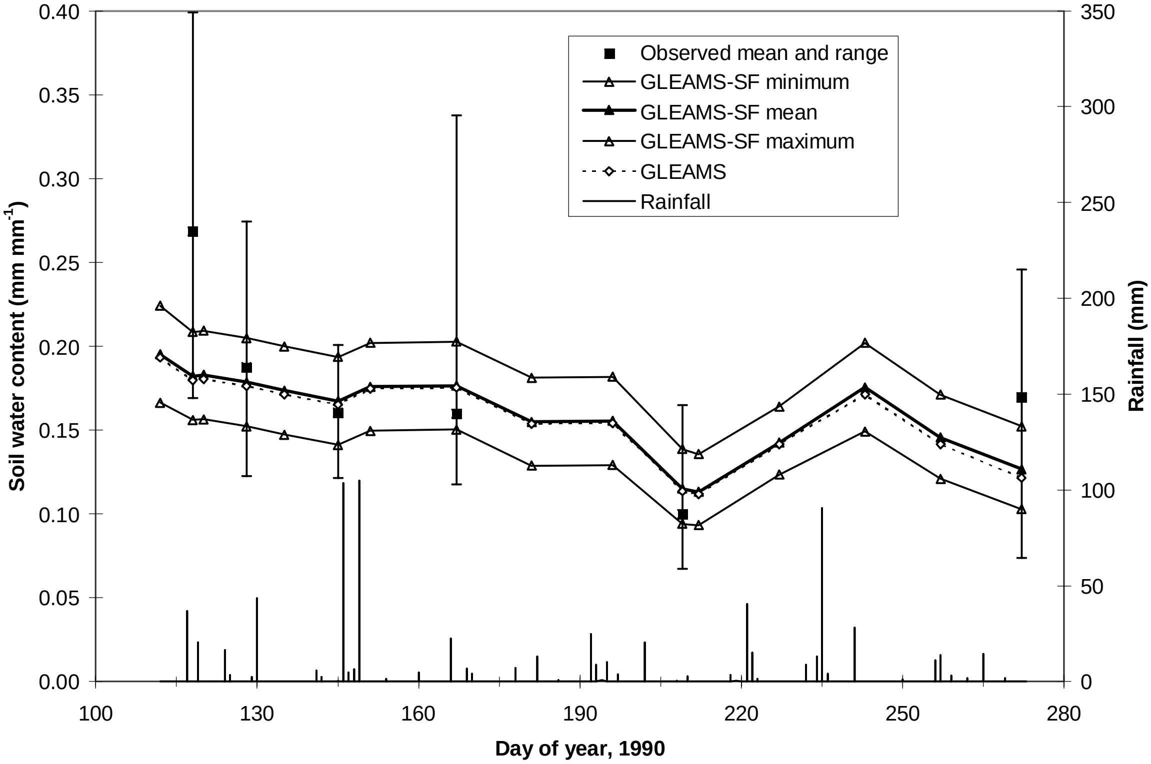

Figure 37. Observed and simulated (GLEAMS-SF) mean and range of depth-averaged soil water content in the root zone (0.9 m) at the Nomini Creek site over the simulation period, along with soil water content predicted by deterministic GLEAMS.

Table 47. Statistical comparison of observed and simulated (GLEAMS-SF) depth-averaged soil water content in the root zone at the Nomini Creek site.

Day of	Observed			GLEAMS-SF			p-value†		Range
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test	Statistic‡
118	0.269	0.267	0.059	0.182	0.182	0.008	0-0.01	0.000	15
128	0.187	0.182	0.038	0.179	0.179	0.008	0.01-0.02	0.506	55
145	0.160	0.161	0.020	0.167	0.168	0.008	0-0.01	0.036	75
167	0.160	0.142	0.050	0.177	0.177	0.008	0-0.01	0.000	25
209	0.100	0.096	0.022	0.115	0.115	0.007	0-0.01	0.000	45
272	0.170	0.157	0.045	0.127	0.127	0.007	0-0.01	0.000	25

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

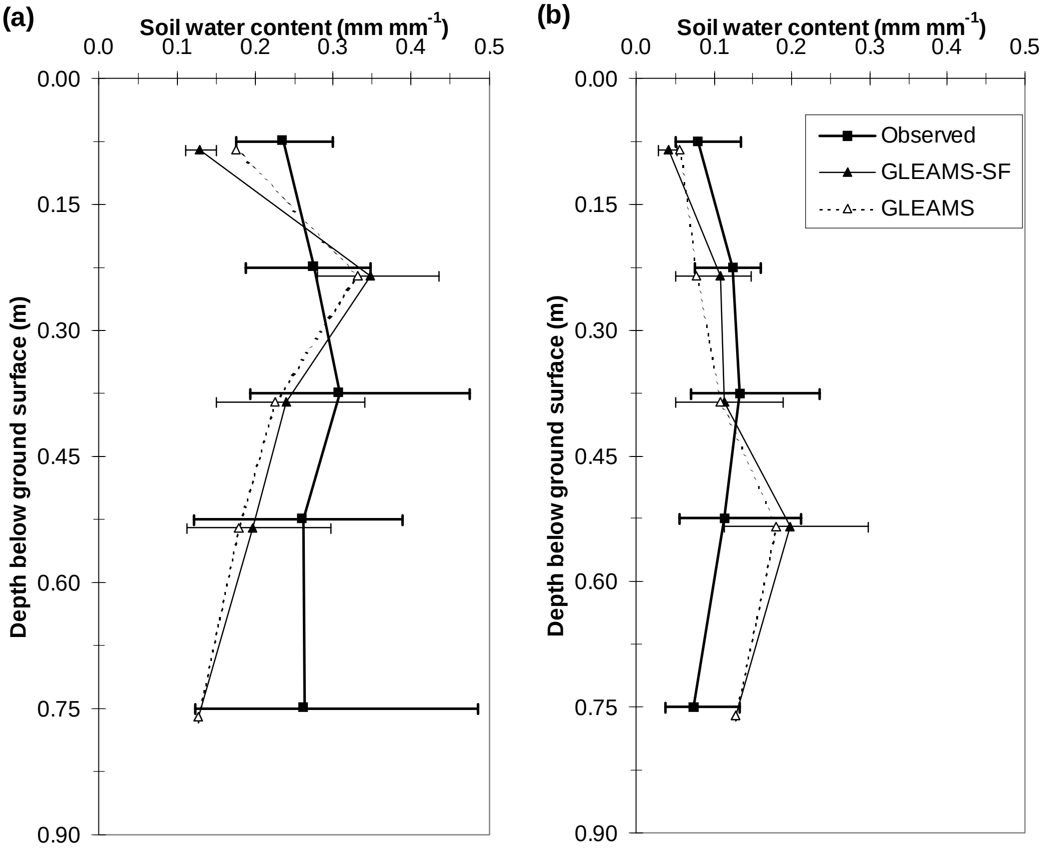

Figure 38. Observed and simulated (GLEAMS-SF) mean and range of soil water content in the root zone at the Nomini Creek site, along with soil water content predicted by deterministic GLEAMS, on: a) day 118 and b) day 209.

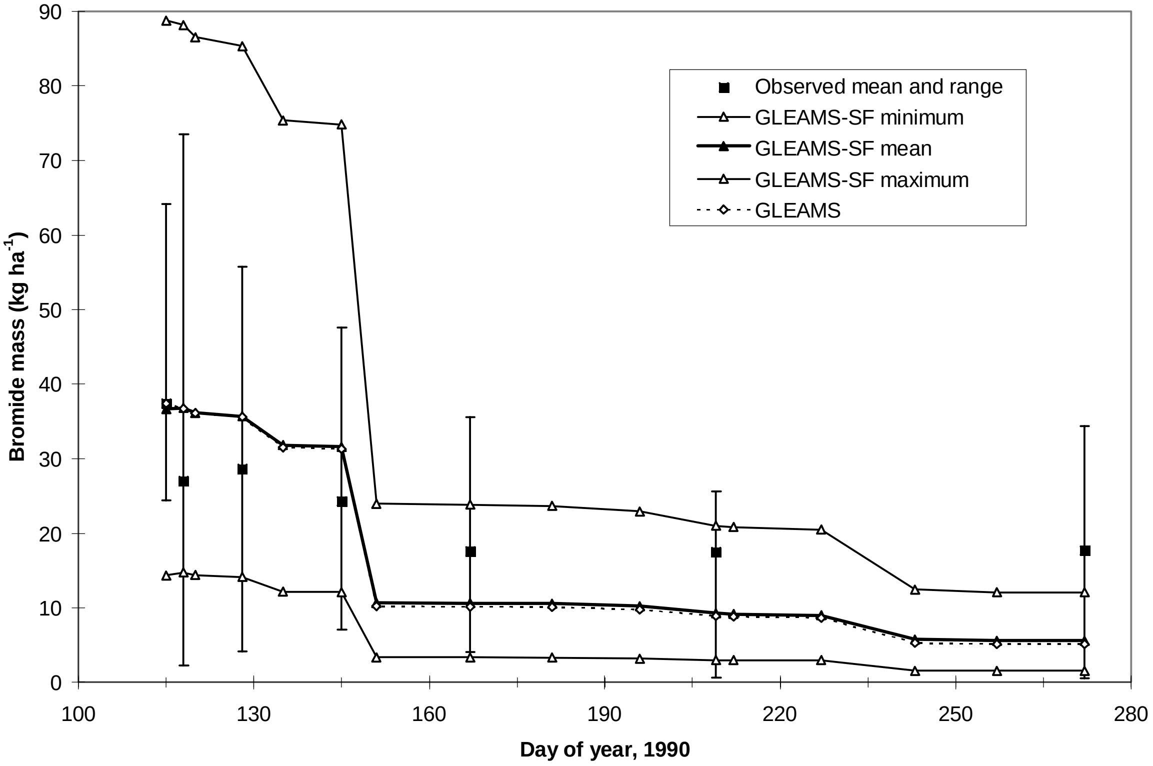

Figure 39. Observed and simulated (GLEAMS-SF) mean and range of total bromide mass in the root zone (0.9 m) at the Nomini Creek site over the simulation period, along with bromide mass predicted by deterministic GLEAMS.

Table 48. Statistical comparison of observed and simulated (GLEAMS-SF) total bromide mass in the root zone at the Nomini Creek site.

Day of	Observed			GLEAMS-SF			p-value†		Range
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test	Statistic‡
118	26.99	24.10	16.56	36.77	35.43	10.24	0-0.01	0.000	80
128	28.64	28.14	11.95	35.68	34.38	9.94	0.01-0.02	0.003	95
145	24.28	24.94	10.92	31.57	30.49	8.79	0.02-0.05	0.003	80
167	17.57	15.91	7.70	10.61	10.30	3.04	0-0.01	0.000	80
209	17.46	18.25	6.32	9.25	8.94	2.66	0-0.01	0.000	55
272	17.70	16.33	9.61	5.57	5.37	1.68	0-0.01	0.000	15

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

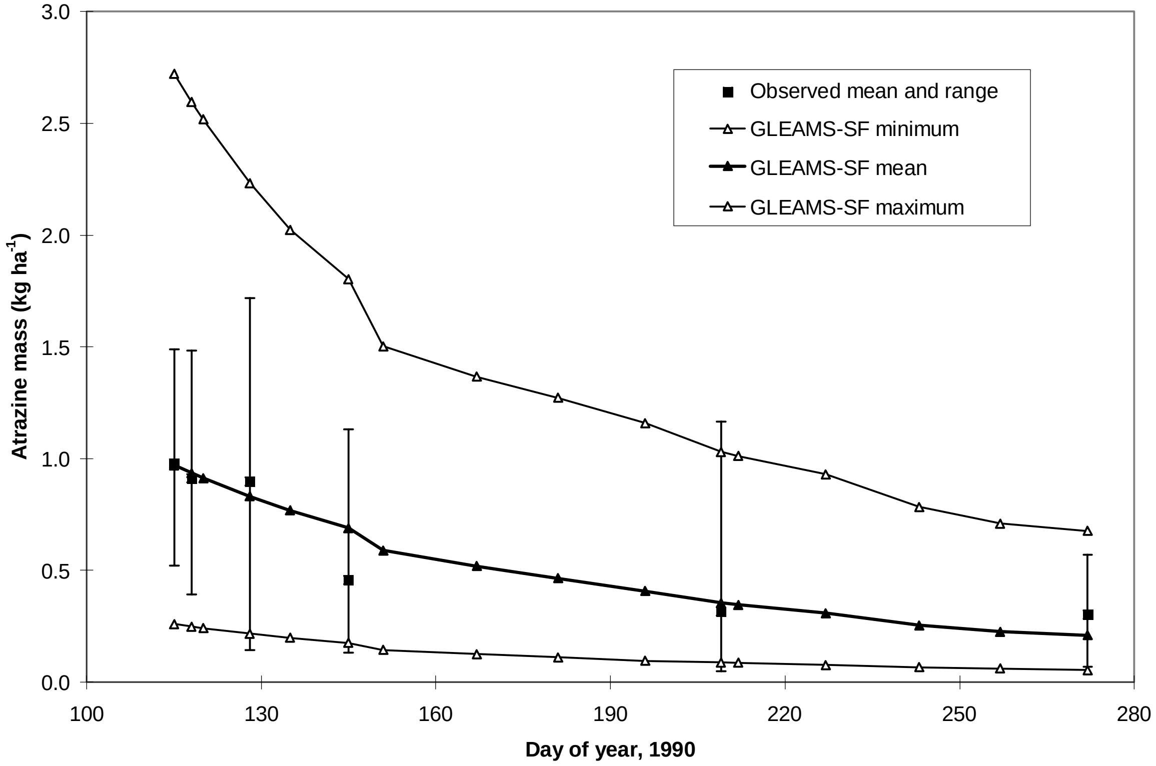

Figure 40. Observed and simulated (GLEAMS-SF) mean and range of total atrazine mass in the root zone (0.9 m) at the Nomini Creek site over the simulation period.

Table 49. Statistical comparison of observed and simulated (GLEAMS-SF) total atrazine mass in the root zone at the Nomini Creek site.

Day of	Observed			GLEAMS-SF			p-value†		Range
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test	Statistic‡
118	0.912	0.886	0.347	0.935	0.883	0.328	0.2-1.0	0.833	100
128	0.898	0.883	0.464	0.832	0.786	0.293	0.1-0.2	0.584	95
145	0.458	0.375	0.266	0.689	0.648	0.246	0-0.01	0.000	90
209	0.315	0.227	0.268	0.355	0.329	0.137	0-0.01	0.018	80
272	0.304	0.293	0.150	0.209	0.194	0.088	0-0.01	0.005	100

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

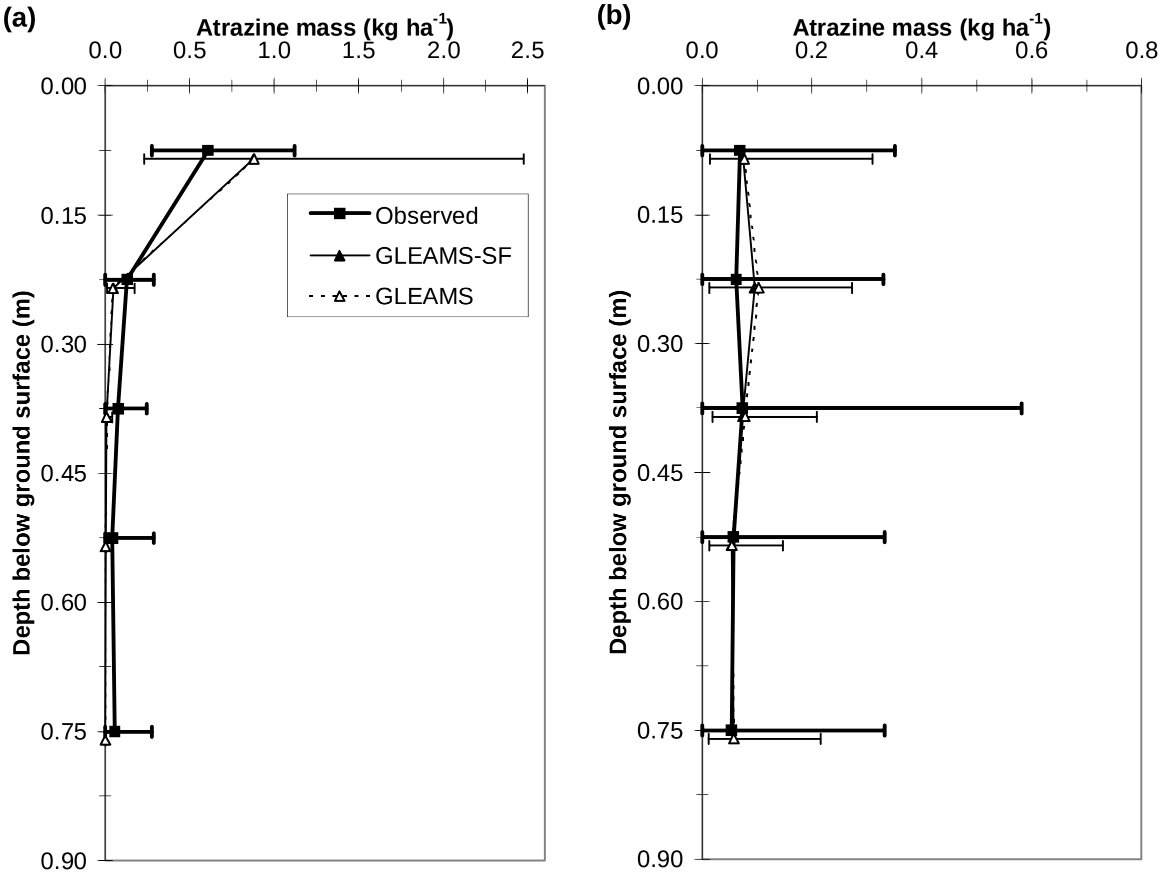

Figure 41. Observed and simulated (GLEAMS-SF) mean and range of atrazine mass in the root zone at the Nomini Creek site, along with soil water content predicted by deterministic GLEAMS, on: a) day 118 and b) day 209. (Note difference in scales).

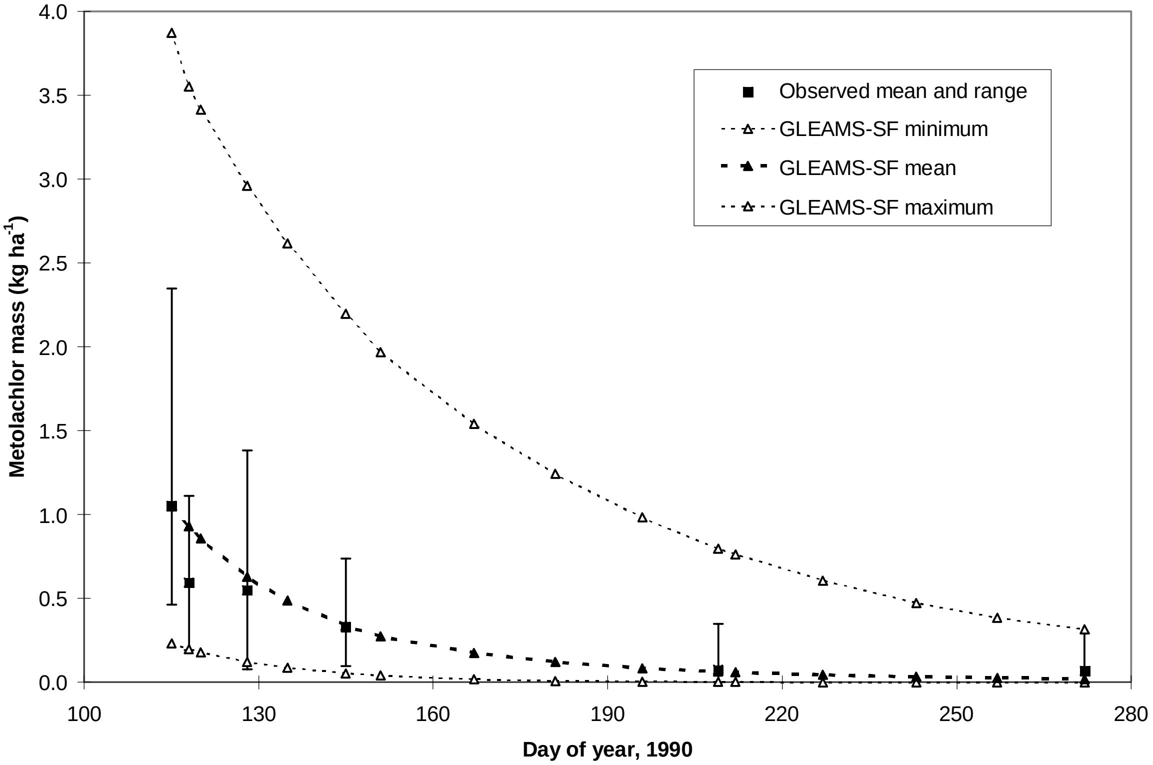

Figure 42. Observed and simulated (GLEAMS-SF) mean and range of total metolachlor mass in the root zone (0.9 m) at the Nomini Creek site over the simulation period.

Table 50. Statistical comparison of observed and simulated (GLEAMS-SF) total metolachlor mass in the root zone at the Nomini Creek site.

Day of	Observed			GLEAMS-SF			p-value†		Range
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test	Statistic‡
118	0.594	0.586	0.211	0.929	0.843	0.432	0-0.01	0.000	95
128	0.549	0.505	0.341	0.630	0.568	0.304	0.1-0.2	0.219	95
145	0.333	0.254	0.177	0.338	0.300	0.182	0.2-1.0	0.771	100
209	0.073	0.043	0.081	0.064	0.053	0.049	0-0.01	0.689	95
272	0.070	0.063	0.058	0.021	0.016	0.020	0-0.01	0.000	95

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

‡ Percentage of observations within simulated range

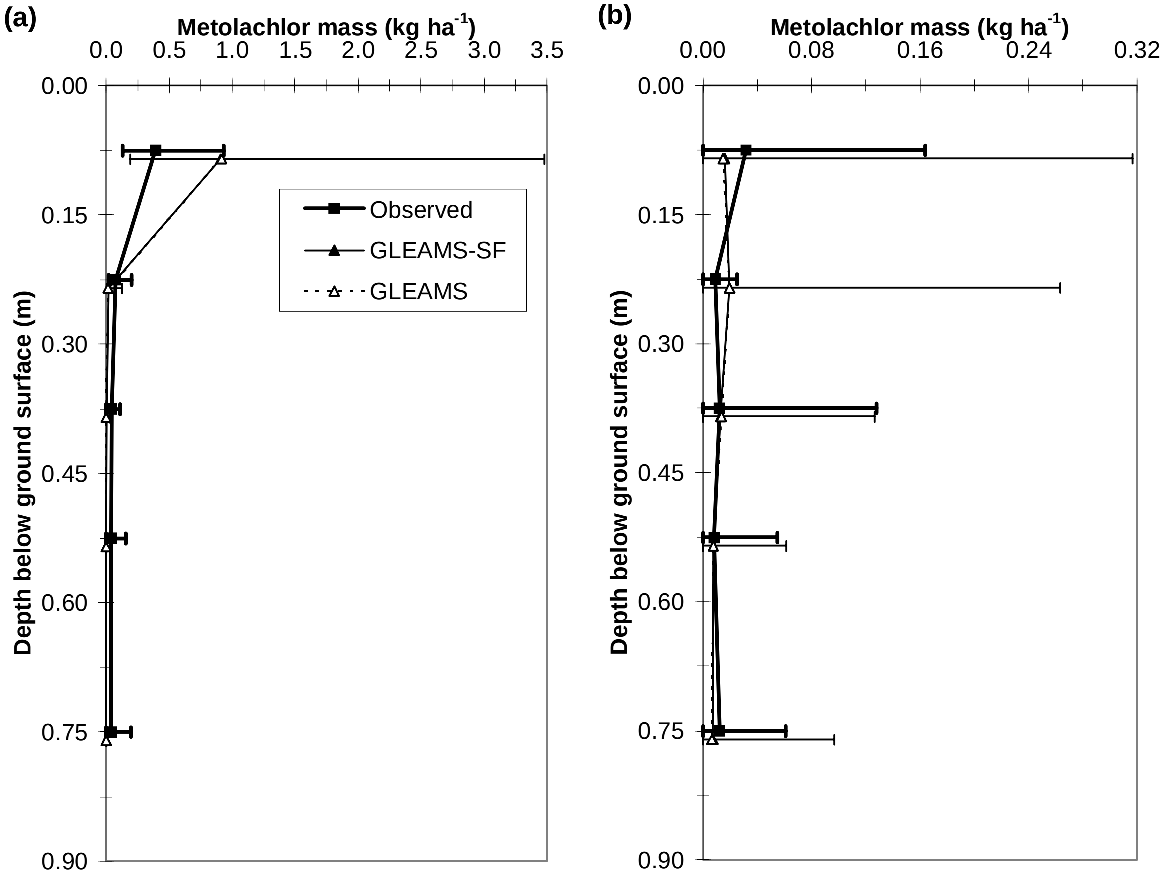

Figure 43. Observed and simulated (GLEAMS-SF) mean and range of metolachlor mass in the root zone at the Nomini Creek site, along with metolachlor mass predicted by deterministic GLEAMS, on: a) day 118 and b) day 209. (Note difference in scales).

Table 51. Mean monthly evapotranspiration (ET) and percolation predicted by GLEAMS-SF and GLEAMS-MC at the Nomini Creek site.

Month-Year	Rainfall (mm)	Runoff (mm)	ET (mm)		Percolation (mm)	
			GLEAMS-SF	GLEAMS-MC	GLEAMS-SF	GLEAMS-MC
Apr-90†	57.4	0.2	17.7	17.7	41.1	41.1
May-90	295.0	41.0	59.3	59.3	198.1	198.1
Jun-90	47.7	0.0	66.6	66.6	0.0	0.0
Jul-90	87.2	0.4	127.0	122.3	0.0	0.0
Aug-90	206.4	13.3	104.3	103.8	32.9	35.1
Sep-90	47.9	0.0	93.3	92.6	0.0	0.0
Total	741.6	54.8	468.1	462.3	272.1	274.4

† April 22-30 only

Table 52. Statistical comparison of depth-averaged soil water content in the root zone predicted by GLEAMS-SF and GLEAMS-MC at the Nomini Creek site.

Day of year, 1990	GLEAMS-SF			GLEAMS-MC			p-value†	
	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
112	0.195	0.195	0.008	0.192	0.192	0.008	0-0.01	0.000
118	0.182	0.182	0.008	0.178	0.178	0.008	0-0.01	0.000
128	0.179	0.179	0.008	0.175	0.175	0.008	0-0.01	0.000
145	0.167	0.168	0.008	0.163	0.164	0.008	0-0.01	0.000
167	0.177	0.177	0.008	0.173	0.173	0.008	0-0.01	0.000
209	0.115	0.115	0.007	0.113	0.113	0.006	0-0.01	0.000
272	0.127	0.127	0.007	0.124	0.124	0.007	0-0.01	0.000

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

Table 53. Statistical comparison of total bromide mass in the root zone predicted by GLEAMS-SF and GLEAMS-MC at the Nomini Creek site.

Day of year, 1990	GLEAMS-SF			GLEAMS-MC			p-value†	
	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
115	36.66	35.30	10.39	37.34	35.98	10.38	0.2-1.0	0.070
118	36.77	35.43	10.24	36.72	35.35	10.22	0.2-1.0	0.898
128	35.68	34.38	9.94	35.56	34.22	9.90	0.2-1.0	0.770
145	31.57	30.49	8.79	31.29	30.24	8.72	0.2-1.0	0.408
167	10.61	10.30	3.04	10.17	9.82	2.94	0-0.01	0.000
209	9.25	8.94	2.66	8.89	8.57	2.57	0.01-0.02	0.000
272	5.57	5.37	1.68	5.16	5.01	1.57	0-0.01	0.000

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

Table 54. Statistical comparison of total atrazine mass in the root zone predicted by GLEAMS-SF and GLEAMS-MC at the Nomini Creek site.

Day of	GLEAMS-SF			GLEAMS-MC			p-value†	
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
115	0.971	0.920	0.340	0.971	0.920	0.340	0.2-1.0	0.978
118	0.935	0.883	0.328	0.935	0.884	0.327	0.2-1.0	0.981
128	0.832	0.786	0.293	0.832	0.786	0.292	0.2-1.0	0.980
145	0.689	0.648	0.246	0.689	0.649	0.245	0.2-1.0	0.985
167	0.520	0.487	0.190	0.519	0.487	0.189	0.2-1.0	0.864
209	0.355	0.329	0.137	0.355	0.329	0.136	0.2-1.0	0.992
272	0.209	0.194	0.088	0.209	0.193	0.088	0.2-1.0	0.813

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests

Table 55. Statistical comparison of total metolachlor mass in the root zone predicted by GLEAMS-SF and GLEAMS-MC at the Nomini Creek site.

Day of	GLEAMS-SF			GLEAMS-MC			p-value†	
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
115	1.048	0.950	0.484	1.046	0.950	0.483	0.2-1.0	0.940
118	0.929	0.843	0.432	0.928	0.843	0.431	0.2-1.0	0.942
128	0.630	0.568	0.304	0.630	0.568	0.304	0.2-1.0	0.949
145	0.338	0.300	0.182	0.338	0.300	0.182	0.2-1.0	0.966
167	0.175	0.153	0.109	0.175	0.153	0.109	0.2-1.0	0.967
209	0.064	0.053	0.049	0.064	0.053	0.049	0.2-1.0	0.997
272	0.021	0.016	0.020	0.021	0.016	0.020	0.2-1.0	0.951

† p-values from two sample Kolmogorov-Smirnov (KS) and Mann-Whitney (MW) tests