Chapter VI

Comparison between Opus-SF and GLEAMS-SF

INTRODUCTION

One of the main conceptual differences between Opus and GLEAMS is how they model water flow in the unsaturated zone. Opus uses the rate-based Richards equation to model water flow, whereas GLEAMS uses the capacity-based approach to model water flow. The rate of change in soil water content in Opus is controlled by hydraulic gradients and a rate parameter, K_s, and redistribution of water is simulated each day on a time step between 0.01 and 1440 minutes (Smith, 1992). The change in soil water content in GLEAMS, on the other hand, occurs on a daily basis only as a result of rainfall and ET. Water moves down from i-th to (i+1)-th layer when water capacity of i-th layer (described by the parameter, water content at field capacity) is reached. Upward flow of water in GLEAMS occurs as a result of transpiration, whereas upward flow of water in Opus can also occur as a result of pressure differences. Solute transport in both models is by convection only. Opus simulates movement of solutes with upward flow of water, apart from plant uptake, whereas GLEAMS simulates upward movement of solutes only through plant uptake.

Water flow (and solute transport) in Opus is controlled by five parameters, K_s, θ_s, θ_r, ψ_b, and λ. On the other hand, water flow (and solute transport) in GLEAMS is controlled by only three parameters, θ_{fc}, θ_{wp}, and ϕ. (In this study, θ_r was considered equal to θ_{wp}, and ϕ was directly related to θ_s). In addition to Opus having more parameters, the rate parameters, K_s, ψ_b, and λ, are generally more variable than the other parameters.

The primary objective of this part of the study was to determine if a model that simulates water flow using a rate-based approach is different and provides more accurate prediction of the average condition and spatial variation of soil water content and solute mass than a model that simulates water flow using a capacity-based approach. This objective, however, could not be fully accomplished due to other differences in the model structure. A more realistic objective was to determine if the more mechanistic model, Opus, resulted in different and more accurate predictions of the average condition and spatial variability of soil water and solute mass than the more functional model, GLEAMS.

In order to accomplish the objective, soil water content, bromide and pesticide mass predictions from Opus-SF and GLEAMS-SF at the Dougherty Plain site and at the Nomini Creek site were compared with each other and with observed data (described in the previous two chapters). The comparison was based on graphical displays, statistical estimators, and statistical tests. The goal was to minimize differences in input data, so that model comparison would represent to the best degree possible, the differences in model structure/formulation.

The differences in model structure other than the conceptual differences in water flow, applicable to this study, include: (i) method used to compute evapotranspiration (ET), (ii) processes and method used to simulate plant growth, (iii) maximum number of soil horizons allowed and number of computational layers used for solution of water flow and solute transport equations, (iv) specification of pesticide degradation rate in subsurface soils, and (v) whether or not degradation rate is varied with respect to temporal variation in the soil environment.

Even though both models use the Priestly-Taylor method to calculate potential ET, solar radiation is specified differently. Daily radiation was provided in Opus for each year, whereas the best data that could be provided in GLEAMS was average monthly radiation for each year. The differences in potential ET, however, were not substantial. Other differences in ET predictions between the two models, besides the differences caused by the rate vs. capacity approach to simulating water flow, are differences in plant growth model and computation of soil evaporation. Opus has a mechanistic plant model that simulates plant growth in response to solar radiation and availability of water, nutrients, and temperature, using mechanistic functions to describe age and size of the crop. A portion of the total plant material is allocated to root mass, according to the plant’s relative age and size, which results in gradual increase in depth of root penetration into the soil until it reaches the maximum potential rooting depth. The plant growth model in GLEAMS is simpler, with crop growth simulated as a function of the leaf area index and evapotranspiration extracted from the active root zone using an exponentially decreasing function. Soil evaporation in Opus and GLEAMS proceeds in the two-stage process proposed by Ritchie (1972). However, there are some differences between the two models in the computation of soil evaporation. The relative amount of ET assigned to soil evaporation in Opus is controlled by the soil water content in the near-surface region, and soil evaporation is estimated from the portion of soil surface not shaded by plants or surface litter (mulch). In GLEAMS, soil evaporation is estimated from the portion of soil surface not shaded by plants only.

The maximum number of soil horizons allowed in Opus is six as compared to five for GLEAMS. To keep inputs similar between models, the root zone was defined by five horizons in both models and comparison of Opus-SF with GLEAMS-SF was based on soil water and solute mass outputs from the upper five horizons (1.2 m at the Dougherty Plain site and 0.9 m at the Nomini Creek site). The rate-based equation used to solve the water flow and solute transport equations in Opus requires more computational layers than the one used in GLEAMS. Opus required 15 computational layers to describe the 1.2 m profile at the Dougherty Plain site, whereas GLEAMS required only 10 layers. Opus required 14 computational layers to describe the 0.9 m profile at the Nomini Creek site, whereas GLEAMS required only 8 layers.

GLEAMS allows pesticide half-life to be input for each soil horizon, whereas Opus computes pesticide degradation rate in each subsurface horizon by multiplying degradation rate in the surface horizon by the ratio of organic carbon in the surface and the subsurface horizon. The above method used in Opus can give reasonable estimates of degradation rate in subsurface horizons for pesticides that degrade primarily by microbial action, when data are not available. This method was used to compute pesticide half-life in subsurface horizons for GLEAMS-SF at the Nomini Creek site, as field-measured data were not available. Since pesticide degradation rates were measured at the Dougherty Plain site, the measured values were used in GLEAMS. Another difference between the pesticide degradation components of the models is that Opus considers the influence of moisture and temperature on pesticide degradation rate, and GLEAMS does not.

Another difference between the model simulations was the manner in which field-measured runoff and pesticide losses in runoff were accounted for in the Nomini Creek simulations. While Opus had the option of specifying field-measured runoff as an input (in the measured data file) for a more direct evaluation of the subsurface component, runoff volume on the runoff-producing days was subtracted from rainfall for GLEAMS. Opus simulated pesticide losses in runoff corresponding to the runoff provided, whereas pesticide losses in runoff were subtracted from the application rate in GLEAMS. Pesticide losses in runoff, however, were minimal and constituted less than 1% of the amount applied.

MODELING FLOW AND TRANSPORT AT THE DOUGHERTY PLAIN SITE

Water Balance

It is evident from Table 56 that the mean monthly ET predicted by Opus-SF is higher than that predicted by GLEAMS-SF in the spring and summer months (March/April to August/September), and lower than GLEAMS-SF predictions in the remaining months. Almost the opposite trend can be seen with the mean monthly percolation values. Over the whole simulation period, Opus-SF predicted 108 mm of ET more than GLEAMS-SF, whereas GLEAMS-SF predicted 97 mm of percolation more than Opus-SF. The highest difference in monthly ET predicted by the two models was approximately 72 mm in July 1987, and the highest difference in monthly percolation was approximately 53 mm in October 1985.

The differences in simulated ET may be attributed to differences in computation of crop growth and soil evaporation (discussed earlier), the difference in the interval of radiation data provided, and the differences in their water flow models. The main reason for the differences in percolation predicted by Opus-SF and GLEAMS-SF is due to differences in their water flow models. GLEAMS-SF predicted larger amount of percolation when the soil layers were at field capacity, as all of the rainfall was being moved down through the layers. For a drier profile, GLEAMS-SF usually predicted less percolation than Opus-SF, which moves water using pressure gradients and gravitational flow. The negative percolation values predicted by Opus-SF indicated upward movement of water to offset the soil water deficit in the summer. GLEAMS-SF, on the other hand, does not simulate upward flow.

Soil Water Content

Depth-averaged soil water content predicted by the models (Fig. 44) also follows most of the differences found in the ET and percolation estimates. The mean values of depth-averaged soil water content decrease in the spring and summer months and increase in the winter months. Opus-SF, with its rate-based water flow model, simulates larger fluctuations in soil water content and appears to be more sensitive to weather variables than the capacity-based algorithm in GLEAMS-SF. Both models responded to rainfall in a similar way if the profile was already at or near field capacity, but depth-averaged soil water content in GLEAMS did not increase as much as in Opus when rainfall occurred when the soil was drier (e.g., soil water content on June 28, 1987 in Figures 44 and 45c). In the latter case, soil water content in the lower layers of GLEAMS did not increase until the upper layers were at field capacity.

The Mann Whitney test and the two sample KS test showed that the medians and EDFs, respectively, of depth-averaged soil water content predicted by Opus-SF and GLEAMS-SF were significantly different ($\alpha = 0.01$) on all dates, except June 17, 1986 and April 28, 1987 (Table 57). Overall, the standard deviations of soil water content predicted by Opus-SF and GLEAMS-SF were similar. The standard deviations predicted by Opus-SF were higher than GLEAMS-SF in 1985 and 1986, with the exception of June 12, 1985, whereas standard deviation predicted by GLEAMS-SF was higher than Opus-SF in 1987. The ranges of depth-averaged soil water content predicted by the two models were also similar, but the minimum and maximum values were different and somewhat proportional to the mean values predicted by the two models (Fig. 44). This shows that the random variations around the mean were predicted somewhat similarly by the two models, even though the average conditions were simulated differently.

Comparison of model results with observed data showed that GLEAMS-SF was able to predict the mean depth-averaged soil water content better than Opus-SF on sampling dates after large rainfall events (e.g., March 24, 1986, June 28, 1987). In a comparison of 14 nitrogen simulation models, de Willigen (1991) noted that mechanistic models were more sensitive to parameter values, and found that their soil water predictions were not better and sometimes worse than that of the simpler functional models.

Statistical test results (Table 6, Table 35) showed that medians and EDFs predicted by Opus-SF were closer to the observed data on June 12, 1985, July 22, 1985, and July 27, 1987, whereas medians and EDFs predicted by GLEAMS-SF were closer to the observed data on Aug. 26, 1985, Mar. 24, 1986, July 8, 1986, and June 28, 1987. Range statistics (Table 6, Table 35) on all sampling dates showed that more observations were contained within the GLEAMS-SF range than the Opus-SF range. The observed mean was within the range predicted by Opus-SF and GLEAMS-SF on all sampling dates. The mean predicted by Opus-SF was within the observed range on all dates except April 30, 1986 and June 28, 1987, whereas the GLEAMS-SF mean was within the observed range on all dates. Therefore, the statistics, along with Figure 44, indicated that GLEAMS-SF predicted spatial variations and average conditions of depth-averaged soil water content in the root zone better than Opus-SF.

Depth-wise distribution of observed and simulated soil water content in the soil profile (Fig. 45), however, shows that the shape of the observed soil water profile was simulated better, as expected, by the rate-based Opus-SF model. Opus-SF predicted the observed mean soil water content well on July 22, 1985 and July 27, 1987, but over-predicted soil water content in all layers on the dates preceded by substantial rainfall, March 24, 1986 and June 28, 1987. GLEAMS-SF, on the other hand, always predicted lower water contents in the upper layers and more water in the lower layers as compared to observed data. The range of soil water content predicted by both models was often greater than the observed range. Opus-SF also seems to have done a better job of predicting the minimum and maximum values of depth-wise soil water content (Fig. 45).

Bromide Mass

Both models predicted bromide mass in the root zone similarly. Bromide loss from the root zone predicted by GLEAMS-SF was slightly higher, as compared to Opus-SF, in the first three months after application (Fig. 46, Table 58), after which Opus-SF predicted slightly less bromide mass in the root zone than GLEAMS-SF. During this period, GLEAMS-SF predicted bromide leaching of approximately 9 g ha^{-1} whereas Opus-SF predicted bromide leaching of less than 1 g ha^{-1}. By February of 1986 (about 300 days after application), both models predicted more than 95% of the bromide to be lost by plant uptake and leaching. The observed data, however, showed bromide to remain in the soil profile in appreciable amounts throughout the study period. As described in Chapter IV and Chapter V, plant uptake accounted for most of the simulated losses during the cropping season and leaching in the high rainfall months of October, November, and December of 1985 accounted for the rest of the bromide losses.

Both KS test and Mann Whitney test showed that the EDFs and medians predicted by Opus-SF and GLEAMS-SF were significantly different ($\alpha = 0.05$) on all dates except Aug. 26, 1985. The bromide medians from the models were also not significantly different on January 13, 1987, after Opus-SF had predicted some of the bromide to move up into the root zone. The standard deviations predicted by Opus-SF were greater than that predicted by GLEAMS-SF until the time that both models had more than 3 kg ha^{-1} of bromide mass remaining in the root zone (Table 58). The ranges and maximum values predicted by the two models were comparable and varied with the mean and median values (Fig. 46).

Aldicarb Mass

Opus-SF predicted higher total aldicarb mass in the root zone than GLEAMS-SF for all three years, with the differences increasing with time in each year (Fig. 47). Opus-SF also predicted larger variations in aldicarb mass than GLEAMS-SF, and the differences in standard deviation and range predicted by the two models increased with time (Fig. 47, Table 59). Except the application dates in each year, the EDFs and medians of aldicarb mass predicted by the two models were not significantly different ($\alpha = 0.05$) on only April 30, 1986 (Table 59).

The mean, standard deviation, and range predicted by GLEAMS-SF was closer to the observed data than the mean and range predicted by Opus-SF on most dates (Fig. 47, Table 8, Table 37). The p-values from Mann-Whitney test and KS test also showed that the median and EDFs predicted by GLEAMS-SF were closer to the observed data than Opus-SF, although results from the statistical tests were not very different (Table 8, Table 37). The range statistics were the same for both models on all field sampling dates. However, it must be noted that even though almost all of the observations were within the simulated range except on one date, the simulated range was much larger than the observed range on many dates. In the case of Opus-SF, the simulated mean was not even contained in the observed range on many dates.

The depthwise distribution of aldicarb mass (Fig. 48) showed that most of the differences between the models occurred beyond the surface horizon (0-0.3 m), with the differences increasing with time. This indicates that the degradation rate of aldicarb in the subsurface horizons computed internally by Opus-SF, which was lower than the values used in GLEAMS-SF based on laboratory measured values, was perhaps the overriding factor in the difference between the models and the overprediction of aldicarb mass by Opus-SF. Other factors such as differences in movement of solutes, due to differences in their water flow models, and the adjustment of degradation rate in Opus-SF with respect to temperature and soil moisture content, would have had a lower effect on the predictions.

Metolachlor Mass

Like aldicarb, Opus-SF predicted higher total metolachlor mass in the root zone than GLEAMS-SF on all three years with the differences increasing with time in each year (Fig. 49). Opus-SF also predicted larger variations in metolachlor mass than GLEAMS-SF, with the differences in standard deviation and range predicted by the two models increasing with time (Fig. 49, Table 60). Except the application dates in each year, both the EDFs and medians of metolachlor mass predicted by the two models were not significantly different ($\alpha = 0.05$) on only June 28, 1987 (Table 60). The median metolachlor mass predicted by the two models on April 30, 1986 were also not significantly different ($\alpha = 0.05$).

With respect to observed data, both models underpredicted the observed metolachlor mass in 1986 and overpredicted mass in 1987 (Fig. 49, Table 9, Table 38). In 1985, Opus-SF overpredicted and GLEAMS-SF underpredicted the mass on the first sampling date (June 12), and both models underpredicted the mass on all of the other dates. Opus-SF was able to predict the observed median better than GLEAMS-SF in 1985 (except for the first date) and 1986, whereas GLEAMS-SF predicted observed median better in 1987. The spatial variations in observed metolachlor mass were much more than that predicted by both models, with standard deviation and range predicted by GLEAMS-SF farther away from the observed variation. The KS test showed that there were no significant differences ($\alpha = 0.01$) between observed EDF and Opus-SF EDF on July 22, 1985 (Table 9, Table 38), while all of the other simulated distributions were significantly different from the observed distribution. The range statistics for Opus-SF were also better than that of GLEAMS-SF in 1985 and 1986.

The depthwise distribution of metolachlor mass (Fig. 50) showed that Opus-SF predicted more metolachlor mass in the top horizon than GLEAMS-SF, with the differences increasing with days after application. Metolachlor, with a higher K_{oc} and a lower half-life (Table 4), leaches much slower than aldicarb and, therefore, most of it remains in the upper 0.3 m and is subject to greater degradation early in the season. Therefore, the effect of degradation rate of metolachlor in the subsurface horizons, computed internally by Opus-SF, which was lower than the values used in GLEAMS-SF based on laboratory measured values, is not as big of a factor as with aldicarb. GLEAMS-SF predicted more leaching of metolachlor from the top horizon than Opus-SF. The adjustment of degradation rate with respect to temperature and soil moisture content may also have had some effect on the Opus-SF predictions. The strongly adsorbed and highly degradable nature of metolachlor may also be the reason why both models (GLEAMS-SF, to a greater extent) underpredicted spatial variability of metolachlor mass in contrast to spatial variability of aldicarb mass.

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Water Balance

Mean monthly ET predicted by the models (Table 61), showed that ET predicted by Opus-SF peaked nearly a month earlier than GLEAMS-SF. While Opus-SF started predicting substantial plant transpiration by June, plant transpiration in GLEAMS-SF became a significant part of the total ET only a month later. The maximum monthly ET of approximately 145 mm predicted by Opus-SF, based on a 0.9 m profile, in June was also greater than the maximum monthly ET of 127 mm predicted by GLEAMS-SF in July. These differences in peak ET and ET amounts can be attributed mainly to differences in crop growth simulated by Opus-SF and GLEAMS-SF, and partially to the water flow models and differences in the interval of radiation data provided to each model. Over the five month study period, Opus-SF predicted approximately 40 mm more ET than GLEAMS-SF. Variation in monthly ET was low in both models, with CVs ranging from 0 to 5% for Opus-SF and 0 to 2% for GLEAMS-SF.

Opus-SF predicted more percolation losses than GLEAMS-SF until the end of June (Table 61). Percolation amounts from Opus-SF based on a 0.9 m profile were not very different (less than 3 mm) from those based on a 1.2 m profile (Table 61) in April and May, but were approximately 18 mm less than the value in Table 61 in June. As discussed in the previous section, the main reason for the differences in percolation predicted by Opus-SF and GLEAMS-SF is due to differences in their water flow models. GLEAMS-SF predicted larger amount of percolation when the soil layers were at field capacity, as all of the rainfall was being moved down through the layers. For a drier profile, GLEAMS-SF usually predicted lower percolation than Opus-SF, which moves water using pressure gradients and gravitational flow. Opus-SF, thus predicted negative percolation values in summer, to offset the soil water deficit in the root zone. GLEAMS-SF, on the other hand, does not simulate upward flow. Deducting runoff, ET, and percolation losses from rainfall shows that both models predicted a reduction in soil water storage in the root zone over the simulation period. The soil water deficit predicted by Opus-SF was approximately 120 mm from the upper 1.2 m, whereas the soil water deficit predicted by GLEAMS-SF was approximately 54 mm from the upper 0.9 m of the soil profile.

Soil Water Content

Depth-averaged soil water content predicted by Opus-SF and GLEAMS-SF (Fig. 51) show clearly the effect of the differences in water balance predicted by the models. The mean values of depth-averaged soil water content predicted by Opus-SF were lower than those predicted by GLEAMS-SF in the months of June, July, and August. The lower soil water content predicted by Opus-SF in the summer months was due to the higher ET predicted by the model during these months. As seen in the Dougherty Plain simulations, the rate-based water flow model in Opus-SF simulated larger fluctuations in soil water content and was more sensitive to weather variables than the capacity-based algorithm in GLEAMS-SF. The sensitivity of Opus-SF predictions to high rainfall (104 mm, 105 mm, and 91 mm of rainfall on days 145, 149, and 235, respectively) can be seen by the sudden increase in soil water content on days 151 and 243 (Fig. 51). These rainfall events did not have as much influence on soil water predictions by GLEAMS-SF, as more of the water percolated out of the root zone.

The Mann-Whitney test showed that the medians of depth-averaged soil water content predicted by the two models were significantly different ($\alpha = 0.05$) on all dates except day 272 (Table 62). The variation in soil water content predicted by the two models was comparable until the end of June, after which the range and standard deviation predicted by Opus-SF were lower than that of GLEAMS-SF (Fig. 51, Table 62). The KS test showed that the EDFs of depth-averaged soil water content predicted by Opus-SF and GLEAMS-SF were significantly different ($\alpha = 0.05$) on all of the field sampling dates (Table 62).

Comparison of model results with observed data on field sampling dates show that observed median was significantly different ($\alpha = 0.01$) from Opus-SF median on all dates except days 128 and 167 and significantly different from GLEAMS-SF median on all dates except days 128 and 145 (Table 20, Table 47). The standard deviation and range of soil water content predicted by Opus-SF and GLEAMS-SF were much lower than the observed standard deviation and range. As a result, the observed mean did not fall within the simulated range on days 118, 209, and 272. Range statistics (Table 20, Table 47) show that 50% of observations fell within the Opus-SF range and GLEAMS-SF range on only two of the six sampling dates. The KS test results (Table 20, Table 47) showed that there were no significant differences ($\alpha = 0.01$) between observed EDF and Opus-SF EDF on day 167 and between observed EDF and GLEAMS-SF EDF on day 128.

The lower soil water content predicted by Opus-SF and GLEAMS-SF early in the study period, as compared to observed data, was partly due to the description of initial water content in the models. In Opus-SF, the user was allowed to input only the initial water content of the surface horizon and the model estimated initial water content for the rest of the layers based on static equilibrium condition. The soil water content estimated thus for the subsurface horizon by Opus-SF led to an underprediction of the soil water profile on day 112 (data not shown). Spatial variations in initial water content were not described in Opus-SF, as there was not enough data to describe its distribution ($n = 4$). This may have been partly responsible for the reduced variation early in the simulation period. As discussed earlier, the initial water content specified in GLEAMS-SF was lower than what was observed in the field, as the model does not allow the user to specify an initial water content above field capacity.

Depth-wise distribution of observed and simulated soil water content on days 118 and 209 (Fig. 52) show that Opus-SF, as expected, was able to predict the shape of the soil water profile in the field better than GLEAMS-SF. The rate based Opus model gave a more uniform soil water profile, whereas the piston flow mechanism in GLEAMS-SF show the water moving downward from layer to layer, when field capacity of each layer is reached. The soil water profile predicted by GLEAMS-SF for most of May show that all layers except the surface layer was at field capacity (data not shown).

The underprediction by both models, GLEAMS-SF to a greater extent, on day 118 (Fig. 52a) may be attributed to the disparity in initial water content specified in the models. Unlike GLEAMS-SF, Opus-SF predicted some variation of soil water content in the 0.6-0.9 m layer on day 118 as a result of the variation in the upper layers. The range of soil water content predicted by both models were less than the observed range in most of the depths on these two dates. The lower variation of soil water content predicted by the models can be attributed mainly to the reduced variation of soil physical properties derived from texture data. The decision to not consider spatial variation of soil properties in the 0.6-0.9 m depth and spatial variation in initial water content in Opus-SF may also have contributed to the lower variation in simulated soil water content.

Bromide Mass

Opus-SF and GLEAMS-SF predicted similar amounts of bromide mass (mean and range) until the end of May (35 days after application), after which Opus-SF predicted more bromide to leave the root zone as compared to GLEAMS-SF (Fig. 53). By day 167, Opus-SF had predicted approximately 80% of bromide to leave the root zone and GLEAMS-SF had predicted approximately 70% of bromide to leave the root zone. The Mann-Whitney and KS tests (Table 63), however, showed that median and EDFs of bromide mass predicted by the two models, from day 145 onwards, were significantly different ($\alpha = 0.05$). The difference between the standard deviations predicted by the two models were less than 5% until day 145, after which bromide mass predicted by GLEAMS-SF was more variable. Some of the differences in bromide mass predicted by the models can be attributed to differences in their water flow models, and hence bromide leaching. The other differences can be explained by differences in plant uptake, as a result of differences in ET predictions. Higher ET predicted by Opus-SF in June could have led to greater uptake losses of bromide. Since the models do not give the amount of uptake losses as an output, the exact amount of losses could not be known. The impact of plant uptake on solute mass predictions and the validity of the uptake coefficient (0.6) used in this study must be investigated further.

The observed data showed bromide to remain in the profile in appreciable amounts throughout the study period, with approximately 50% of the applied tracer remaining in the root zone. Even though Opus and GLEAMS were not able to retain most of the bromide in the root zone (as discussed in earlier chapters), simulation of spatial variability allowed some of the observations to be contained within the simulated range. On day 167, 45% and 80% of the observations were contained in the range predicted by Opus-SF and GLEAMS-SF, respectively (Table 21, Table 48). The range statistics reduced to 5% and 55% for Opus-SF and GLEAMS-SF, respectively, on day 209, and 10% and 15% on day 272. Overall, GLEAMS-SF seems to have predicted bromide mass better than Opus-SF.

Atrazine Mass

The difference between Opus-SF and GLEAMS-SF in predicting pesticide mass was not as distinct as bromide mass, like in the Dougherty Plain simulation (Figs. 54 and 55, Table 64). This is mainly because of the moderating effect of adsorption and degradation processes on pesticide transport as compared to bromide transport. Except for the application date, Opus-SF continuously predicted lower atrazine mass than GLEAMS-SF even though the differences in mean and median were always less than 10%. The Mann-Whitney test showed that the median predicted by the two models were significantly different ($\alpha = 0.01$) on days 128, 145, 167, and 209 (Table 64). The standard deviation and range of atrazine mass predicted by Opus-SF were also lower than that of GLEAMS-SF. The KS test showed that EDFs of atrazine mass predicted by the two models were significantly different ($\alpha = 0.05$) on days 145, 167, and 209 (Table 64).

GLEAMS-SF predicted faster leaching of atrazine than Opus-SF during most of the rainfall events in April and May, as the soil layers were at field capacity. GLEAMS-SF predicted a small amount of atrazine to leach below the root zone by April 30 (average of 0.16 g ha^{-1}), whereas Opus-SF predicted a much lower amount (average of less than 0.0001 g ha^{-1}). By May 31, GLEAMS-SF predicted 0.068 kg ha^{-1} of atrazine leaching losses from the root zone as compared to 0.01 kg ha^{-1} by Opus-SF. In June and July, GLEAMS-SF predicted no leaching losses as percolation was zero (Table 61), whereas Opus-SF predicted another 5-10 g ha^{-1} of leaching losses. Because of the slower downward movement of atrazine in Opus-SF, more atrazine was degraded in the upper layers (degradation rates decrease with depth), resulting in lower mass remaining in the root zone.

Greater atrazine losses due to plant uptake, because of higher ET predicted by Opus-SF in June, may explain for the additional differences between the models in June (Fig. 54). The effect of modifying degradation rate by temperature and moisture in Opus-SF is not obvious from the mass values. By the end of the simulation period, degradation and plant uptake accounted for more than 95% of atrazine losses predicted by Opus-SF, whereas they accounted for approximately 89% of atrazine losses predicted by GLEAMS-SF. By day 272, however, most of the differences between the models had evened out, and both predicted approximately 0.2 kg ha^{-1} to remain in the root zone as compared to 0.3 kg ha^{-1} in the field.

Both models underpredicted the observed standard deviation but overpredicted the range (maximum) in the first two months after application. Towards the latter half of the season, the simulated standard deviation was half or less than half of the observed standard deviation. Overall, statistical tests (Table 22, Table 49) show that Opus-SF did a slightly better job of predicting average conditions and distribution of atrazine mass than GLEAMS-SF.

Metolachlor Mass

Most of the differences between metolachlor mass predictions by Opus-SF and GLEAMS-SF were similar to that of atrazine (Figs. 56 and 57, Table 65). Metolachlor, with a larger K_{oc}, can be retained in the soil longer than atrazine, but will be degraded faster due to its smaller half-life. Opus-SF predicted lower metolachlor mass than GLEAMS-SF until the end of June, after which there were not much differences between the model predictions. The Mann-Whitney test showed that the median metolachlor mass predicted by the two models were not significantly different ($\alpha = 0.05$) on days 118, 209, and 272, besides the application date (Table 65). Differences in standard deviation and range were on the same lines as the mean, with GLEAMS-SF predicting more variation until the end of June, after which the variation predicted by both models were more or less the same. The maximum value of metolachlor mass predicted by GLEAMS-SF was always greater than that of Opus-SF. The KS test showed that EDFs of metolachlor mass predicted by the two models were not significantly different ($\alpha = 0.05$) on days 118, 209, and 272 (Table 65).

As with atrazine, the lower metolachlor mass predicted by Opus-SF can be attributed to more degradation of the herbicide in the upper layers as a result of the slower movement of water and solutes in April and May, as compared to GLEAMS-SF. Plant uptake would be less of a difference between the models in the case of metolachlor, as the uptake coefficient was only 0.32, as compared to 0.59 for atrazine. Leaching losses of metolachlor were also much lower than atrazine, with GLEAMS-SF predicting 6.5 g ha^{-1} by May, as compared to approximately 0.2 g ha^{-1} by Opus-SF. By the end of the five month period, metolachlor leaching losses predicted by GLEAMS-SF was 7.5 g ha^{-1} and by Opus-SF was approximately 9 g ha^{-1}. Degradation was the main loss pathway for metolachlor, which explains the lower difference between the model predictions in the latter half of the season. By the end of the simulation period, degradation and plant uptake accounted for more than 99% of metolachlor losses predicted by both models.

In comparison with observed data, there were no significant differences ($\alpha = 0.05$) between observed medians and corresponding model predictions on days 128, 145, and 209 (Table 23, Table 50). Both models underpredicted the observed standard deviation but overpredicted the range (maximum) throughout the study period. Towards the latter half of the season, the simulated standard deviation was close to half of the observed standard deviation. The KS tests showed that observed EDFs were not significantly different ($\alpha = 0.05$) from EDFs predicted by Opus-SF on days 128, 145, and 209, and they were not significantly different ($\alpha = 0.05$) from EDFs predicted by GLEAMS-SF on days 128 and 145 (Table 23, Table 50).

SUMMARY

Opus-SF was more sensitive to weather variables than GLEAMS-SF, and predicted higher ET and lower percolation than GLEAMS-SF. Seasonal fluctuations of soil water content was greater in Opus-SF than in GLEAMS-SF. The medians and EDFs of soil water content predicted by Opus-SF and GLEAMS-SF were significantly different on most sampling dates at both sites. GLEAMS-SF predicted depth-averaged soil water content on the field sampling dates better than Opus-SF. Opus-SF, on the other hand, predicted the depth distribution of soil water better than GLEAMS-SF.

GLEAMS-SF predicted faster leaching of solutes than Opus-SF, especially when the soil was at or above field capacity at the time of a rainfall event. The medians and EDFs of pesticide mass predicted by the two models were closer, but significantly different on most sampling dates at the Dougherty Plain site and on about half of the sampling dates at the Nomini Creek site. As compared to observed data, GLEAMS-SF predicted aldicarb mass at the Dougherty Plain site better than Opus-SF whereas Opus-SF predicted metolachlor mass at the same site better than GLEAMS-SF. Atrazine and metolachlor mass at the Nomini Creek site was predicted closer to observed data by Opus-SF on some sampling dates and GLEAMS-SF on other dates. Hence, it was difficult to determine which model predicted pesticide fate and transport at the Nomini Creek site.

Spatial variability of soil water content predicted by the two models, expressed by its standard deviation, range, and coefficient of variation, was comparable at both sites. Spatial variability of bromide mass at both sites and metolachlor mass at the Dougherty Plain site, predicted by Opus-SF, was greater than that predicted by GLEAMS-SF. On the other hand, spatial variability of aldicarb mass at the Dougherty Plain site and atrazine and metolachlor mass at the Nomini Creek site, predicted by GLEAMS-SF, was greater than that predicted by Opus-SF. Therefore, the greater number of spatially variable parameters and the more variable parameters in Opus-SF did not translate into a consistent difference in spatial variability of model output.

In conclusion, the more functional GLEAMS-SF model simulated depth-averaged soil water content in the root zone better than the more physically based Opus-SF, although it was not able to simulate the depth distribution of soil water as accurately as Opus-SF. This conclusion agrees with previous studies comparing such models in a deterministic context (Nicholls et al., 1982; de Willigen, 1991; Hutson and Wagenet, 1993). GLEAMS-SF was also able to predict solute movement at least as well as Opus-SF. GLEAMS-SF was able to simulate spatial variations of depth-averaged soil water content and pesticide mass in the field with reasonable accuracy employing fewer parameters that exhibit relatively less spatial variability.

Table 56. Mean monthly evapotranspiration (ET) and percolation predicted by Opus-SF and GLEAMS-SF at the Dougherty Plain site.

Month-Year	Rainfall, mm	.....ET, mm….. Opus-SF	GLEAMS-SF	.....Percolation, mm….. Opus-SF	GLEAMS-SF
Apr-85	47.2	60.9	46.6	1.3	0.4
May-85	81.5	76.8	63.5	1.0	4.3
Jun-85	106.1	132.0	130.2	-12.3	0.0
Jul-85	94.3	150.2	114.6	-14.2	0.0
Aug-85	100.9	60.1	49.3	-13.4	1.8
Sep-85	31.1	102.0	87.0	-10.7	0.0
Oct-85	176.0	17.7	33.6	9.1	61.7
Nov-85	187.3	18.2	32.1	170.2	138.6
Dec-85	149.9	18.2	30.3	152.3	117.5
Total-85	974.3	636.1	587.1	283.4	324.4
Jan-86	76.3	22.8	30.7	70.5	53.9
Feb-86	133.7	28.7	38.5	101.7	92.0
Mar-86	89.8	44.0	39.2	44.7	52.1
Apr-86	14.9	33.2	20.5	3.3	0.0
May-86	4.4	25.9	23.8	-5.3	0.0
Jun-86	65.4	161.0	96.7	-25.5	0.0
Jul-86	63.3	94.8	56.9	-27.3	0.0
Aug-86	108.6	93.8	80.0	-21.7	0.0
Sep-86	57.5	64.8	93.1	-9.2	0.0
Oct-86	77.8	25.6	40.0	6.5	0.0
Nov-86	150.1	18.4	33.8	49.3	82.4
Dec-86	110.8	16.4	30.5	124.0	80.7
Total-86	952.6	629.5	583.6	310.9	361.2
Jan-87	177.3	20.0	31.5	165.1	146.9
Feb-87	142.5	22.2	35.7	89.4	105.4
Mar-87	62.7	46.0	52.7	60.7	15.1
Apr-87	28.9	55.9	34.7	5.9	8.3
May-87	79.2	78.8	69.6	1.9	10.2
Jun-87	135.1	94.2	159.7	21.4	8.6
Jul-87	165.7	203.3	131.8	-21.6	0.4
Aug-87	204.7	180.2	152.0	-6.2	34.1
Sep-87†	12.7	35.2	54.6	6.6	0.0
Total-87	1008.8	735.7	722.4	323.1	329.1

† September 1-10 only

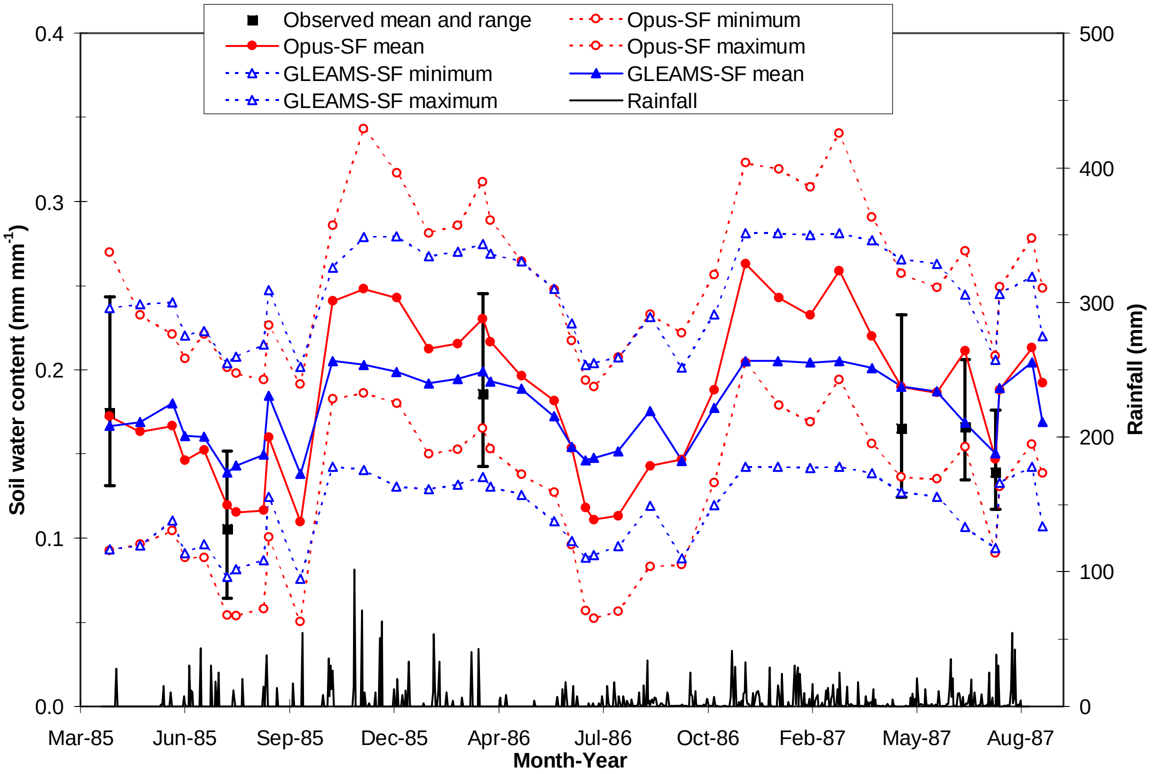

Figure 44. Observed and simulated mean and range of depth-averaged soil water content in the root zone at the Dougherty Plain site.

Table 57. Statistical comparison of depth-averaged soil water content in the root zone predicted by Opus-SF and GLEAMS-SF at the Dougherty Plain site.

	Opus-SF			GLEAMS-SF			p-value†	
Date	**Mean**	**Median**	**St.dev.**	**Mean**	**Median**	**St.dev.**	**KS Test**	**MW Test**
4/1/85	0.172	0.172	0.025	0.167	0.167	0.022	0-0.01	0.0000
6/12/85	0.077	0.075	0.017	0.041	0.036	0.021	0-0.01	0.0000
7/22/85	0.103	0.101	0.019	0.115	0.116	0.014	0-0.01	0.0000
8/26/85	0.092	0.091	0.015	0.089	0.088	0.014	0-0.01	0.0000
3/24/86	0.230	0.230	0.020	0.199	0.199	0.019	0-0.01	0.0000
4/30/86	0.125	0.128	0.035	0.070	0.067	0.029	0-0.01	0.0000
6/17/86	0.077	0.075	0.024	0.034	0.031	0.015	0.05-0.10	0.1129
7/8/86	0.039	0.036	0.016	0.039	0.036	0.015	0-0.01	0.0000
4/28/87	0.190	0.189	0.018	0.190	0.190	0.019	0.2-1.0	0.5139
6/28/87	0.211	0.210	0.017	0.169	0.169	0.019	0-0.01	0.0000
7/27/87	0.147	0.146	0.017	0.150	0.151	0.017	0-0.01	0.0000

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

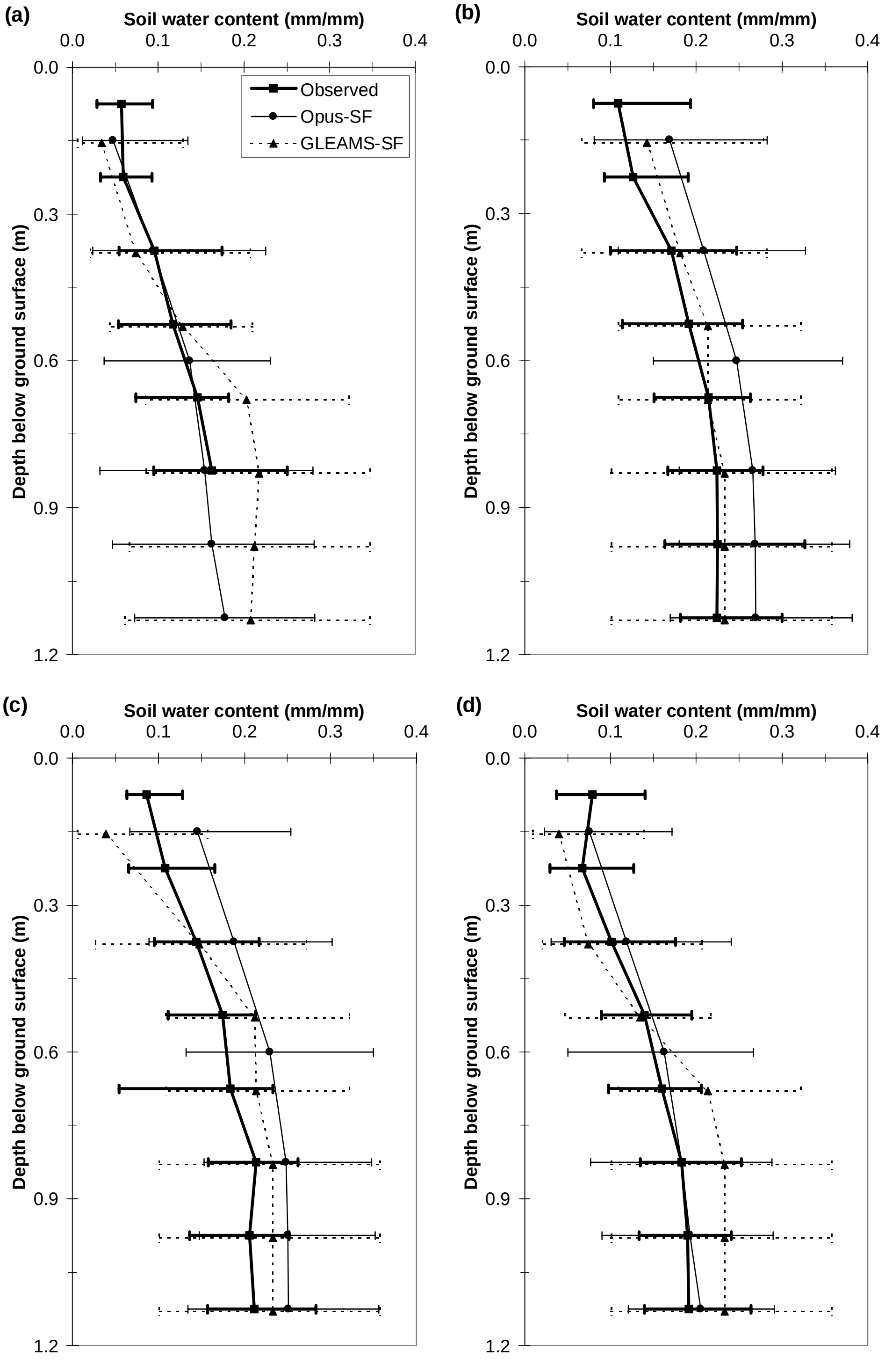

Figure 45. Observed and simulated mean and range of soil water content in the root zone at the Dougherty Plain site on: a) July 22, 1985, b) March 24, 1986, c) June 28, 1987, and d) July 27, 1987.

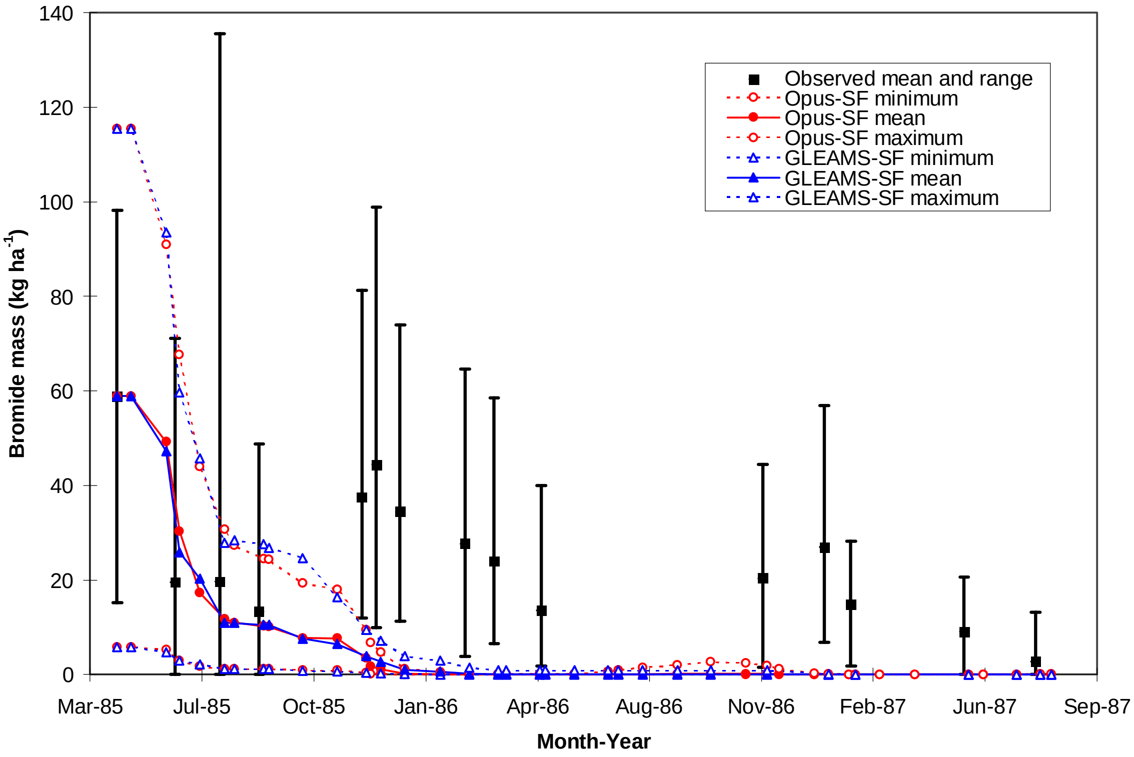

Figure 46. Observed and simulated mean and range of bromide mass in the root zone at the Dougherty Plain site.

Table 58. Statistical comparison of total bromide mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Dougherty Plain site.

	Opus-SF			GLEAMS-SF			p-value†	
Date	**Mean**	**Median**	**St.dev.**	**Mean**	**Median**	**St.dev.**	**KS Test**	**MW Test**
6/12/85	30.37	30.02	9.89	25.84	25.08	7.67	0-0.01	0.0000
7/22/85	11.82	11.41	4.27	10.96	10.62	3.73	0-0.01	0.0000
8/26/85	10.20	9.89	3.46	10.50	10.12	3.66	0.2-1.0	0.0958
11/26/85	3.40	3.15	1.56	3.90	3.77	1.37	0-0.01	0.0020
12/9/85	1.13	0.97	0.69	2.73	2.59	1.04	0-0.01	0.0000
12/30/85	0.19	0.14	0.16	1.08	1.01	0.49	0-0.01	0.0000
2/26/86	0.01	0.01	0.01	0.20	0.17	0.13	0-0.01	0.0000
3/24/86	0.00	0.00	0.01	0.10	0.08	0.07	0-0.01	0.0000
5/5/86	0.01	0.00	0.01	0.10	0.08	0.07	0-0.01	0.0000
11/19/86	0.17	0.09	0.20	0.09	0.07	0.07	0-0.01	0.0000
1/13/87	0.01	0.00	0.01	0.01	0.00	0.01	0-0.01	0.1004
2/6/97	0.00	0.00	0.00	0.00	0.00	0.00	0-0.01	0.0000
5/18/97	0.00	0.00	0.00	0.00	0.00	0.00	0-0.01	0.0000
7/21/87	0.00	0.00	0.00	0.00	0.00	0.00	0-0.01	0.0000

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

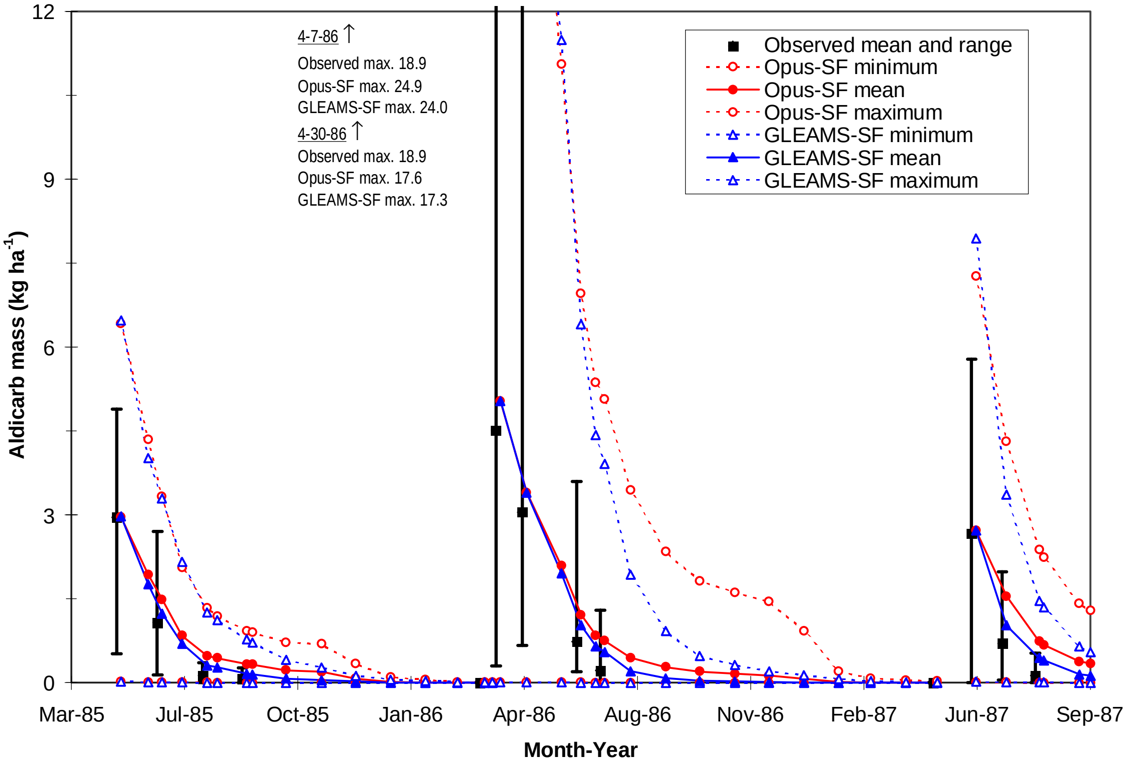

Figure 47. Observed and simulated mean and range of aldicarb mass in the root zone at the Dougherty Plain site.

Table 59. Statistical comparison of total aldicarb mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Dougherty Plain site.

	Opus-SF			GLEAMS-SF			p-value†	
Date	**Mean**	**Median**	**St.dev.**	**Mean**	**Median**	**St.dev.**	**KS Test**	**MW Test**
5/7/85	2.964	2.958	1.037	2.966	2.960	1.035	0.2-1.0	0.9483
6/12/85	1.490	1.474	0.560	1.236	1.224	0.480	0-0.01	0.0000
7/22/85	0.487	0.464	0.222	0.316	0.295	0.159	0-0.01	0.0000
8/26/85	0.334	0.315	0.162	0.162	0.145	0.094	0-0.01	0.0000
3/24/86	0.001	0.000	0.001	0.000	0.000	0.001	0-0.01	0.0000
4/7/86	5.031	3.560	4.425	5.038	3.560	4.423	0.2-1.0	0.9699
4/30/86	3.399	2.404	2.990	3.396	2.379	2.991	0.2-1.0	0.7785
6/17/86	1.209	0.850	1.131	1.025	0.718	0.963	0-0.01	0.0000
7/8/86	0.749	0.506	0.733	0.551	0.372	0.551	0-0.01	0.0000
4/28/87	0.001	0.000	0.002	0.000	0.000	0.001	0-0.01	0.0000
6/1/87	2.726	2.695	1.212	2.724	2.690	1.214	0.2-1.0	0.9570
6/28/87	1.550	1.502	0.717	1.030	1.003	0.500	0-0.01	0.0000
7/27/87	0.738	0.700	0.368	0.436	0.412	0.233	0-0.01	0.0000

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

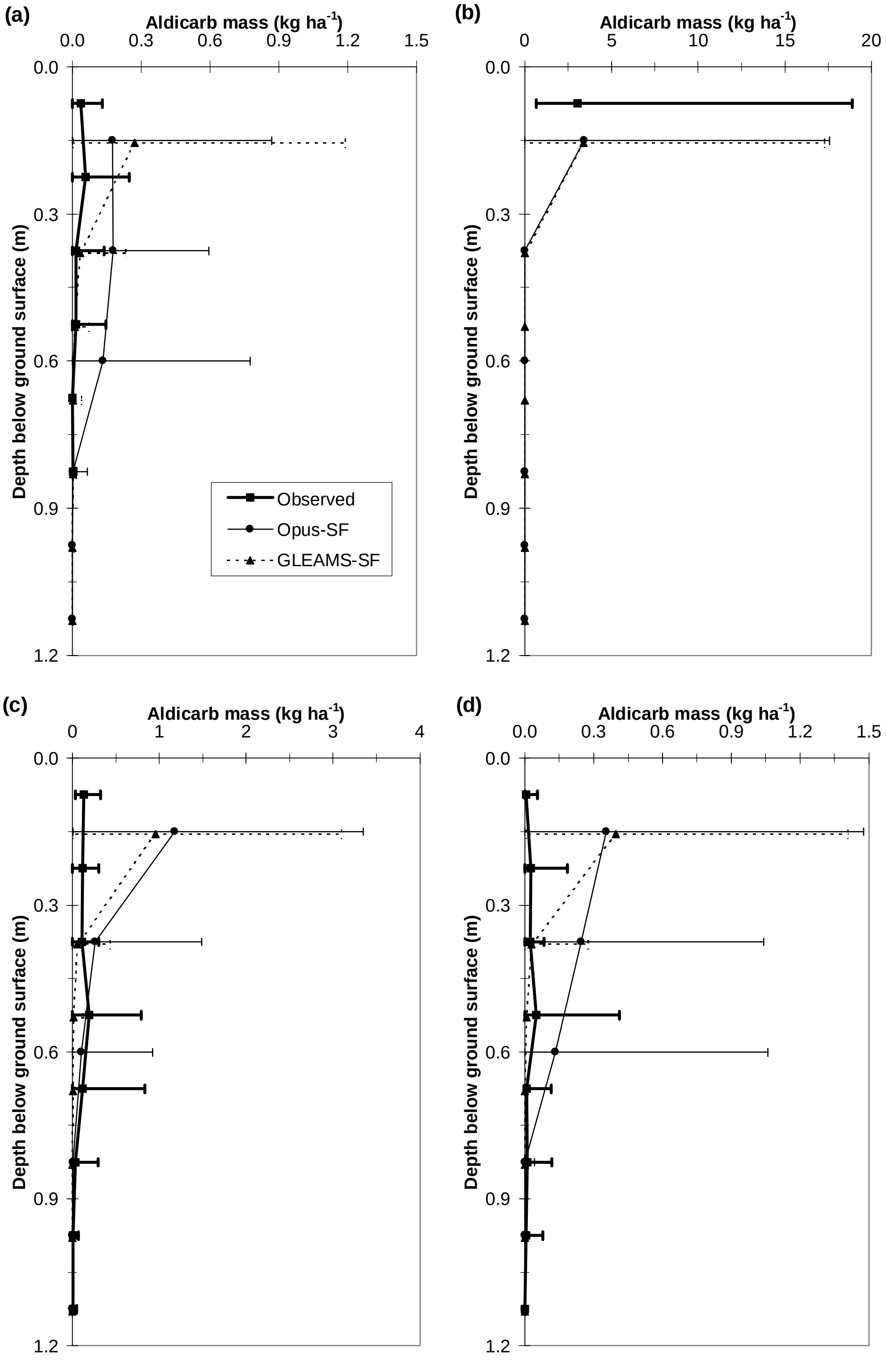

Figure 48. Observed and simulated mean and range of aldicarb mass in the root zone at the Dougherty Plain site on: a) July 22, 1985, b) April 30, 1986, c) June 28, 1987, and d) July 27, 1987. (Note difference in scales).

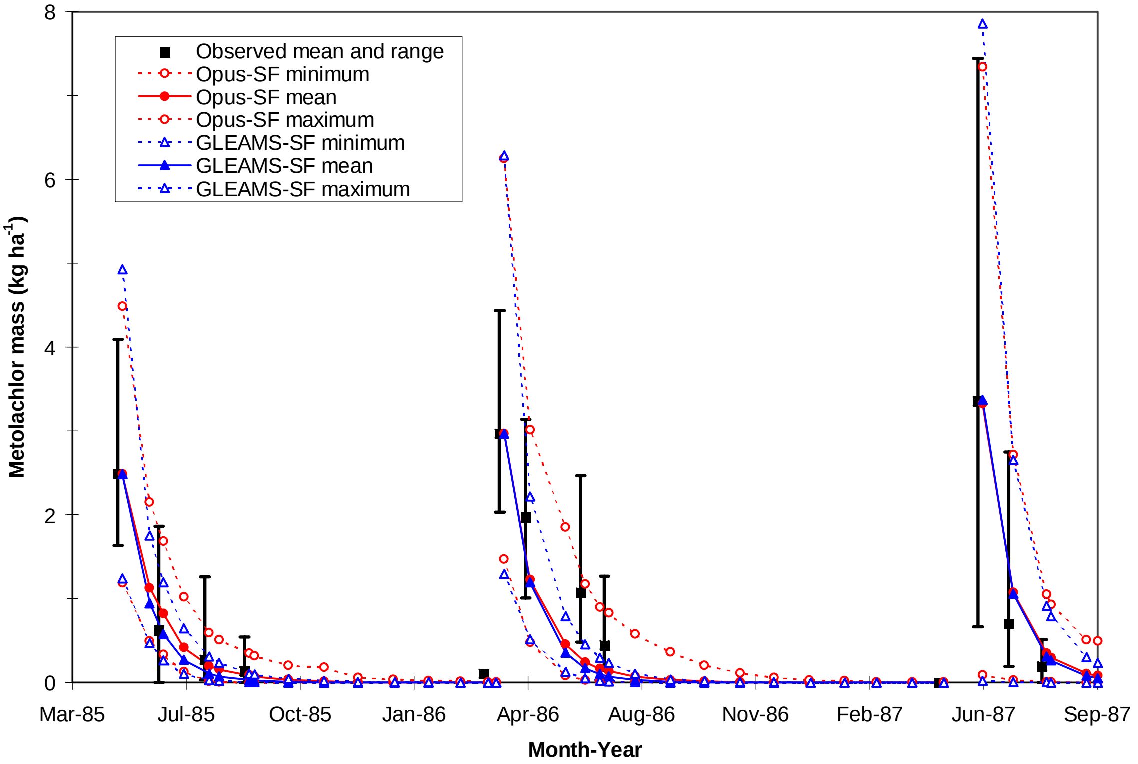

Figure 49. Observed and simulated mean and range of metolachlor mass in the root zone at the Dougherty Plain site.

Table 60. Statistical comparison of total metolachlor mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Dougherty Plain site.

	Opus-SF			GLEAMS-SF			p-value†	
Date	**Mean**	**Median**	**St.dev.**	**Mean**	**Median**	**St.dev.**	**KS Test**	**MW Test**
5/7/85	2.487	2.442	0.479	2.485	2.440	0.477	0.2-1.0	0.9368
6/12/85	0.824	0.804	0.211	0.582	0.566	0.142	0-0.01	0.0000
7/22/85	0.200	0.188	0.081	0.108	0.102	0.041	0-0.01	0.0000
8/26/85	0.088	0.079	0.048	0.028	0.025	0.014	0-0.01	0.0000
3/24/86	0.001	0.000	0.001	0.000	0.000	0.000	0-0.01	0.0000
4/7/86	2.964	2.902	0.625	2.966	2.900	0.627	0.2-1.0	0.9304
4/30/86	1.227	1.179	0.343	1.198	1.171	0.277	0-0.01	0.2829
6/17/86	0.244	0.200	0.149	0.175	0.166	0.065	0-0.01	0.0000
7/8/86	0.139	0.110	0.098	0.076	0.070	0.034	0-0.01	0.0000
4/28/87	0.000	0.000	0.000	0.000	0.000	0.000	—‡	—
6/1/87	3.327	3.321	1.218	3.373	3.360	1.241	0.2-1.0	0.3449
6/28/87	1.076	1.065	0.431	1.059	1.044	0.414	0.2-1.0	0.4426
7/27/87	0.354	0.331	0.175	0.314	0.298	0.143	0-0.01	0.0000

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

‡ The test could not be performed as all GLEAMS-SF values were zero

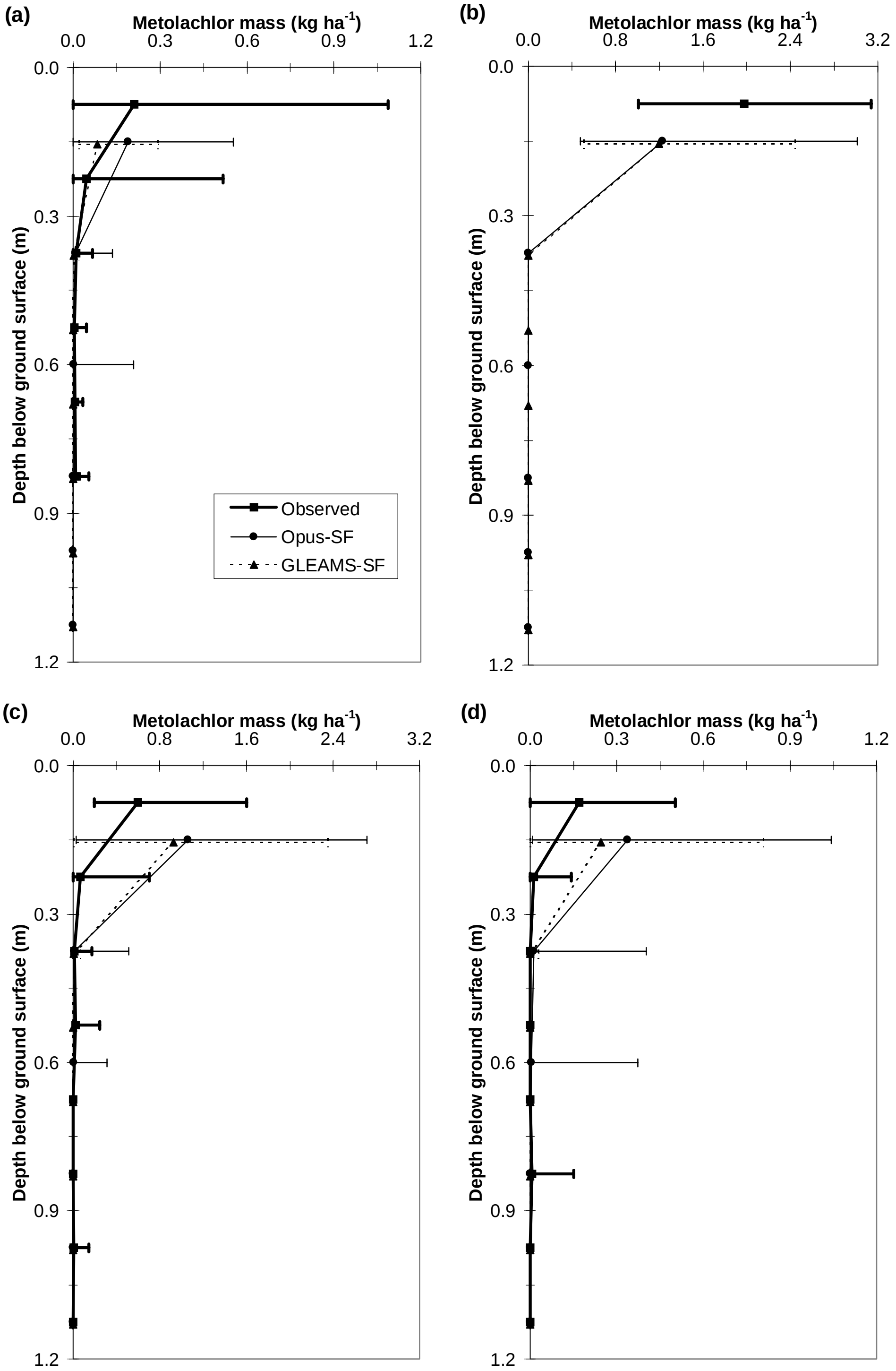

Figure 50. Observed and simulated mean and range of metolachlor mass in the root zone at the Dougherty Plain site on: a) July 22, 1985, b) April 30, 1986, c) June 28, 1987, and d) July 27, 1987. (Note difference in scales).

Table 61. Mean monthly evapotranspiration (ET) and percolation predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site.

Month-	Rainfall	Runoff	ET† (mm)		Percolation† (mm)	
Year	**(mm)**	**(mm)**	**Opus-SF**	**GLEAMS-SF**	**Opus-SF**	**GLEAMS-SF**
Apr-90‡	57.4	0.2	10.7	17.7	45.6	41.1
May-90	295.0	41.0	50.3	59.3	215.8	198.1
Jun-90	47.7	0.0	151.7	66.6	35.9	0.0
Jul-90	87.2	0.4	103.8	127.0	-3.1	0.0
Aug-90	206.4	13.3	97.7	104.3	-2.0	32.9
Sep-90	47.9	0.0	101.3	93.3	-0.2	0.0
Total	741.6	54.8	515.4	468.1	291.9	272.1

† ET and percolation from Opus-SF is based on a 1.2 m profile, whereas percolation from GLEAMS-SF is based on a 0.9 m profile.

‡ April 22-30 only

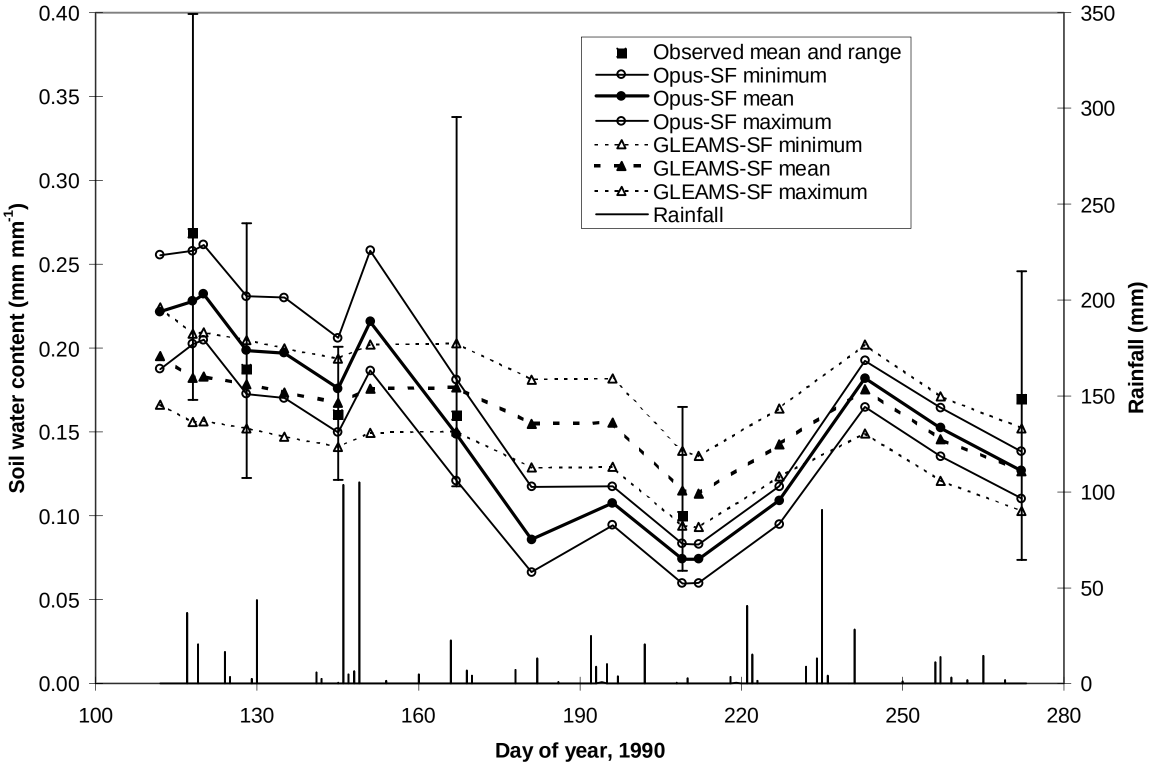

Figure 51. Mean and range of depth-averaged soil water content in the root zone (0.9 m) predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site, along with observed data.

Table 62. Statistical comparison of depth-averaged soil water content in the root zone predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site.

Day of	Opus-SF			GLEAMS-SF			p-value†	
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
112	0.222	0.222	0.010	0.195	0.195	0.008	0-0.01	0.000
118	0.228	0.228	0.008	0.182	0.182	0.008	0-0.01	0.000
128	0.199	0.198	0.008	0.179	0.179	0.008	0-0.01	0.000
145	0.176	0.176	0.008	0.167	0.168	0.008	0-0.01	0.000
167	0.149	0.148	0.009	0.177	0.177	0.008	0-0.01	0.000
209	0.074	0.074	0.003	0.115	0.115	0.007	0-0.01	0.000
272	0.127	0.127	0.004	0.127	0.127	0.007	0-0.01	0.214

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

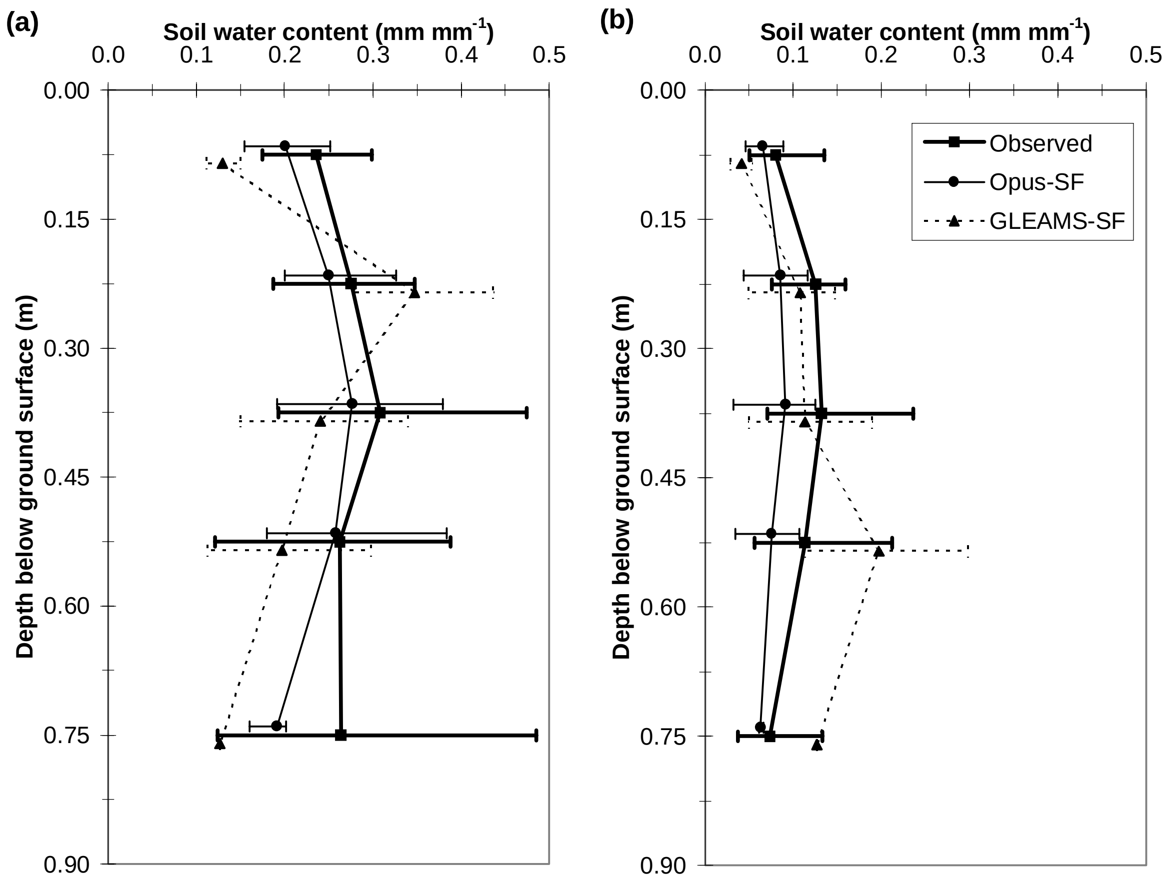

Figure 52. Mean and range of soil water content in the root zone predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site, along with observed data, on: a) day 118 and b) day 209.

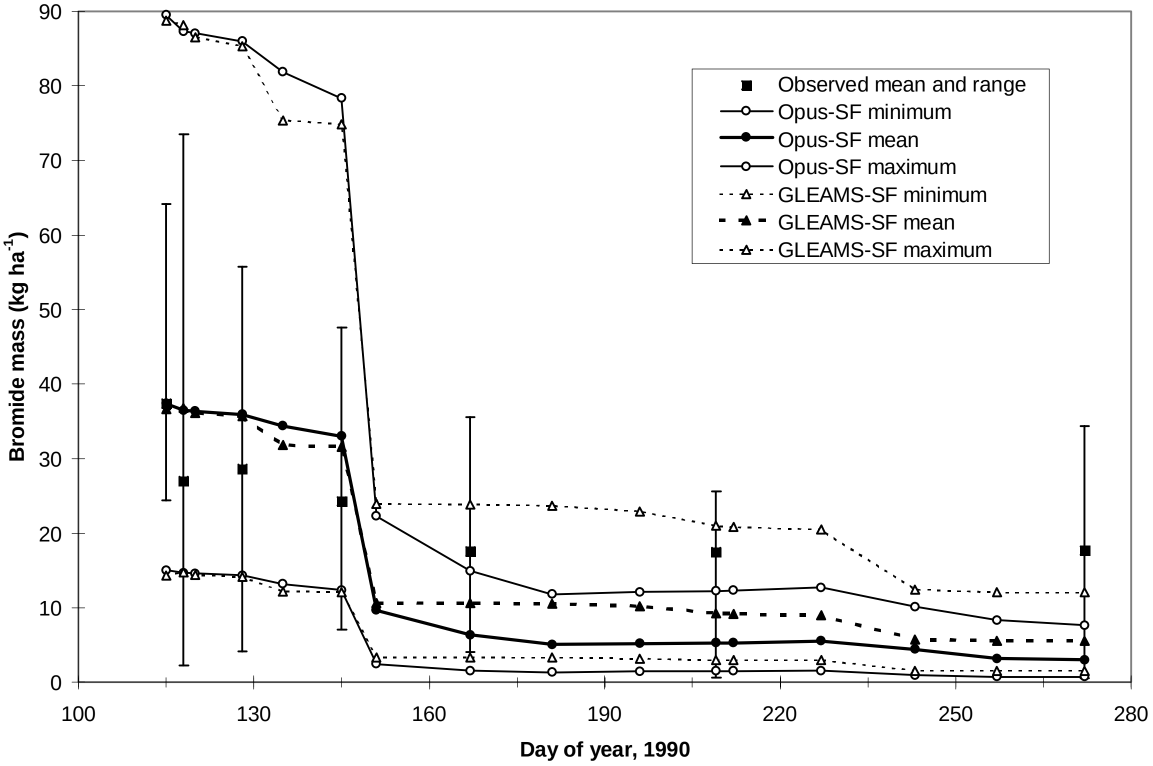

Figure 53. Mean and range of total bromide mass in the root zone (0.9 m) predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site, along with observed data.

Table 63. Statistical comparison of total bromide mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site.

Day of	Opus-SF			GLEAMS-SF			p-value†	
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
115	37.37	35.97	10.39	36.66	35.30	10.39	0.2-1.0	0.057
118	36.47	35.10	10.14	36.77	35.43	10.24	0.2-1.0	0.486
128	35.93	34.59	9.99	35.68	34.38	9.94	0.2-1.0	0.465
145	33.01	31.88	9.18	31.57	30.49	8.79	0-0.01	0.000
167	6.39	6.11	2.01	10.61	10.30	3.04	0-0.01	0.000
209	5.28	5.12	1.57	9.25	8.94	2.66	0-0.01	0.000
272	3.00	2.85	0.98	5.57	5.37	1.68	0-0.01	0.000

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

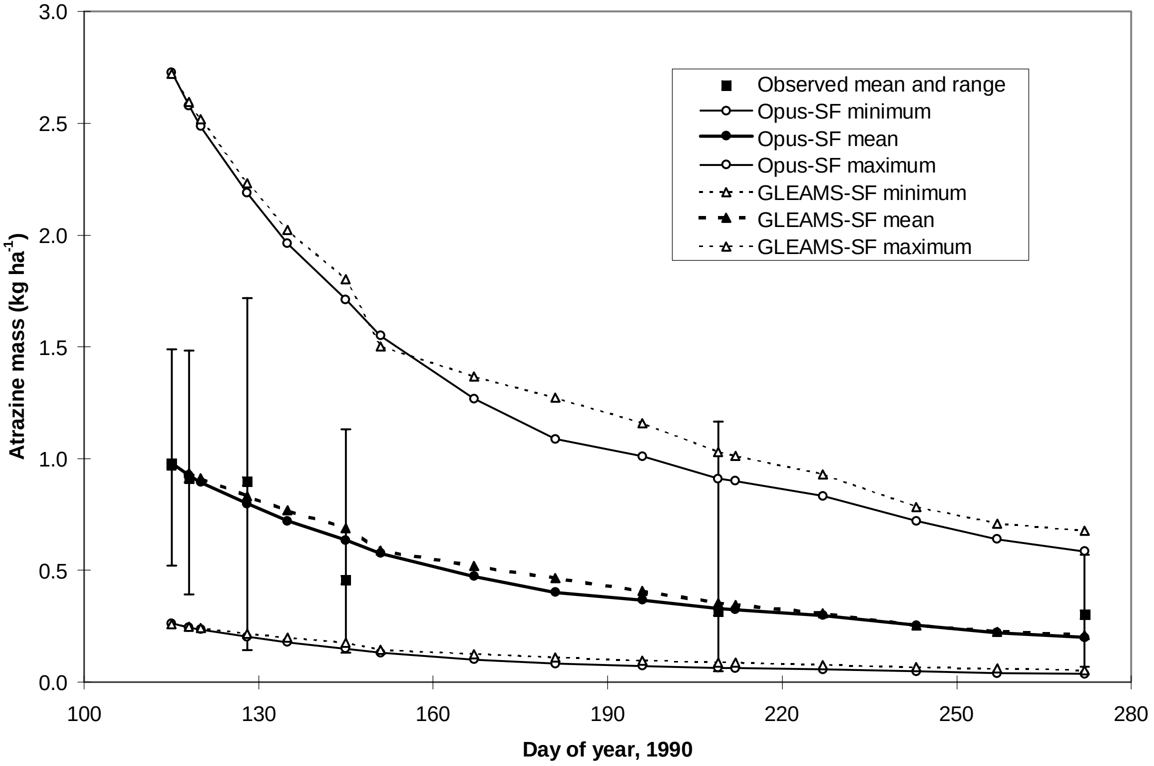

Figure 54. Mean and range of total atrazine mass in the root zone (0.9 m) predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site, along with observed data.

Table 64. Statistical comparison of total atrazine mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site.

Day of	Opus-SF			GLEAMS-SF			p-value†	
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
115	0.978	0.923	0.340	0.971	0.920	0.340	0.2-1.0	0.552
118	0.926	0.872	0.322	0.935	0.883	0.328	0.2-1.0	0.530
128	0.797	0.752	0.278	0.832	0.786	0.293	0.2-1.0	0.002
145	0.635	0.603	0.225	0.689	0.648	0.246	0-0.01	0.000
167	0.474	0.448	0.173	0.520	0.487	0.190	0-0.01	0.000
209	0.329	0.308	0.124	0.355	0.329	0.137	0-0.01	0.000
272	0.200	0.187	0.081	0.209	0.194	0.088	0.05-0.10	0.021

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

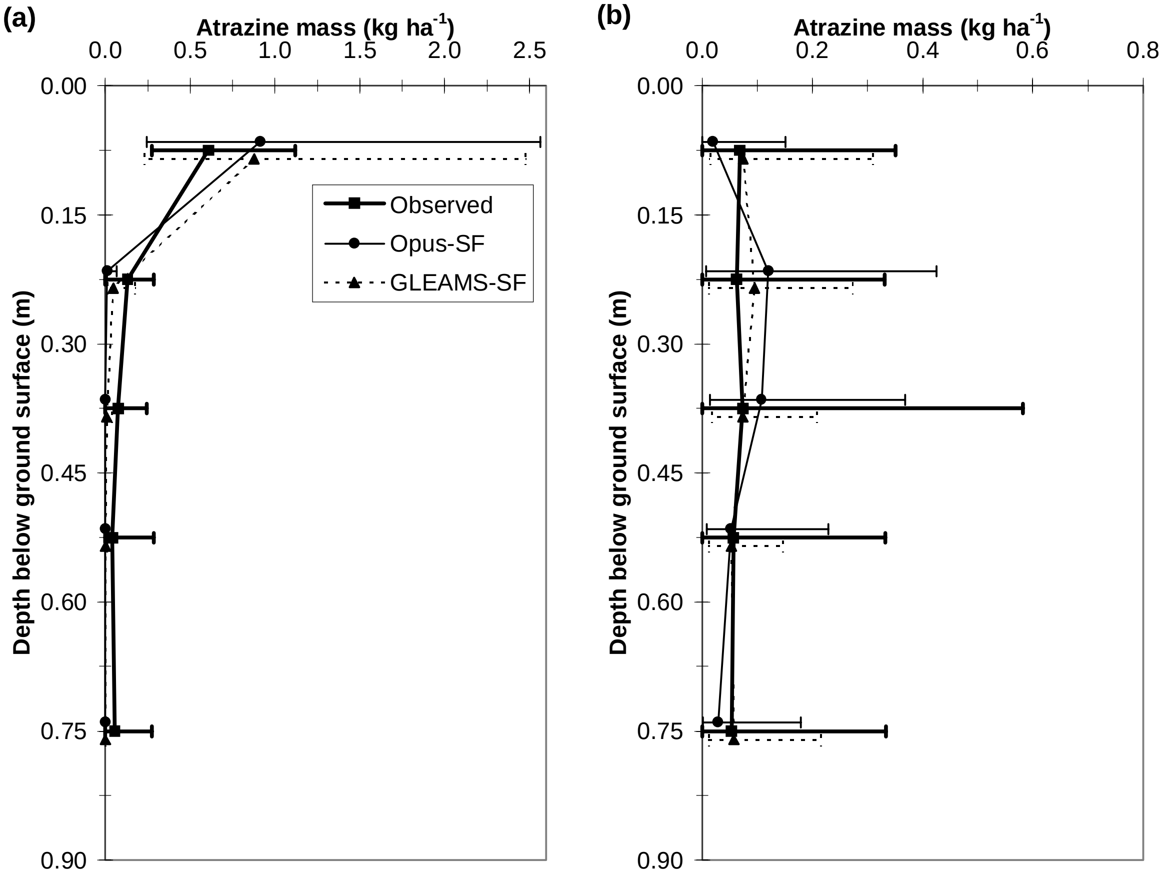

Figure 55. Mean and range of atrazine mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site, along with observed data, on: a) day 118 and b) day 209. (Note difference in scales).

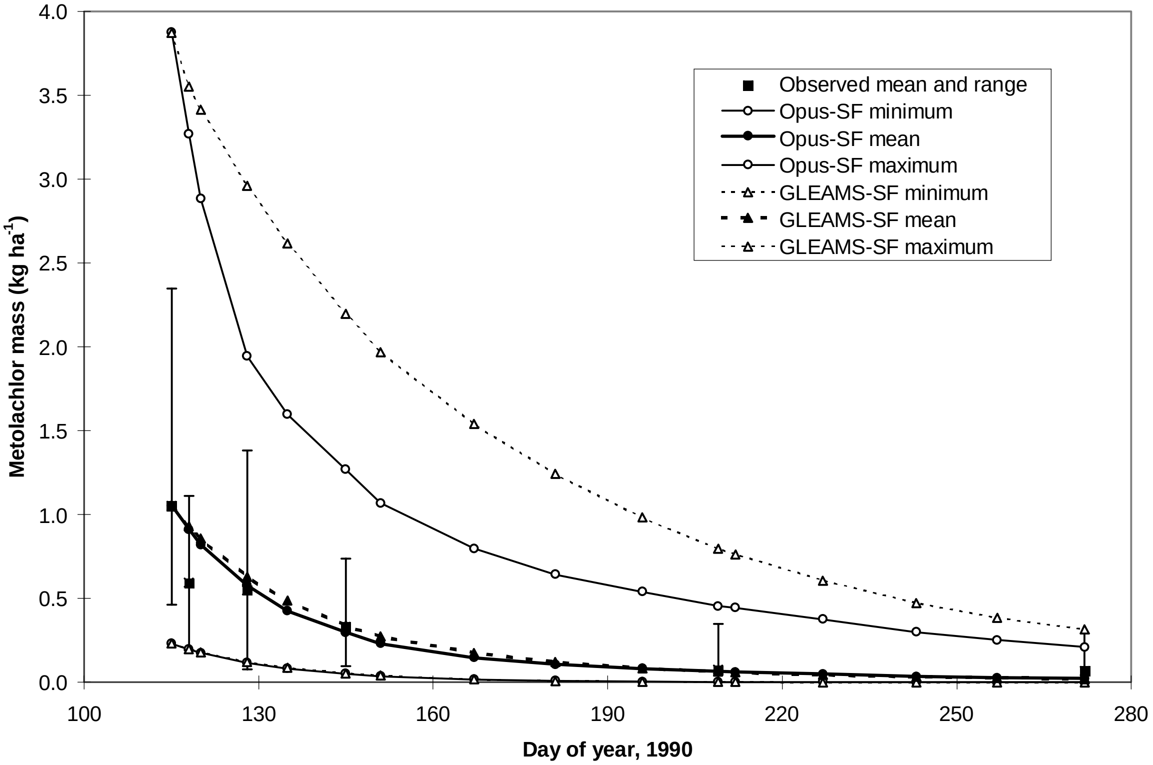

Figure 56. Mean and range of total metolachlor mass in the root zone (0.9 m) predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site, along with observed data.

Table 65. Statistical comparison of total metolachlor mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site.

Day of	Opus-SF			GLEAMS-SF			p-value†	
year, 1990	Mean	Median	St.dev.	Mean	Median	St.dev.	KS Test	MW Test
115	1.053	0.957	0.484	1.048	0.950	0.484	0.2-1.0	0.731
118	0.911	0.829	0.418	0.929	0.843	0.432	0.2-1.0	0.289
128	0.577	0.518	0.272	0.630	0.568	0.304	0-0.01	0.000
145	0.298	0.264	0.156	0.338	0.300	0.182	0-0.01	0.000
167	0.147	0.127	0.089	0.175	0.153	0.109	0-0.01	0.000
209	0.065	0.053	0.048	0.064	0.053	0.049	0.2-1.0	0.580
272	0.022	0.015	0.022	0.021	0.016	0.020	0.2-1.0	0.606

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

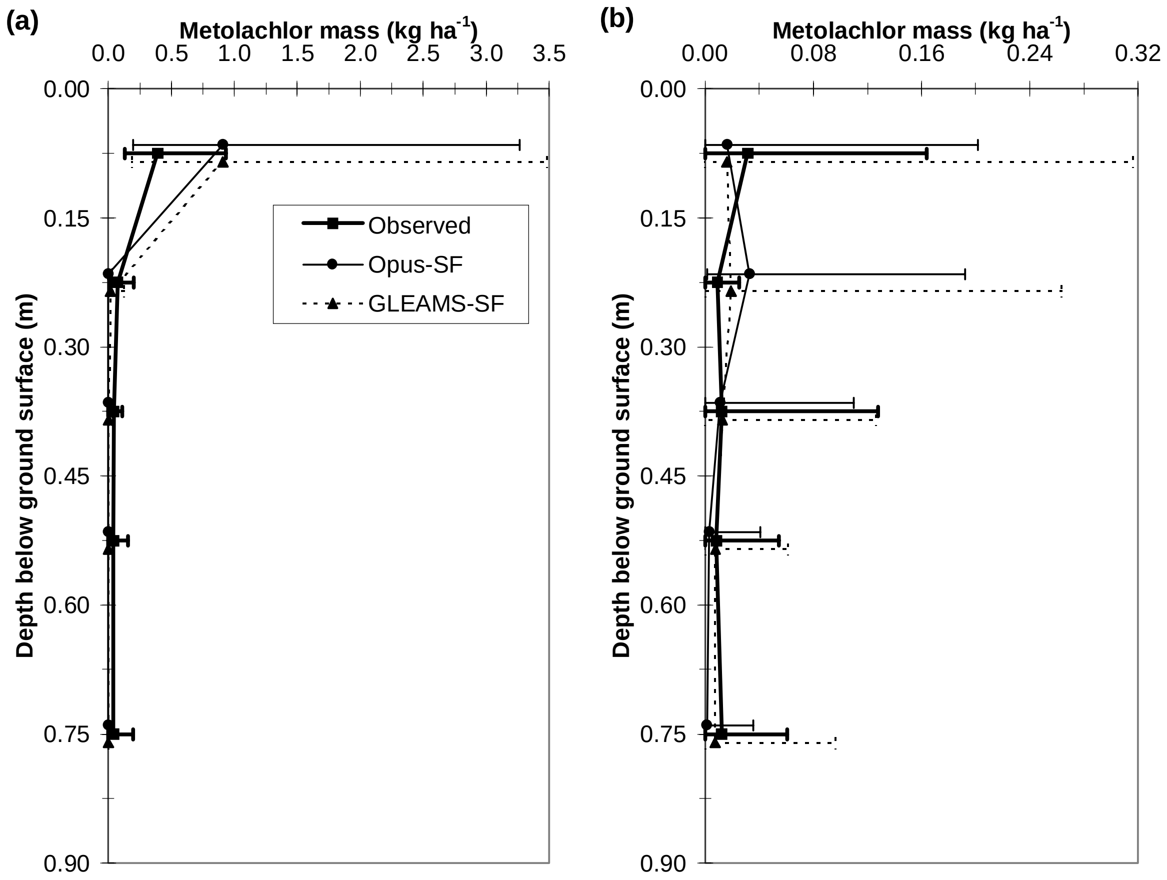

Figure 57. Mean and range of metolachlor mass in the root zone predicted by Opus-SF and GLEAMS-SF at the Nomini Creek site, along with observed data, on: a) day 118 and b) day 209. (Note difference in scales).