Chapter VII

Summary, Conclusions, and Recommendations

SUMMARY AND CONCLUSIONS

Spatial heterogeneity in the soil system has a profound influence on the flow of water and chemicals in the unsaturated zone. Incorporating this variability in solute leaching models could lead to more realistic predictions of contaminant levels in the unsaturated zone and will provide improved predictions in assessing risks associated with contaminants in the unsaturated zone. It will also enhance the credibility of pesticide and other solute leaching models as tools for making regulatory and management decisions.

In this study, a stochastic framework was developed to represent spatial variability in one-dimensional solute leaching models. In the stochastic approach, the heterogeneous field is conceptualized as a collection of one-dimensional, independent, non-interacting soil columns (stream tubes) differing in soil properties. The horizontal variations of soil hydraulic and retention properties in each horizon are treated as random functions of zero transverse spatial correlation length, after accounting for any spatial trends. Unlike previous stochastic simulation studies with solute leaching models, parameters exhibiting spatial trends are described by a deterministic (trend) component and a zero mean, random component. The solution to the field scale problem is then considered to be equal to the ensemble average of the solutions at the stream tube scale.

The implementation of the stochastic framework consisted of four steps: statistical/ geostatistical analysis of data, generation of input parameter sets, repeated executions of the model, and analysis of output. Statistical/geostatistical analysis included determination of probability density functions and cross-correlation between spatially variable parameters from field-measured data, and analysis of their spatial structure. The independent/correlated spatially variable input parameters were then generated using the Latin hypercube sampling method. Parameters exhibiting spatial trends were detrended before input parameter generation, and the trends were reinstated afterward using a spatial grid that covered the entire field. Repeated executions of the model were performed using Monte-Carlo simulation techniques. Analysis of output consisted of summarizing the output variables using graphical displays, statistical descriptors and goodness-of-fit measures.

Two existing root zone leaching models, Opus and GLEAMS, were incorporated in the stochastic framework. The stochastic version of Opus (Opus-SF) was conducting by using an external model-specific routine and modifications in the model. The stochastic version of GLEAMS (GLEAMS-SF) was implemented using a general-purpose batch routine that used 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.

Intrinsic and extrinsic variability in soil and chemical properties from a 3.9-ha agricultural field in the Dougherty Plain region of Georgia and a 0.05-ha agricultural field plot in Nomini Creek watershed in the Virginia Coastal Plain were incorporated in Opus-SF and GLEAMS-SF to simulate spatial variations in water flow and solute transport. Soil hydraulic and retention properties, soil organic carbon content, pesticide degradation rates in different soil layers, and chemical application rates were treated as spatially variable parameters in Opus-SF and GLEAMS-SF. The accuracy of Opus-SF and GLEAMS-SF were evaluated using soil water, bromide and pesticide mass data observed at the two sites.

Model validation results must be viewed considering the assumptions invoked in the modeling approach and limitations in the observed data. The one-dimensional assumption used in the stochastic approach may be violated in areas of the heterogeneous field where there is lateral flow. The assumption of not simulating runoff at the Nomini Creek site may increase infiltration and induce some errors in the water and chemical balance. The simulations of using Opus, a rate-based model, was based on daily rainfall, and did not include rainfall rate information. In addition to field measurement errors, comparisons with observed data must consider the fact that there were only limited number of sampling points available in each year and that observed data on each of these dates were based on a sample size of 20. While a sample size of 20 may be considered adequate to provide a good description of average conditions and variability in a 0.05-ha field plot (Virginia), it may not be large enough to describe variability in a 3.9-ha field (Georgia). Field measurements of soil and pesticide properties (input parameters) at the Nomini Creek site were also limited. However, these are some of the most extensive data currently available for pesticide fate and transport at the field-scale.

Considering the above-mentioned drawbacks, the main findings from the comparison of the models with observed data can be summarized as follows:

1) While the statistical tests indicate that the models could not predict equality of median of depth-averaged soil water content and total pesticide mass observed in the field on most sampling dates, the observed mean and median were predicted within a factor of two. Therefore, for most practical applications, Opus-SF and GLEAMS-SF are capable of predicting the average of soil water content and pesticide mass in the root zone.

2) The distribution of depth-averaged soil water content and total pesticide mass in the root zone predicted by the models on the field sampling dates were not equivalent to the observed data, according to the statistical tests. However, the simulated standard deviations were within a factor of two of the observed standard deviations and a majority of the observations were contained in the simulated range on most sampling dates for four out of six output variables (exceptions being metolachlor mass at the Dougherty Plain site and soil water content at the Nomini Creek site). Therefore, Opus-SF and GLEAMS-SF can provide reasonable estimates of spatial variability of soil water content and pesticide mass for most practical applications.

3) Soil hydraulic and retention properties derived from texture data substantially reduced the variability of soil water content from Opus-SF and GLEAMS-SF, but had less impact on bromide and pesticide mass predictions from both models.

4) Bromide transport in the root zone was modeled similarly by both models but did not compare well with the field data. Apparent inconsistencies in the data, including the retention of significant bromide in the profile after three years make it questionable to assign all the error to the models. Clearly, the field data did not follow the assumptions of a non-reactive, conservative tracer which the models represent.

5) Pesticide transport in the root zone was predicted much better than bromide mass by both models for both field studies. The sink terms, degradation and uptake, accounted for over 94% of the aldicarb and atrazine losses, and over 99% of the metolachlor losses. Thus, the quality of pesticide fate and transport predictions was largely dependent on obtaining good estimates of degradation and adsorption parameters.

Results from the deterministic version of the models were similar, but not equal to the mean values from the stochastic version of the models. The differences between the two versions were more distinct in the case of soil water content and bromide mass than in the case of pesticide mass, for both models and at both sites. These differences show that either characterization of the spatially variable parameters and non-linearities in the models had a greater impact on the soil water and bromide predictions than on the pesticide results, or that their effect was averaged out more in the case of pesticide mass predictions. Differences between deterministic Opus and Opus-SF (mean) were greater than differences between deterministic GLEAMS and GLEAMS-SF (mean), but still did not exceed 10%.

Results from the proposed stochastic framework (Opus-SF and GLEAMS-SF) were compared with results from the traditional Monte-Carlo approach (Opus-MC and GLEAMS-MC), where spatial trends are not considered and all variation is described as random. Overall, the differences in soil water and solute transport predictions by the two approaches were not substantial. The soil water content predictions by Opus-SF and Opus-MC were, however, significantly different for the first 150 days at the Dougherty Plain site and most of the 152 day simulation period at the Nomini Creek site. The soil water content predictions by GLEAMS-SF and GLEAMS-MC were significantly different throughout the simulation period at the Nomini Creek site. However, neither of the modeling approaches gave predictions consistently closer to the observed data. Therefore, including spatial trends of a few soil properties in some of the horizons in the spatial variability representation, did not result in a more accurate prediction of soil water content than considering only random variation of the soil properties. There was also very little difference in solute transport predictions predicted by the two approaches. A more complete evaluation of the stochastic framework approach suggested in this study (considering spatial trends) is possible only in cases where a majority of the soil properties possess spatial trends.

A direct comparison between the rate-based approach used in Opus-SF and capacity-based approach used in GLEAMS-SF could not be performed as originally planned, because other differences in the model often masked the effect of the water flow models. The results from the two models show that the average conditions and distributions of soil water content predicted by Opus-SF and GLEAMS-SF were significantly different on most sampling dates at both sites. The average conditions and distributions 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. Other major findings from the comparison between Opus-SF and GLEAMS-SF are as follows.

1) 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.

2) 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.

3) 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.

4) 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. There were no consistent differences between the model predictions of atrazine and metolachlor mass at the Nomini Creek site.

5) Spatial variability of soil water content predicted by the two models 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, root zone leaching models, Opus and GLEAMS, were incorporated in a stochastic framework that describes the spatial variability of soil properties as the sum of a deterministic trend component and a random component. Opus-SF and GLEAMS-SF were able to predict the average and spatial variations of soil water content and pesticide mass at the Dougherty Plain and Nomini Creek sites with accuracy sufficient for most management-type applications. 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. 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.

LIMITATIONS OF OPUS AND GLEAMS

The major limitations or weaknesses of the deterministic versions of Opus and GLEAMS identified in this study include: (i) Opus does not have an option to specify initial water content in all horizons, which may be limiting for site specific applications; (ii) the initial water content parameter (BST) in GLEAMS cannot take values greater than the field capacity and less than the wilting point (this may affect the results in the first one or two months of simulation); (iii) Opus does not have an option to specify degradation rate for the subsurface horizons, which may be limiting for site specific applications; (iv) preferential movement of solutes cannot be simulated in either model; (v) upward movement of solutes from the lower boundary in Opus can lead to unrealistic prediction of solute mass in the lower soil horizon(s); (vi) amount of pesticide or solute losses by plant uptake is not provided in the regular or detailed output of either model.

IMPLICATIONS OF THE RESEARCH

The major outcome from this dissertation is a research and management tool that can be used to provide reasonable estimates of soil water and pesticide distribution variance, to compute worst-case leaching scenarios, and to assess risks associated with agrochemicals in the groundwater. The research has provided stochastic versions of two management/research type root zone leaching models and a stochastic framework that can be implemented with other one dimensional solute transport models. As with any solute transport model, the use of these tools without a good understanding of its strengths and weaknesses is not encouraged.

The accuracy of the model in predicting average conditions as well as spatial variability of output variables is dependent on the amount and quality of data available to characterize the input parameters of the model. The similarity between the mean values from the stochastic versions and the deterministic simulation results suggest that the stochastic versions are versatile and can be used to predict the average conditions.

Expressing spatial structure of a soil property in terms of deterministic trends and random variation is theoretically more sound than considering only random variations, and less sound than the common geostatistical approach of describing spatial variations in terms of both large scale and small scale variations. The deterministic trend approach used in this study, however, does not require a direct estimate of spatial correlation length and hence, requires a smaller sample size. The sample size required to describe the PDFs of the model parameters is often adequate to detect spatial trends as long as the sample locations cover a majority of the areal extent of the domain. Incorporation of trend, however, may not improve the prediction of mean and variance estimates from these models if the trend phenomena is not distinct over all or most of the soil horizons.

A major implication of the study is that the more functional and capacity-based models like GLEAMS will be as good a tool as the more mechanistic and rate-based models like Opus for management type applications (e.g., estimating water and pesticide amounts in the soil) in sandy soils in the Coastal Plain region of the eastern United States. Capacity-based models require fewer soil water parameters that tend to be less variable, and therefore, require fewer samples to describe spatial variability in soil water parameters. The use of capacity-based models over rate-based models will lead to a significant savings in computer resources also, especially in long-term and multiple simulations.

RECOMMENDATIONS FOR FUTURE RESEARCH

The following are the recommendations for future research:

- More extensive comparison of the stochastic framework must be conducted under different soil types and under different climatic regimes. Comparison must be made with field studies that have sufficient data to capture and describe the spatial variability of key soil properties and field processes, and sufficient amount of contaminant concentration measurements. A common limitation of field studies involving NPS pollutants is the imbalance between the number of property measurements and the number of contaminant concentration measurements available for output analysis. The minimum sample size can be computed from both the coefficient of variation of the property and the correlation length of the property, relative to the length scale of the field and the error in estimating the ensemble average of a spatially variable property (Dagan et al., 1990).

- More simulation studies are needed to establish whether or not there are significant differences between results from the stochastic framework proposed in this study and the traditional Monte Carlo approach which considers only random variation and does not consider spatial trends. These studies can be conducted initially using hypothetical data with varying degrees of trend and then using field data where distinct trends can be identified in most or all of the soil horizons.

- The stochastic framework can be extended to the watershed scale or applied to fields, which have the potential for considerable amounts of runoff, by accounting for spatial variability of runoff (and rainfall). Runoff occurring in the stream tubes at higher elevations would have to be routed to adjacent stream tubes at lower elevations, so that the water balance in each tube is maintained.

- Better guidelines and techniques for evaluating the performance of stochastic solute leaching models are needed. Guidelines for evaluating stochastic models must consider the inexact nature of modeling and field measurement errors, and should preferably be suggested by a panel of experts who have experience with modeling and field studies. A combination of statistical tests, quantitative and visual techniques must then be devised to test the accuracy of the model, based on the guidelines. The stochastic approach to model validation suggested by Luis and McLaughlin (1992) is a step in the right direction.

- Further studies must be conducted to determine the amount of bromide and pesticide uptake by plants. This will help to verify and probably improve the approach currently used in solute leaching models, and provide better estimates of the controlling model parameter, the plant uptake coefficient.