Chapter I
Introduction

Background and Justification

Agricultural activities form one of the wide-spread sources of diffuse or non-point source (NPS) pollution of surface water bodies and groundwater. According to the 1990 National Water Quality Inventory Report to Congress (EPA, 1992), agricultural pollutants affected 60% of the impaired river miles in the United States. In the groundwater quality section of the report, 19 states in the U.S. identified agricultural activities as a source of contamination out of which eight states ranked them as the most important source of contamination. Pesticides and nitrates were identified as groundwater contaminants by 32 and 37 U.S. states, respectively, while 17 states reported the occurrence of other agrochemicals in the groundwater. Although some of these occurrences may be due to point sources, transport of field-applied agrochemicals appears to be an important factor leading to groundwater contamination.

Assessment of groundwater contamination by pesticides, nitrates, and other agrochemicals primarily involves characterizing the transport of these compounds through the vadose zone (the root zone and the underlying unsaturated zone). The most direct way of characterizing the transport of these pollutants is through field monitoring studies. Monitoring studies, however, are extremely time consuming and often very expensive. Although computer simulation models cannot replace monitoring studies, they provide an efficient and cost-effective alternative that can be easily adapted to many field situations with varying soil types and different land uses. The U.S. Environmental Protection Agency's report on NPS pollution (EPA, 1989a) suggests the use of hydrologic models to predict possible contamination from agrochemical use on agricultural sites. As a result, some of these models are being used by industry and government agencies for regulatory purposes and by planners for making management decisions.

CMLS [Chemical Movement through Layered Soils] (Nofziger and Hornsby, 1987), GLEAMS [Groundwater Loading Effects of Agricultural Management Systems] (Leonard et al., 1987), LEACHM [Leaching Estimation and Chemistry Model] (Wagenet and Hutson, 1986), Opus (Smith, 1992), PRZM [Pesticide Root Zone Model] (Carsel et al., 1985), and RZWQM [Root Zone Water Quality Model] (USDA, 1992) are examples of computer simulation models that have been used to predict the movement of pesticides and other NPS pollutants through the unsaturated zone at the field scale. All of these models are deterministic and use input parameters that are assumed to be representative of the natural heterogeneous system. Hence, they do not consider the uncertainties and variabilities in the natural system. The fate and transport of agrochemicals in soils are, however, greatly influenced by intrinsic variations in soil properties as well as extrinsic variations caused by activities such as chemical application and tillage (Rao and Wagenet, 1985). Incorporating these variations in solute transport models will provide a more realistic representation of the pollutant distribution in the field.

Rao and Wagenet (1985) suggested that characterizing spatial variability in pesticide transport will also lead to a more direct evaluation of pesticide simulation models, as well as improve field sampling design and interpretation of results from field studies. Model validation studies involving deterministic NPS models have also indicated that representing spatial variability can lead to a more direct comparison of observed and simulated data, and may improve predictions (Pennell et al., 1990; Parrish et al., 1992; Zacharias and Heatwole, 1993, 1994). Sound procedures to represent spatial variability in NPS models are also required, as planners look for tools to evaluate new spatially-oriented management strategies such as precision farming.

Soil scientists have used a stochastic approach to model field-scale solute transport in heterogeneous soils for about two decades (e.g., Dagan and Bresler, 1979, 1983; Bresler and Dagan, 1979, 1981, 1983; Jury, 1982; Simmons, 1982; Russo, 1984a; Sposito et al., 1986; Jury and Roth, 1990; Russo, 1991; Russo and Dagan, 1991; Destouni, 1993; Jury and Scotter, 1994). These studies have provided a framework for representing spatial variability in the unsaturated zone and established important concepts in applying stochastic principles. However, most of these studies have not dealt with transient models and have used non-reactive solutes.

With respect to reactive solutes, a number of researchers have investigated the effect of parameter uncertainty on model predictions (Carsel et al., 1988; Zhang et al., 1993; Kumar and Heatwole, 1996) by lumping the effect of spatial variability with information uncertainty. Studies examining the direct effect of spatial variability on pesticide leaching using screening models have illustrated that spatial variability can have a significant impact on the leached fractions of pesticides (Small and Mular, 1987; Jury and Gruber, 1989; van der Zee and Boesten, 1991, 1993). However, these studies did not provide any analysis in terms of actual field-observed spatial variability.

Wu et al. (1997) applied stochastic simulation techniques to the GLEAMS model and provided analysis in terms of actual field-scale spatial variability. They represented spatial variability of intrinsic soil parameters and runoff curve number in predicting spatial variations in subsurface water flow and nitrate leaching from three 10-ha agricultural fields in southern Ohio. In the stochastic approach they used, a hydrologic environment (field) was decomposed into sub-environments based on the knowledge of the domain's deterministic spatial variability (soil series) and each sub-environment was divided into three layers to form a modeling unit. The modeling units were assumed to be spatially independent of each other, and selected soil properties in each modeling unit were described with a multivariate normal random vector. Monte-Carlo runs of GLEAMS were then carried out to provide prediction bands for soil water content and nitrate concentration at various depths in the three fields. One of the limitations of the study identified by Wu et al. (1997) was the inability of the GLEAMS model to accurately account for subsurface water flow and nitrate transport and transformation processes.

The number of processes and the degree of complexity with which flow and transport are represented in solute transport models vary. One major distinction is in the way these models handle water flow and solute leaching. Rate-based models are mechanistic models that define rates of change of water content and solute concentration by rate parameters, such as the hydraulic gradient and hydraulic conductivity, whereas capacity-based models are functional models that define changes rather than rates of change, using capacity factors such as volumetric water content at field capacity (Addiscott and Wagenet, 1995). Even though these definitions seem to represent distinct categories of models, in actuality, it is better to regard them as being at different ends of a modeling spectrum, with a number of hybrids in between (Wagenet and Hutson, 1996).

Rate-based and capacity-based (or, mechanistic and functional) models have been compared in a deterministic context (Nicholls et al., 1982; Smith and Ferreira, 1989; Pennell et al., 1990; de Willigen, 1991; Hutson and Wagenet, 1993). However, no study has compared such models in a stochastic context. With growing integration of simulation modeling and geographic information systems (GISs) to provide spatial estimates of NPS pollutants in the vadose zone over a large area, there is considerable discussion on the choice of model to use for a given application (Hutson and Wagenet, 1993; Wagenet and Hutson, 1996). A comparison between existing NPS models in a stochastic framework using actual field data would provide valuable insight.

There are a number of reasons for lack of sufficient studies involving stochastic models that have looked at the effect of actual field-observed spatial variability on transport of agricultural chemicals in heterogeneous field soils. One of the major constraints to advancing our knowledge in this area has been the limited number of detailed datasets available. Among the unresolved issues with respect to representing spatial variability in NPS models are clear guidelines on which method and what level of detail are needed for describing spatial variability of soil properties and field processes. Procedures that take into account spatial trends along with probability density functions (PDFs) to describe spatial variability have not been applied to transient solute leaching models. Previous research efforts to model the effect of spatial variability have mainly concentrated on intrinsic variations and have very seldom considered extrinsic variations such as variations in chemical application. Stochastic soil water and chemical output from a mechanistic model that uses highly variable rate parameters has not yet been compared with stochastic output from models that use less variable capacity parameters.

OBJECTIVES

The overall goal of this research was to assess the significance of actual field-observed spatial variability of soil properties and field processes on prediction of subsurface water flow and chemical transport from one-dimensional solute transport models. The specific objectives of this research were to:

1. Develop a stochastic framework to represent spatial variability of subsurface soil properties and chemical application for deterministic, one-dimensional solute transport models.
2. Evaluate stochastic versions of the solute transport models, Opus (Opus-SF) and GLEAMS (GLEAMS-SF):

a) Test the accuracy of their central tendency and spatial variability predictions with field-measured soil water content, bromide, and pesticide mass data;

b) Compare the central tendency predictions from the stochastic models with predictions from the deterministic models; and

c) Compare the central tendency and spatial variability predictions from the models using the proposed stochastic framework with corresponding predictions from the models using traditional Monte-Carlo simulation.

3. Determine if the more mechanistic rate-based Opus-SF would yield more accurate predictions of central tendency and spatial variability of soil water content and solute mass than the capacity based GLEAMS-SF.

OVERALL APPROACH

A stochastic framework was developed to incorporate spatial variability information in one-dimensional root zone leaching models. The stochastic approach used conceptualizes the heterogeneous field as a collection of vertical, non-interacting stream tubes. Spatial variability of soil properties in each horizon is described by probability density functions fitted to measured field data, after removing spatial trends. Thus, spatial variability is described by a deterministic (trend) and stochastic (random) component in the horizontal direction and deterministic (soil layering) in the vertical direction. The solution to the field scale problem is considered to be equal to the ensemble average of the solutions at the local scale.

Selection of models for the study was influenced by the requirement of obtaining a rate-based and a capacity-based root zone leaching model that used similar methods to model ET and surface hydrology. The daily version of the Opus model (Smith, 1992; Ferreira and Smith, 1992) and the GLEAMS model (Leonard et al., 1987; Knisel, 1993) met this qualification. Both are USDA models with similar objectives and comparable model structures. Both Opus and GLEAMS were developed to study the effect of management practices on the pollution aspects of agricultural hydrology (Smith and Ferreira, 1989). The daily version of Opus and GLEAMS simulate potential ET, runoff, and erosion processes using similar methods. The major difference between the models is in the way they describe water flow and, as a result, solute transport in the unsaturated zone. Opus simulates the unsaturated flow of water by a finite difference solution of the rate-based Richards' (1931) equation, whereas GLEAMS uses a capacity-based storage routing technique to simulate water movement through the soil profile. Thus, by implementing Opus and GLEAMS models in a stochastic framework, this study provides the basis for evaluating the impact of spatial variability on the subsurface water components of a rate model versus a capacity model.

Spatial variability of important soil physical, biological, and pesticide properties and chemical application from two sites, a 3.9-ha agricultural field in Georgia (Hook, 1987; Smith and Parrish, 1993) and a 0.05-ha agricultural field plot in Virginia (Heatwole et al., 1992; 1997; Zacharias et al., 1997), were used to assess its significance on model predictions. Model performance was evaluated using soil water content, bromide and pesticide mass data from the two field sites. At each site, twenty locations were sampled on several dates after chemical application. The two sites represented agricultural fields of different sizes in different climatic regions, with soil and chemical properties (input parameters for the model) collected at different levels of detail and soil water content and bromide and pesticide concentrations (for comparison with output from the model) collected over different time intervals. Both studies provide information on intrinsic factors as well as extrinsic factors (chemical application) affecting spatial variability of pesticides in soil. Soil hydraulic and retention properties at the Dougherty Plain site was measured at twenty locations, whereas these properties were derived from texture data measured at 35 locations at the Nomini Creek site.

The performance of Opus-SF and GLEAMS-SF was assessed using graphical displays, statistical estimators, and statistical tests. In addition to comparison with observed data, central tendency predictions from Opus-SF and GLEAMS-SF were compared with deterministic predictions from the models. Predictions from Opus-SF and GLEAMS-SF were also compared with predictions from a traditional Monte Carlo simulation of the models, in which spatial variability is described only as random variation and the deterministic trends are not considered. Finally, soil water and chemical mass predictions from the two models were compared to each other, in the light of observed data. The objective there was to examine if the more mechanistic representation of subsurface flow and transport used in Opus-SF led to a more accurate description of spatial variability as compared to the more functional representation used in GLEAMS-SF.