1. INTRODUCTION

In recent years consideration of the unsaturated zone has received increasing attention among scientists, regulators, and engineers involved with subsurface contaminant transport. Regarding groundwater pollution, the unsaturated zone acts as buffer but also as conveyor belt between the land surface, where most contaminants originate, and groundwater, which is a resource protected under a number of environmental regulations. Pesticides and fertilizers leach to the water table from agricultural areas; underground storage tanks leak petroleum products; landfills, septic tanks, waste water lagoons, and other man-made features are potential hazards to drinking water if the underlying aquifer is used as a potable water resource. For the cleanup of soil contamination and for the evaluation and control of waste storage and disposal sites, flow and transport processes in the area between the actual or potential contaminant source and the groundwater table must be well understood. Unsaturated flow processes above the water table play an important role in determining the pathways of a contamination plume before it reaches the aquifer, particularly in semiarid and arid regions where the unsaturated zone may be several tens of meters thick.

Modeling unsaturated flow and transport with mathematical or numerical methods is an important tool for predicting the infiltration and redistribution of soil water and the transport of solutes in the unsaturated zone. Flow and transport models are commonly used to support the decision making process in agricultural management, environmental impact assessment, toxic waste control, remediation design, and subsurface cleanup monitoring.

The modeling process, however, requires knowledge of the fundamental properties of porous media. Field research has shown that these porous media properties change continuously from location to location ("spatial heterogeneity"). Spatial heterogeneity may significantly influence flow and transport processes in the vadose zone. Modeling efforts must inherently cope with "uncertain" information i.e., information that has been extrapolated from measurement locations to the surrounding areas because it is impossible to measure all soil properties at all locations. Since the model input is uncertain, the model results are uncertain and the validity of the modeling may be questioned.

In the past two decades, research efforts have been directed towards developing general quantitative concepts to describe the spatial heterogeneity of subsurface porous media. With mathematical tools the impact of model input uncertainty (due to heterogeneity) on the uncertainty of flow and transport predictions is quantified. Many of these research efforts have applied the so-called "geostatistical" description of porous media properties and used it for the "stochastic analysis" of model uncertainty. Geostatistics is a tool to quantify spatial variability of natural phenomena in terms of statistical parameters. Given the spatial variability of some environmental properties (model input) stochastic analysis, a particular form of mathematical analysis, finds the statistical parameters describing the spatial variability of and the prediction uncertainty about other environmental phenomena (model output). Most applications of the stochastic analysis of subsurface flow and transport processes have been with respect to groundwater.

Moisture movement in unsaturated or variably saturated soils is a physically more complex process than water flow in saturated porous media. The stochastic analysis of such processes in heterogeneous soils has therefore been limited to a relatively few, simplified analytical models. These models ar known to be valid only if the spatial heterogeneity of the soil is moderate. None of the analytical stochastic models describing variably saturated flow and transport in heterogeneous porous media have been rigorously verified.

This work is an attempt to partially remedy the lack of stochastic tools that predict not only the most likely path and rate of water and solute movement in soils but also the spatial variability (i.e. uncertainty) of water movement and solute transport in the unsaturated zone. Combined analytical-numerical stochastic methods are developed, with which the characteristics and the prediction uncertainty of steady-state flow and transient transport in highly heterogeneous soils can be assessed. The stochastic methods developed in this work are also able to predict the uncertainty about water movement and contaminant transport as a function of the number, location, and type of measurements taken at a particular field site of interest.

The scope of this work is two-fold: In part II, the stochastic framework is defined, within which the rest of this study operates. Analytical, quasi-analytical, and numerical tools are developed for the highly flexible analysis of many unsaturated flow and transport problems in moderately and strongly heterogeneous soils. In part III, these mostly numerical (computer modeling) tools are applied to verify existing analytical models of unsaturated flow and transport, to implement a numerical stochastic analysis of the spatial heterogeneity of soil hydraulic conductivity, soil water tension, soil water flux, and solute (or contaminant) transport as a function of the soil heterogeneity, and to demonstrate how the design of measurement and monitoring networks in the unsaturated zone may or may not reduce the uncertainty about these flow and transport variables.

The dissertation is organized into ten chapters. This introduction is both chapter one and part I. Part II consists of six chapters: In chapter 2, the concepts of probability and random variables are introduced. An attempt is made to link the physical phenomena "spatial heterogeneity" and "uncertainty" with the conceptual rigor of probability theory and stochastic analysis. The chapter is intended to give a detailed answer to the question of why we use stochastic analysis to understand model uncertainty. Chapter 3 then introduces, compares, and validates several numerical methods to artificially generate random, spatially heterogeneous soils that can be used to study the effects of soil heterogeneity on flow and transport variability. These methods are of very general nature and have found applications in a wide range of physics, engineering and earth-sciences applications and are commonly known as "random field generators". In chapter 4 a purely analytical stochastic theory of flow in unsaturated soils is developed based on similar work by other authors. The analytical unsaturated stochastic flow theory serves three important purposes: it is an inexpensive, approximate method to assess the spatial variability of soil water tension and soil water flux; it is necessary for the application of existing transport theories to heterogeneous, unsaturated soils; and - as will be shown in chapter 7 - it is an invaluable catalyst needed to reduce the computation time associated with the numerical (computer) solution of the unsaturated, steady-state flow problem to just a fraction of the time hitherto necessary. In chapter 5 a computer simulation program is introduced that solves the physical equations governing variably saturated, flow and transport for any given random realization of a heterogeneous soil. Chapter 6 investigates several aspects of the numerical grid design for the finite element flow model introduced in chapter 5. Finally in chapter 7 an efficient combined analytical-numerical computer solution algorithm is described for the unsaturated stochastic flow problem based on the methods introduced in chapters 3 through 6.

Part III consists of three chapters, all of which are based on the conceptually simple but computationally expensive Monte Carlo method: a large number of "random" soils that are statistically identical to the field site of interest are generated. The flow and transport problems are solved for each soil, the individual results are compiled, and eventually analyzed statistically to give an overall assessment of the spatial variability of flow and transport in heterogeneous soils. The key to a successful Monte Carlo simulation is a high number of realizations (repetitions) such that the Monte Carlo results are truly representative of the stochastic nature of spatial heterogeneity and uncertainty. Monte Carlo analysis is therefore only possible with the efficient computational algorithms introduced in part II.

Chapter 8 is dedicated to the analysis of spatial variability and uncertainty of the unsaturated hydraulic conductivity, the soil water tension, and the soil moisture flux in a steady-state unsaturated flow regime. It compares the highly accurate numerical solutions with the analytical solutions of chapter 4 to discern the strengths and weaknesses of the analytical stochastic approach. In chapter 9 the nature of solute transport in heterogeneous soils is described and both the spatial variability of solute concentration as a function of time and the temporal variability of solute flux as a function of space in heterogeneous soils is investigated. The analysis is specifically applied to a point or small pollution source (as opposed to a spatially extensive non-point pollution source). This chapter also compares the highly accurate numerical results with approximate analytical stochastic transport theories to highlight their advantages and disadvantages. Finally, in chapter 10, I investigate how prediction uncertainty can be reduced by measuring various soil properties in situ and by using a conditional stochastic method that honors the degree of deterministic knowledge available about a soil site. The results are contrasted with the unconditional stochastic analyses of chapters 8 and 9.