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Simulating Radionuclide Fate and Transport in the Unsaturated Zone: Evaluation and Sensitivity Analyses of Select Computer Models

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Simulating Radionuclide Fate and Transport in the Unsaturated Zone: Evaluation and Sensitivity Analyses of Select Computer Models

by

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NOTICE

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FOREWORD

The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air, and water resources. Under a mandate of national environmental laws, the Agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. To meet these mandates, EPA's research program is providing data and technical support for solving environmental problems today and building a science knowledge base necessary to manage our ecological resources wisely, understand how pollutants affect our health, and prevent or reduce environmental risks in the future.

The National Risk Management Research Laboratory is the Agency's center for investigation of technological and management approaches for reducing risks from threats to human health and the environment. The focus of the Laboratory's research program is on methods for the prevention and control of pollution to air, land, water, and subsurface resources; protection of water quality in public water systems; remediation of contaminated sites and ground water; and prevention and control of indoor air pollution. The goal of this research effort is to catalyze development and implementation of innovative, cost-effective environmental technologies; develop scientific and engineering information needed by EPA to support regulatory and policy decisions; and provide technical support and information transfer to ensure effective implementation of environmental regulations and strategies.

Mathematical models are useful tools for determining soil screening levels of radionuclides in the unsaturated zone. However, models require users to specify various parameters characteristic of the site and chemical of interest. These parameters are not known without error. Many parameters vary over time and space in manners which are unknown. This is especially true when models are used to predict future events. This uncertainty in input parameters is associated with an uncertainty in model output which should be recognized by the model user. This report analyzes several transport models for unsaturated soils and quantifies the sensitivity of model outputs to changes in input parameters. This information will help users understand the importance of different parameters, identify parameters which must be determined at the site, interpret model results and apply their findings to specific problems.

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ABSTRACT

Numerical, mathematical models of water and chemical movement in soils are used as decision aids for determining soil screening levels (SSLs) of radionuclides in the unsaturated zone. Numerous transport and fate modeling codes exist for predicting movement and degradation of these hazardous chemicals through soils. Many of these codes require extensive input parameters which include uncertainty due to soil variability and unknown future meteorological conditions. The impacts of uncertain model parameters upon pertinent model outputs are required for sound modeling applications. Model users need an understanding of these impacts so they can collect the appropriate parameters for a given site and incorporate the uncertainties in the model predictions into the decision making process. This report primarily summarizes the findings which address the uncertainties and sensitivities of model outputs due to uncertain input parameters. However, the report also addresses the sensitivity of simulated results to conceptual model selection, and the comparison of sensitivity results between models, illuminating numerical differences and errors.

The objective of the parameter sensitivity studies was to determine the sensitivities and uncertainties of peak contaminant concentrations and time to peak concentrations at the water table, as well as those for the time to exceed the contaminant's MCL at a representative receptor well. The five models selected for these analyses were CHAIN, MULTIMED-DP 1.0, FECTUZ, CHAIN 2D, and HYDRUS. All of these are designed to estimate movement and fate of radionuclides through unsaturated soils. The models span a range in detail and intended use. This report presents information on the sensitivity of these codes to model conceptualization of radionuclide transport in the vadose zone, to numerical differences and errors, and to changes and uncertainties in input parameters, as well as presenting information concerning the analysis and interpretation of certain modeling components. The report does not intend to assess the appropriateness of any model for a particular use nor the uncertainty due to the model chosen, but it does indicate the problems and limits of using certain modeling components for certain physical applications.

Model parameters investigated include soil properties such as soil structure and texture, bulk density, water content, and hydraulic conductivity. Chemical properties examined include distribution coefficient, degradation half-life, dispersion coefficient, and molecular diffusion. Other site and soil characteristics such as equilibrium/nonequilibrium sorption sites, rooting depth, recharge rate, hysteretic effects, and precipitation/evapotranspiration were examined. Model parameter sensitivity was quantified in the form of sensitivity and relative sensitivity coefficients. The sensitivity coefficient is useful when calculating the absolute change in an output due to a known change in a single parameter. Relative sensitivity is useful in determining the relative change in an output corresponding to a specific relative change in one input parameter. Relative sensitivities are also used to compare the sensitivities of different parameters. These results are presented in graphical and tabular forms.

This study identified the limitations and advantages of using the selected codes for assessing the transport and fate of radionuclides in the unsaturated zone. This study also found the degree of uncertainty that exists in various model output parameters due to the combination of sensitivities of input parameters, high parameter variabilities, model type with its particular set of components, and the specific properties of the radionuclides. In addition, the study found that predicted movement of radionuclides was greater when the natural variability of daily rainfall was incorporated into the model than when only an annual flux was used. This is because major precipitation events (their daily averages in this case) result in larger fluxes of water and higher leaching rates that are essentially smoothed over when annual averaged fluxes are used. The study reaffirms that uncertainty is pervasive in natural systems and that results of modeling efforts presented in a deterministic fashion may be misleading, unless the results of modeling studies are presented in terms of probabilities of various outcomes. Further, this report evaluates model parameter sensitivity for a specific scenario, that is, radionuclide transport and fate through a 6 m homogeneous soil column at the Las Cruses Trench Site in New Mexico. For other scenarios, the general model user should take great care in the use of the results of the current study. Other sensitivity and uncertainty estimates may be required for the specific conditions and parameters of interest.

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