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Robert S. Kerr Environmental
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Project Summary

CHEMFLO: One-Dimensional Water and Chemical Movement in Unsaturated Soils

D. L. Nofziger, K. Rajender, Sivaram K. Nayudu, and Pei-Yao Su

This user's guide serves the purpose of instructing the user in the execution of a software package CHEMFLO for simulating water and chemical movement in unsaturated soils. The guide should allow easy access to information critical to the development of an understanding of the transport and fate of chemicals for point and non-point sources.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Understanding the movement of water and chemicals into and through soils is of great importance in managing, utilizing, and protecting our natural resources. These processes are very dynamic, changing dramatically over time and space. Soil properties, chemical properties, and water and chemical application rates interact in complex ways within the soil system to determine the direction and rate of movement of these materials. Researchers have worked many years to understand the physical and chemical mechanisms responsible for the movement of these materials. They have developed mathematical models describing these processes and compared the predictions of these models with field and laboratory measurements. The resulting mathematical models form a basis for predicting the behavior of water and chemicals in soils.

The full manual describes a software system designed to enable persons to define water and chemical movement systems, to solve the mathematical models, and to display the results of the simulations in graphical and tabular forms. This software expands on that of Nofziger[1] by reducing limitations in simulating water movement, adding chemical movement, and expanding the graphical and tabular output options. The manual describes the mathematical models used in the software and their limitations. The computer hardware and software required are then described. Simulations for several flow systems are included as the use of the software is described. Other features of the software are then illustrated. Finally, a set of numerical experiments is included. These experiments are designed to illustrate flow and transport in different types of soil systems and to enable users to assess the importance of different soil properties and other physical and chemical parameters upon water and chemical movement.

The software is intended for use by students, regulators, consultants, scientists, and persons involved in managing water and chemicals in soil who are interested in understanding unsaturated flow and transport processes. A limited amount of technical terminology is used in the software and manual, but the user need not understand the mathematics of the model in order to effectively use the software. As is the case in any model, the user is urged to become familiar with the limitations of the model and to assess their significance for the situation of interest before using it for decision making.

Conclusions

An interactive software system was developed to enable decision-makers, regulators, policy-makers, scientists, consultants, and students to simulate the movement of water and chemicals in unsaturated soils. Water movement is modeled using Richards[2] equation. Chemical transport is modeled by means of the convection-dispersion equation. These equations are solved numerically for one-dimensional flow and transport using finite differences. Results of the water model can be displayed in the form of graphs of water content, matric potential, driving force, conductivity, and flux density of water versus distance or time. Graphs of concentration, and flux density of chemical as functions of distance or time can also be displayed. Cumulative fluxes of water and chemical and total mass of chemical in the soil can be displayed as functions of time. Tabular outputs are also available. The full manual presents the mathematical equations and the numerical techniques used in the software. Limitations of the model are presented. Instructions for installing the software on your computer are given along with illustrations of its use. Finally, a set of numerical experiments are presented to enable the user to gain an understanding of the dynamic processes involved in water movement and chemical transport in soils. The software was written for use with IBM compatible microcomputers with 640 K bytes of random access memory, two floppy disk drives or one floppy disk and one fixed disk, or CGA, EGA, or VGA graphics cards, and an 80x87 math coprocessor.

References

1. Nofziger, D. L. 1985. Interactive simulation of one-dimensional water movement in soils: user's guide University of Florida, Institute of Food and Agricultural Sciences, Cir. 675 56 pp.
2. Richards, L. A. 1931. Capillary conduction of liquids through porous mediums. *Physics* 1:318-333.

D. L. Nofziger, K. Rajender, Sivaram K. Nayudu, and Pei-Yao Su are with Oklahoma State University, Stillwater, OK 74078.
***Joseph R. Williams** is the EPA Project Officer (see below).*

The complete report, entitled "CHEMFLO: One-Dimensional Water and Chemical Movement in Unsaturated Soils," (Order No. PB 90-126 020/AS; Cost: $23.00, subject to change) will be available only from:
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at:
Robert S. Kerr Environmental Research Laboratory
U.S. Environmental Protection Agency
Ada, OK 74820

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