

A General Approach to Modeling Chemical Transport and Transformation in the Vadose Zone

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Good morning.

In this presentation I am going to talk about a method of modeling – but not about any particular model as a software package.

My use of the term “vadose zone” refers to the region between the land surface and the top of the groundwater in a saturated aquifer.

The essential characteristic of the vadose zone is that water flows at varying degrees of saturation.

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Summary of approaches.

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There are two parts to this approach:

Describe solute transport & transformation with ordinary differential equations, linear or nonlinear.

Solve these ODE's with standard mathematical software.

I use MATLAB – but I don't have any experience with other similar software.

I do not have shares in Mathworks, so this is not an endorsement, just a reporting of my experience.

The exclusive use of ordinary differential equations may be a surprise to those of you who are used to seeing these time- and spatially-varying process as partial differential equations. I will explain soon!

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Plenty of good models available for describing transport and transformation of chemicals – some of which we will hear about during this meeting?

Easy to construct a new model for a specific purpose:

example of a model designed for the application of control theory to chemical transport in the soil.

One parameter for adsorption-desorption or mobile-immobile water.

Breakthrough curve data: these processes are distinguishable only by the magnitude of one model parameter.

Coding of the model is simplified, and consists only of instructions for the mathematical software platform.

Advective-dispersive solute transport, with rate-limited linear absorption-desorption, can be described with about 15 statements in MATLAB.

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Now, I am going to talk about how to model transport processes with ordinary differential equations.

For the purpose of groundwater protection, water flow in the vadose zone is one-dimensional vertical, and therefore a function of time and depth.

The usual description by a partial differential equation is replaced by a concept called cells-in-series, which can be written as ordinary differential equations.

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CIS concept has history of at least 50 years in modeling dispersion

Cells considered as slices of the vadose zone, volume determined by the fraction of water in the transport process.

Thickness of the slices determined by the amount of dispersion

Solute is completely mixed within each cell.

Discrete in space, but continuous in time: this is a departure from previous use of this concept, in which the model was developed in discrete-time form.

The continuous-time description has major computational advantages.

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Now consider advection-dispersion in the vadose zone

The cells-in-series model is a very good analogue of advection-dispersion when the cell thickness is set equal to twice the dispersivity.

Established experience in soil science that unsteady, non-uniform solute transport analysed as steady-state in cumulative drainage.

Hydrodynamic dispersion is directly proportional to the pore-water velocity by a fixed value of dispersivity.

The differential equations are linear in terms of cumulative drainage

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The cells-in-series concept transforms the spatially-varying solute transport into a series of mixing tanks.

This mixing tank series is a concept favoured by chemical engineers.

Chemical transformations are lumped for each cell, so that ordinary differential equations are written for each cell. These may be linear or non-linear.

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I would now like to present the results of two examples of modeling by using this General Approach.

The first is solute transport through soil by drainage from rainfall and irrigation onto pasture.

The second example is a model of soil-water flow through macropores with sorption loss to the soil matrix.

These results are from experiments with replicated columns of field soil about 1000 mm in diameter and about 1000 mm deep.

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The model structure shown here can represent all or any of the listed processes.

Each cell in the transport series on the left (where equilibrium processes occur) is connected with a non-equilibrium cell, on the right by rate-limited transfer.

Adsorption-desorption can occur within the equilibrium, transport cells or within the non-equilibrium cells, or both.

If the adsorption isotherms are linear, then the whole model forms a linear system, with the cell concentrations as the system states.

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When a system model is linear, standard mathematical software gives some very useful results.

One of these is that stable model predictions can be done for any time interval.

This is especially useful for practical monitoring because the transport processes are driven by uneven amounts of drainage and there may be only one bulk solute sample for each drainage event.

The state-space description of the CIS model enables any input and initial condition.

Forecasting under uncertainty can be done with Kalman filter methods.

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This is the solute breakthrough curve of ^{35}S -labelled sulphate which was initially resident at the land surface.

The model response was calibrated with other solute data from the same experiment as well as the ^{35}S , and includes advection-dispersion, mobile-immobile diffusion, and rate-limited linear adsorption-desorption.

The model is not a good fit to the data because of soil-water movement in the upper soil layers which is not represented by drainage from the bottom of the soil columns.

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Calibrated model is a good representation of prior knowledge about the processes.

The solute concentrations in the cells near the land surface are least known because the vertical transport processes are only partially represented by drainage at the observation depth, and other processes such as plant uptake are not modeled.

Below the plant root zone, solute transport is more predictable and uncertainty is less.

Uncertainty is quantified as the variance of estimation of each state (cell concentration), and can be a subjective assessment.

This kind of approach is useful for monitoring and management.

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The estimation part of this plot shows the one-step-ahead predictions as the model uses each new data value to improve the estimate of the system states, which are the solute concentrations of each cell.

At the end of the data record, the current cell concentrations are the initial states of the model for creating the forecasts.

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My second example is a model of soil-water flow in macropores.

This particular application does not include solute transport, because the experimental data were for only the drainage amounts at five-minute time intervals.

The differential equations here are with respect to time not cumulative drainage.

This is a non-linear model, both in terms of the local water flow law and sorption of water from the macropores into the soil matrix.

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The cellular structure of the model allows the states, in this case macropore water content, to be displayed.

This 3-D view shows the complex nature of the non-linear water wave response to an intermittent sequence of irrigation pulses.

This model does not have the linear system property of prediction over uneven, specified time intervals.

However, the mathematical software takes care of the time step for integration and the model demonstrated 100% conservation of water mass.

The next slide shows the model prediction and observed data at the bottom of the soil column.

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The arrival and recession of the wave are reasonably well predicted, but the multiple peaks are possibly subject to chaotic behaviour.

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In conclusion, I want to summarise some features of this general approach to modeling with respect to contributing to assessment of pesticide impact on groundwater.

This is a relatively easy way of constructing and coding models for complex, chemical transformations

After transformations in the organic soil layers near the land surface, the remaining transport phase through the vadose zone to groundwater is easily computed for the intermittent and uneven intervals of drainage which drive the process.

The transport phase can be represented by linear system models which are well suited to the requirements of monitoring and management of groundwater protection