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

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Summary

- The general approach
- Modeling chemical transport
- Modeling chemical transformation
- Example results:
- Case 1: Advection-dispersion with linear sorption
- Case 2: Macropore flow with sorption

General Approach

- Describe transport and transformation processes as first-order ordinary differential equations (ODE-1’s)
- Use mathematical software for integration of the ODE-1’s, and graphical display (MATLAB®)

Advantages

- Model constructed to suit purpose -
  e.g., monitoring and management
- Appreciation of dynamic behaviour -
  may have fewer model parameters
- Simplified coding of computer program -
  access to analytical and graphical tools

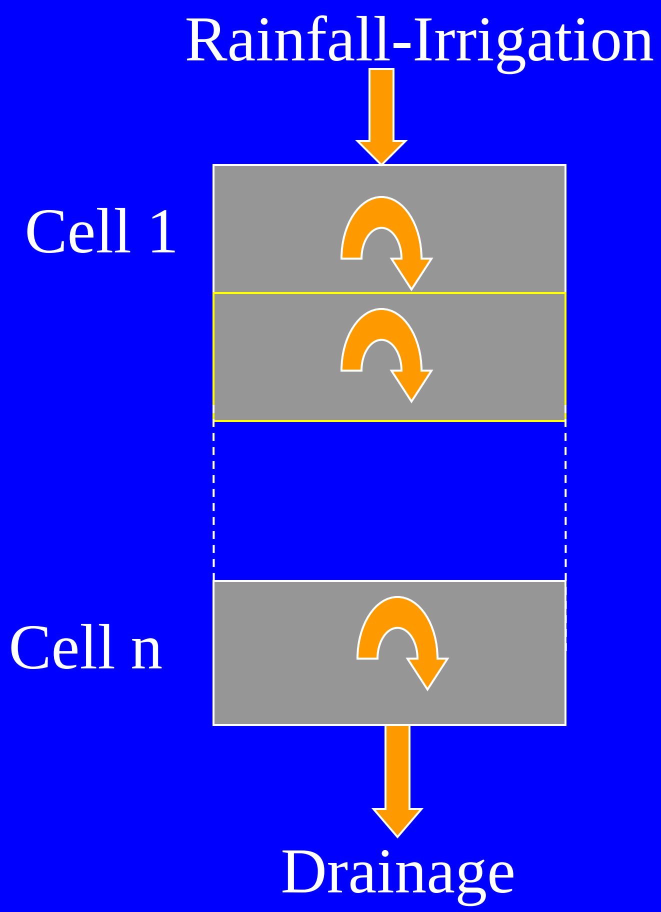
Transport in the vadose zone

- One-dimensional, vertical
- Function of time and depth

- Partial differential equations replaced by a **cells-in-series** model described with ODE's

Cells-in-series models (CIS)

- Cell thickness depends on dispersion
- Complete solute mixing within cell
- Discrete in space
- Continous in time



CIS example: Advection-dispersion

- Cell thickness=2 x dispersivity
- Dispersion= water velocity x dispersivity
- “Time” index is cumulative drainage
- Unsteady flow (in time) becomes steady (in drainage)
- Model is now continuous in drainage

Chemical transformations

- CIS model accounts for spatial distribution due to transport, with ODE-1's
- Transformations are lumped at the cell level
- Transformation processes are described by coupled, linear or non-linear ODE-1's

Some modeling results

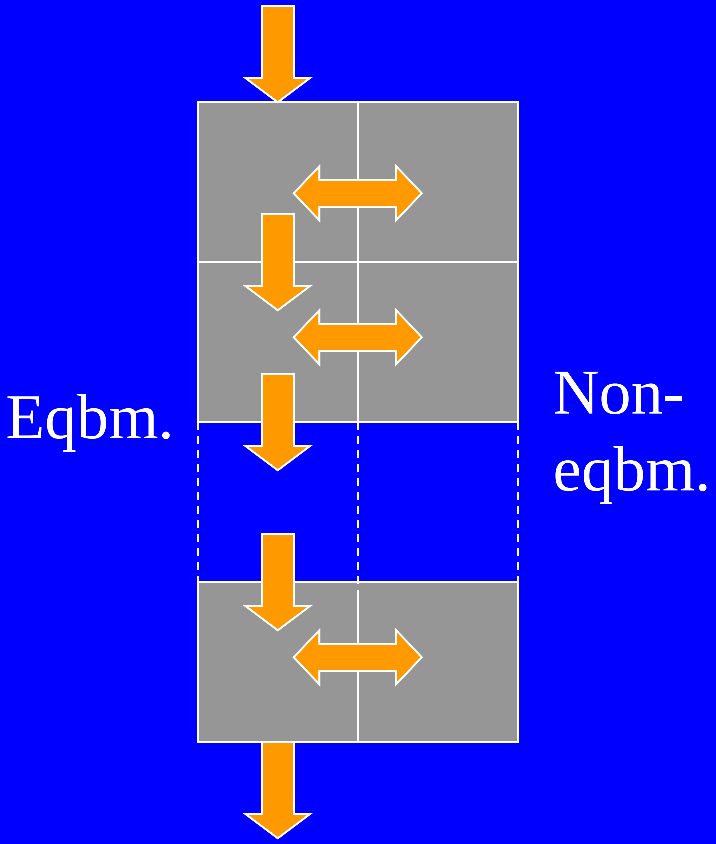
- Case 1: solute breakthrough curves
- Case 2: macropore drainage from high-rate irrigation

- Undisturbed field soils under pasture
- Soil columns:

  ~1000 mm diameter, ~1000 mm depth

Case 1: Solute Transport
advection-dispersion & linear sorption

- **Processes:**
- Advection-dispersion
- Adsorption-desorption (linear)
- Mobile-immobile water
- Rate-limited diffusion
- **Linear system**



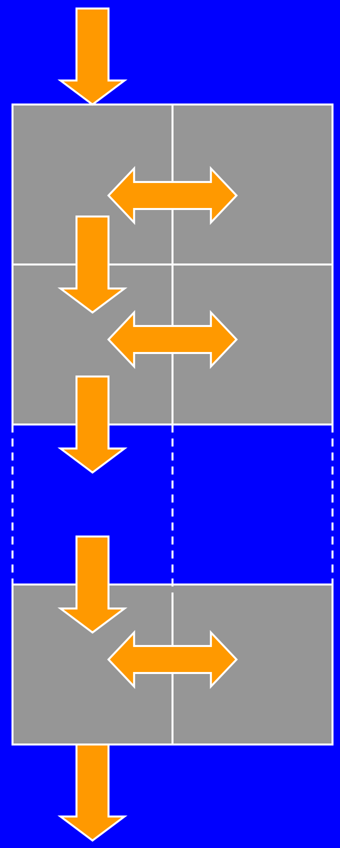
Linear system capability

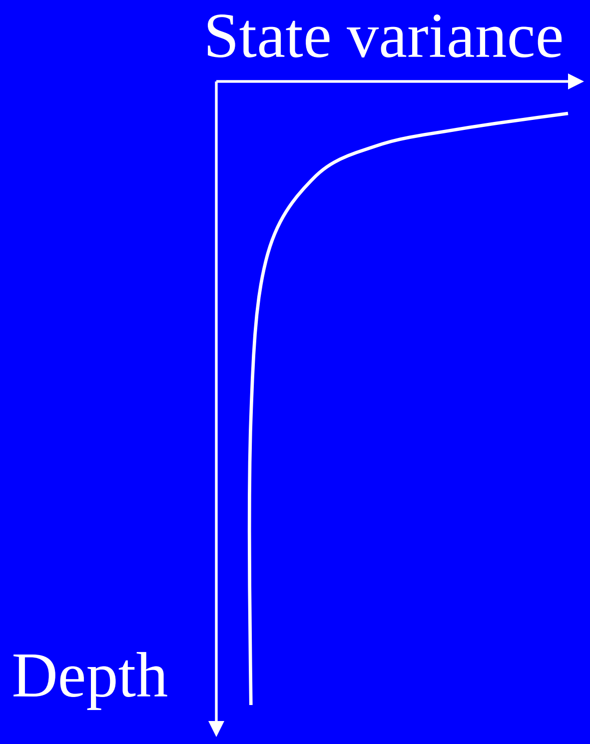
- Solute flux inputs for uneven drainage intervals
- Computational stability
- Initial conditions of any
  concentration-depth profile
- Process parameters can vary with depth
- Enables forecasting under uncertainty (Kalman filter methods)

Response to ^{35}S-labelled sulphate

Knowledge and Uncertainty

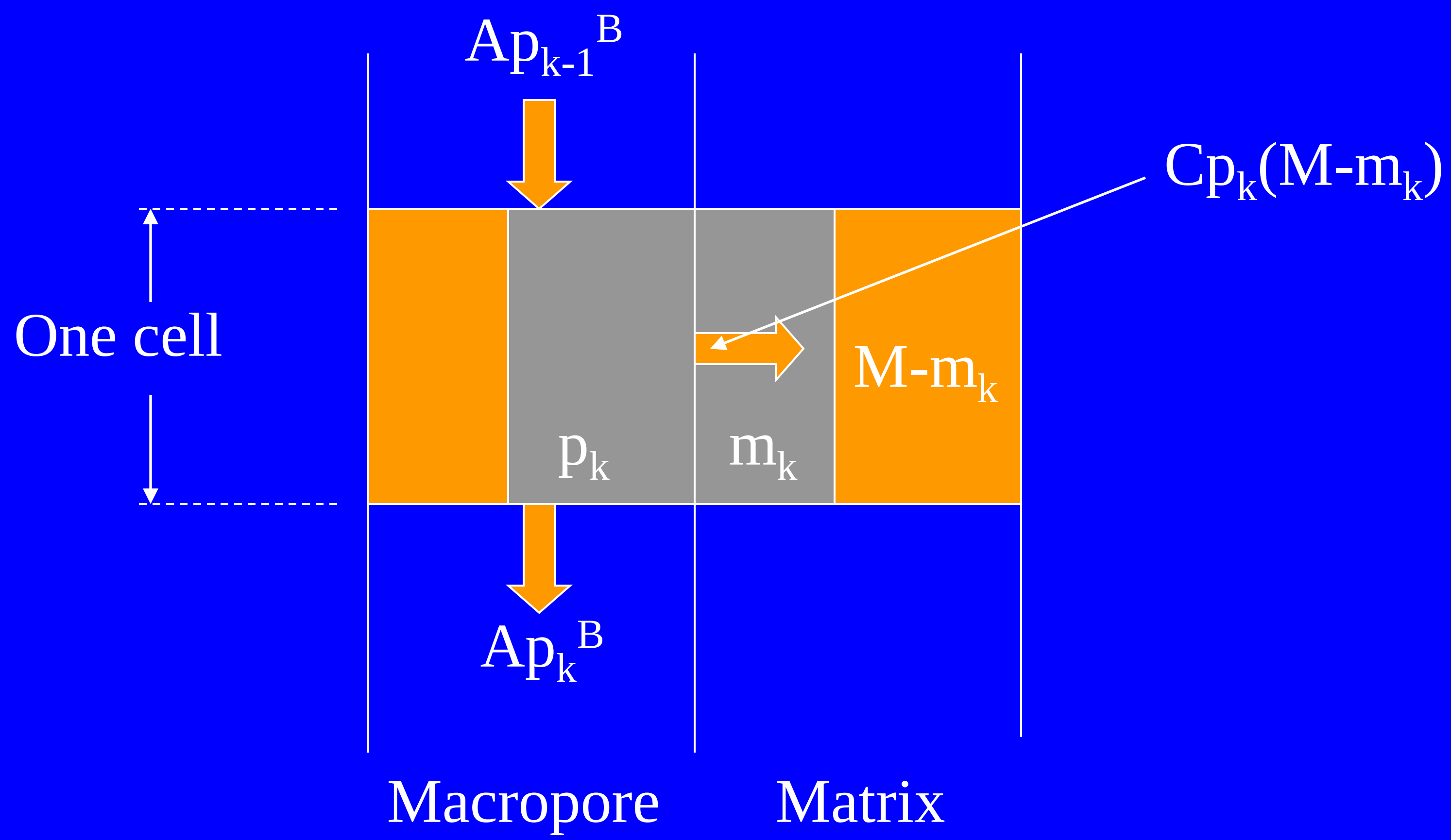
Cell concentrations are the system states





State estimation and forecasting

Case 2: Macropore Water Flow kinematic wave & non-linear sorption



3-D view of kinematic macropore water wave

Simulation of macropore drainage

Conclusions:
Protecting groundwater from pesticides

- This general modeling approach enables easier coding of complex chemical transformations
- Transportation through the vadose zone can be easily modeled in terms of uneven drainage intervals
- Model structures are suited to monitoring and management