Model Abstraction Techniques for Predicting Subsurface Contaminant Transport

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SUMMARY

Model abstraction is a methodology for reducing complexity of a simulated domain while maintaining the validity of the simulation results with respect to the questions that the simulation is aimed at addressing. The need for model abstraction stems from the needs to improve reliability and to reduce uncertainty of simulations, to make modeling and its results more understandable and transparent to the end users, and to enable more efficient use of available resources in data collection and computations.

This study focuses on applications of model abstraction to contingency planning and management of potential and actual contaminant release sites within the scope of the US NRC operations.

The OPE3 experimental field site near Beltsville, MD, has been extensively studied for more than 10 years using geophysical, biophysical, remote sensing, soil and groundwater monitoring methods. A major focus of the data analysis was on the existence of subsurface structural units and features that may drastically change the fate and transport of contaminants in the vadose zone, as well as of projected trajectories of the contaminant plume in groundwater. We found that solute transport in soils and shallow groundwater at the site was affected by (i) the presence of a restrictive fine-textured layer that was not fully continuous laterally; (ii) the complex topography of the restrictive layer favoring preferential flow and transport along preferred pathways along its surface relief; (iii) the presence of natural capillary barriers; and (iv) possible funnel flow in a coarse-textural layer located between fine-textured layers. New field experimental study was designed to observe the lateral transport of a surface-applied conservative tracer pulse when transport was controlled by regular irrigation pulses and natural precipitation. The results of the experiment were used to test applicability of three of model abstraction techniques, specifically: (A-1) aggregation, i.e. replacement heterogeneous soil profile with a homogeneous soil, (A-2) parameter determination, i.e. replacement of calibrated parameters with values estimated using pedofransfer functions; (A-3) model conceptualization, i.e. ignorance of the unsaturated zone by locating source of release within the saturation zone. Different initial and boundary conditions were generated to run calibrated and abstracted HYDRUS-3D model. Applicability of model abstractions was evaluated using performance indicators (PI): peak concentrations, time of peak concentrations, and total fluxes computed in 100 locations across the simulation domain. Abstractions A-1 and A-2 resulted in inadequate predictions of all PI, indicating high model sensitivity to the transport parameters and complexity of the simulated system, while results of abstraction A-3 did not deviate significantly from the calibrated model. Overall, this work demonstrated the usefulness of model abstraction in simulations of flow and transport in variably-saturated subsurface.

FIELD EXPERIMENT AND SUBSURFACE TRANSPORT SIMULATION

Site Characteristics and Probes Locations

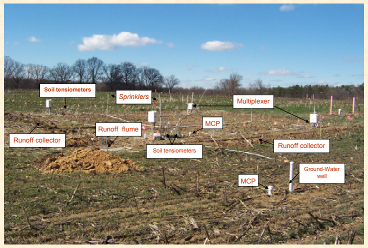


Fig.1 Lateral flow experimental setup

- Location: OPE3, USDA, Beltsville Agricultural Research Center, MD
- Soil: sandy loam, Typic Hapludult
- Soil horizons: Ap - 0-25 cm, Bt - 25-80 cm,C – 80-120 cm;
- Groundwater depth: Divers at 12 locations, every 30 min;
- Cl^- concentrations: ion chromatography, daily.
- Water content measurements:
  - MCPs (SENTEK) at depths 10-100 cm every 10 cm;
  - 4 probes at irrigated plot size of 10x10 m;
  - 8 probes beyond the irrigated plot;
  - measurements every 15 min from March 25 through August 4, 2008;
- Rainfall measurements: Pluviograph

Tracer transport simulation

For For HYDRUS-3D calibration we considered a 3-D layered domain that extended laterally for 55 m in the x (east-west) direction and for 50 m in the y (north-south) direction. The thickness (z direction) of the domain varied from 3.12 m to 5.18 m. Soil texture measured at 12 locations from depth of 0.2 m through 2.0 m with 0.2 m increment was grouped into 9 classes: three Sandy Loam classes (sL1, sL2 and sL3), two Sandy Clay Loam classes (scL1 and scL2), two Loam classes (L1 and L2), and two Silt Clay Loam classes (sicL1 and sicL2). The soil materials were distributed at each computational layer based on measured soil texture data.

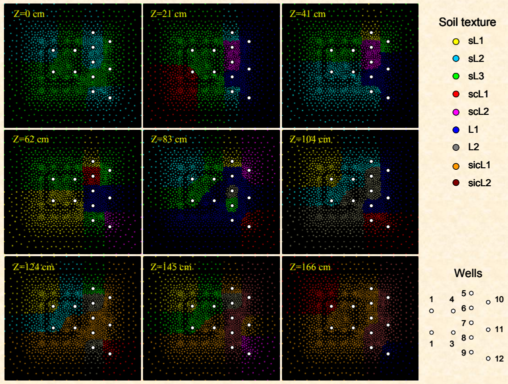


Fig.2 Material distribution in the simulated domain

HYDRUS-3D calibration

ROSETTA estimated parameters of van Genuchten equation were set fixed for the water retention in the HYDRUS-3D simulations. Saturated hydraulic conductivity (K_{sat}), parameters of longitudinal (*DispL*) and transverse (*DispT*) dispersivity were fitted to the Cl^- concentrations measured in water samples taken every 24 hours from 12 wells during the experiment. The model reasonably well described the dynamics of groundwater depth and Cl^- concentrations in the observation wells.

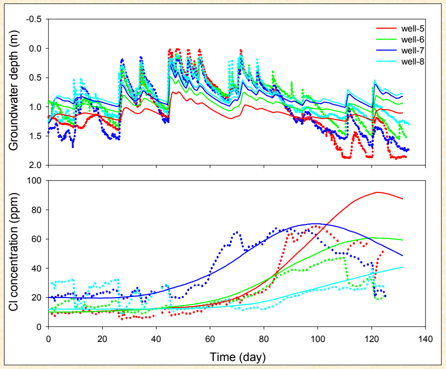


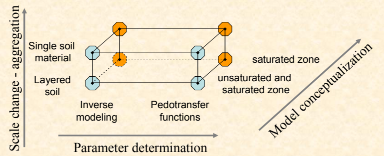
Fig.3 Measured (symbols) and simulated (lines) dynamics of groundwater depth (top) and Cl^- concentrations at 4 locations

THEORY OF MODEL ABSTRACTION

The base model should be abstracted if it:

- includes descriptions of processes that cannot be observed well;
- creates an unacceptable uncertainty in the key output;
- has an unacceptable demand for resources in multiple simulations;
- produces inexplicable results in terms of the key output;
- is too complex to be explicable and believable for the users;
- is to be discarded in favor a preferred simple model.

Design of Model Abstraction via Model Conceptualization, Scale Change and Parameter Determination Abstractions



Model Scenarios

- Source: an accidental release from point source at locations well-1 or well-2.
- Groundwater depth: 1.7 and 2.7 m below the surface at the lowest point of the simulation domain
- Groundwater slope: (a) 1.6% in West-East direction, 0.4% in North-South direction
  (b) 1.6% in West-East direction, 1.0% in North-South direction
- Weather conditions: precipitation corresponding to 25%, 50% and 75% probabilities of 60-years monitoring period in Beltsville, MD

Performance Indicators and Statistics

Indicators

- Peak concentration
- Time of peak concentration
- Total flux

Statistics

- Correlation coefficient
- Nash-Sutcliffe efficiency $E = 1 - \frac{\sum (O_i - P_i)^2}{\sum (O_i - \overline{O})^2}$
- Index of agreement $d = 1 - \frac{\sum (O_i - P_i)^2}{\sum (|P_i - \overline{O}| + |O_i - \overline{O}|)^2}$

Abstraction techniques

- **A-1**: Aggregation: replacement of a heterogeneous soil profile with a homogeneous soil
- **A-2**: Parameter determination: replacement of the fitted K_{sat} with pedotransfer function (PTF) estimated values (Rawls et al., 1983)
- **A-3**: Model conceptualization: ignoring the unsaturated zone by locating source of release within the saturation zone

RESULTS OF HYDRUS-3D SIMULATIONS

Water flow and Cl^- transport were simulated using the calibrated and abstracted HYDRUS-3D model for the specified scenarios. Spatial distributions of the performance indicators were plotted for each simulation to evaluate visually the subsurface passways of the applied tracer. Visual examination of the performance indicators pointed to discrepancy between abstracted models A-1 (homogeneous soil), A-2 (K_{sat} from PTFs) and the calibrated model. Ignoring the unsaturated zone (abstracted model A-3) did not change significantly the spatial patterns of the performance indicators obtained with the calibrated model.

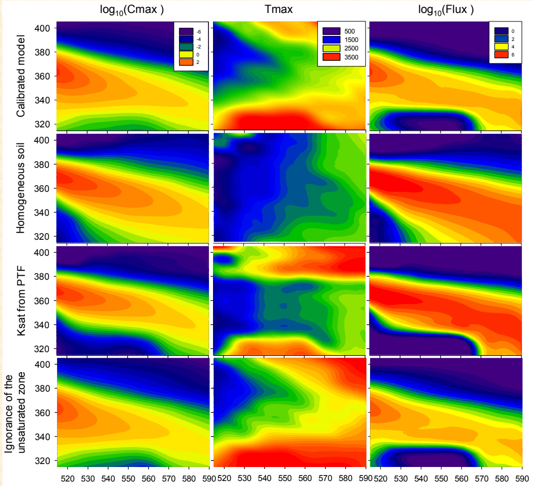


Fig.4 Example of the spatial distribution of the performance indicators simulated with the calibrated and abstracted HYDRUS-3D models

A total of 48 scenarios were used to evaluate correctness of the three abstractions. All three considered statistics, i.e., correlation coefficient, Nash-Sutcliffe efficiency and index of agreement d., indicated inappropriateness of the abstractions A-1 and A-2 reflecting high model sensitivity to the transport parameters and complexity of the simulated system. PI obtained for the abstraction A-3 did not deviate significantly from the calibrated model, indicating importance of the saturated flow in this particular study. Abstraction by ignoring the unsaturated zone appeared to be efficient to simplify the simulation domain.

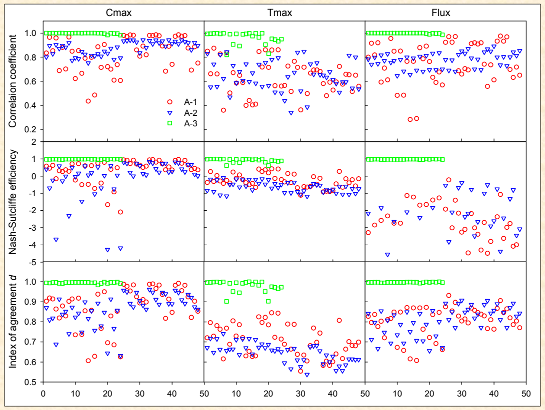


Fig.5 Statistics of the performance indicators for three model abstractions

CONCLUSIONS

- This work demonstrated the usefulness of model abstraction in simulations of flow and transport in variably-saturated subsurface. Whereas multidimensional and multi-process representations leave room for several competing conceptual models for flow and transport, simpler models that retain the most essential features of those representations could provide meaningful alternatives.
- Model abstraction has a great potential for reducing complexity and uncertainty of models predicting water, heat, gas and chemical transport in diverse environments.
- Model abstraction is a powerful tool for evaluation of parameter upscaling effects on model prediction accuracy in highly heterogeneous systems.