Model Abstraction: Background, Approaches, and Confirmation

YAKOV PACHEPSKY, USDA-ARS

Contributors and collaborators

- Ralph Cady, Tom Nicholson – U.S. NRC
- Tim Gish, Andrey Guber – USDA-ARS
- Jirka Simunek – UC Riverside
- Alexander Yakirevich, Mikhail Kuznetsov – Ben Gurion University, Israel
- Diederick Jacques – Nuclear Research Centre, Belgium
- Jung-Woo kim – Atomic Energy Research Institute, Korea
- Rien van Genuchten – Fed. University of Rio de Janeiro/Nuclear Energy Commission, Brazil

Comprehensive Publications

NUREG CR-6884. Model Abstraction Techniques for Soil Water Flow and Transport. U. S. NRC 2006.

NUREG CR-7026. Application of Model Abstraction Techniques to Simulate Transport in Soils U.S. NRC. 2011.

Model Abstraction - Definition

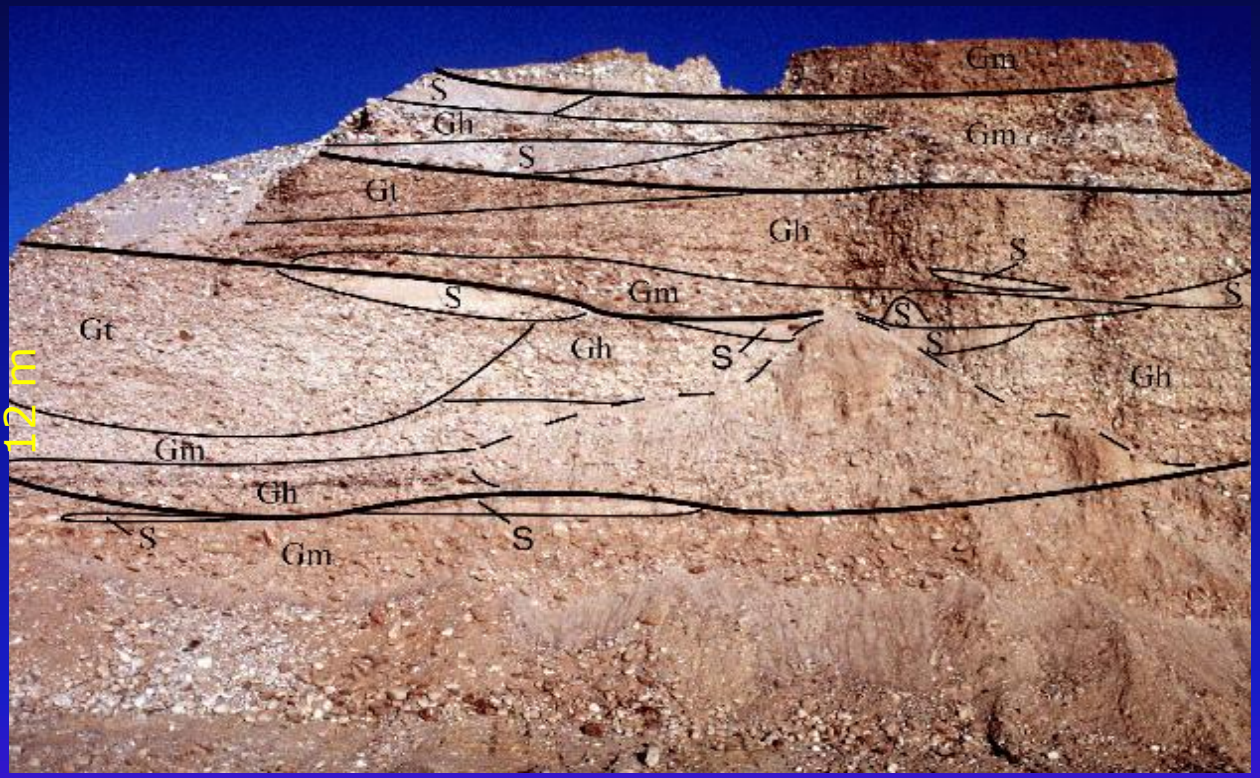
Model abstraction (MA) is a methodology for
reducing the complexity of a simulation model
while maintaining the validity of the simulation results
with respect to the question that the simulation is being used to address.

Model Abstraction – Why may be desirable

- The base model includes descriptions of processes that cannot be observed well; calibration is problematic.
- The base model propagates uncertainty in inputs a manner that creates unacceptable uncertainty in the key output.
- The base model produces inexplicable results in terms of the key output.
- The base model requires an unacceptable amount of resources to be parameterized and/or run.
- The base model lacks transparency to make the model and its results explicable and believable to customers.
- Benefits from the concurrent use of models of different complexity.

Model Abstraction – Why possible?

Complexity is easy to perceive but difficult to represent in mathematical terms.



Quarry exposure of braided-stream deposits:

S - disconnected sand lenses
Gm - poorly-sorted massive units
Go - moderately-sorted horizontally-bedded units
Gt - crossbedded units.

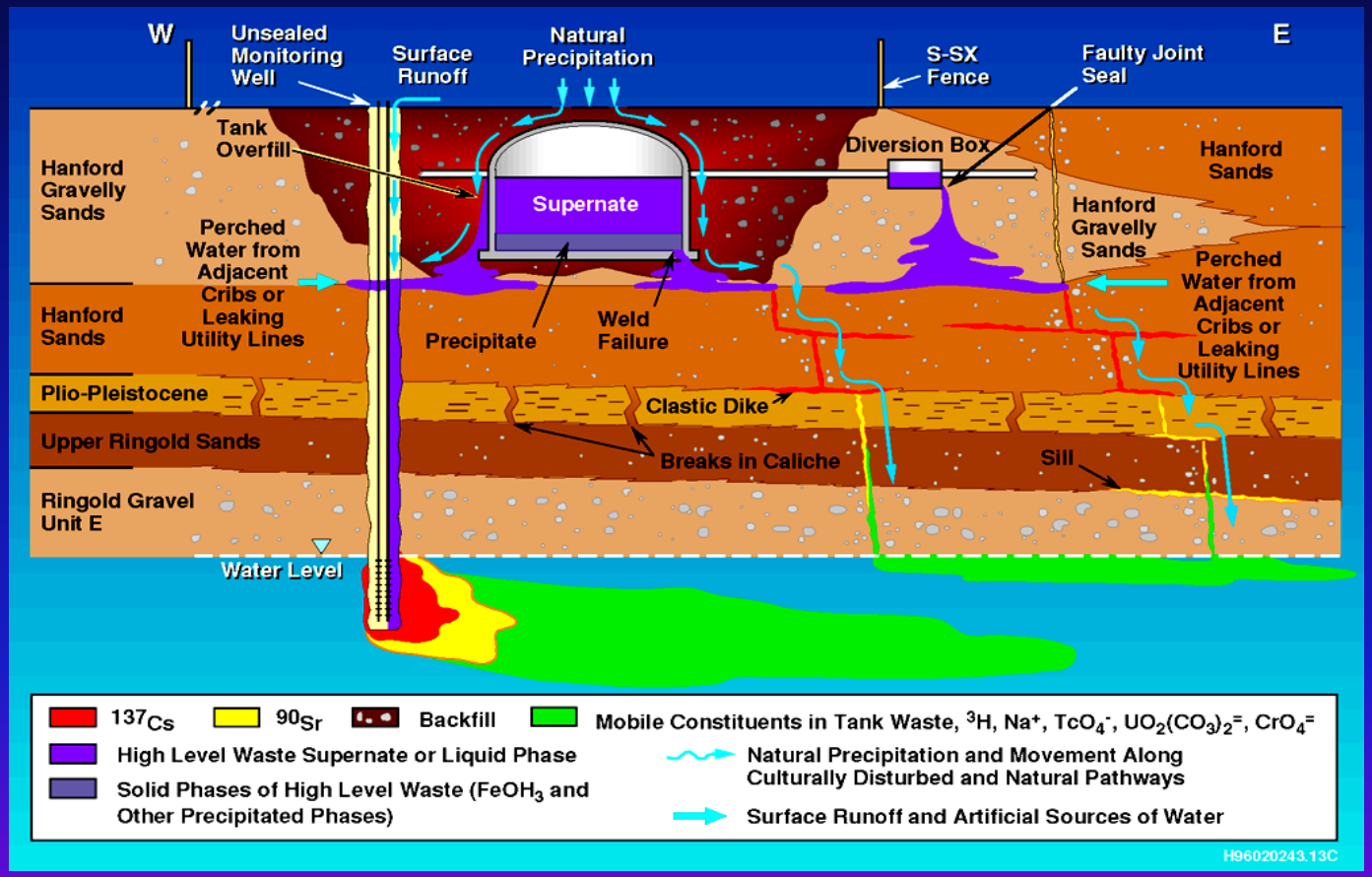
Boise hydrogeophysical research site

Warren Barrash, BSU

Mathematical models different by their concepts can result in the same accuracy in terms of residual errors.
There is no such thing as “the best model”

Complexity - Hanford site

Conceptual model of the contaminant transport in unsaturated zone



Ward et al. (1997) after Caggiano et al. (1996)

Low and intermediate level waste disposal site – El Cabril , Hornachuelos, Spain

Developments and milestones in MA theory and applications

	Refsgaard et al., '12	Multimodeling in groundwater monitoring network design
	Alexandrov et al., '11	Multimodeling in technical assessment and evaluation of environmental models and software
	Jacques et al., '11	MA to assess the spatial-temporal evolution of chemical degradation fronts in real-size concrete structures typical of a near-surface radioactive waste disposal facility.
2010		
	Van Ness & Scheffer '05	The concurrent use of complex and simple models
	Neuman & Wierenga, '03 '	The model simplification has to be systematic and comprehensive
	Davies&Bigelow, '03	Strategy-level analysis and decision support require simpler models
2000	Chwif et al, '00	Sources and consequences of the excessive model complexity
	Cauglin & Sisti, 97 Fishwick, 1995;	General taxonomies of model simplification methods. Term "model abstraction"
	Beven et al., '92	Recognition that the multiplicity of models is a norm
1990		
	Innis & Rextad, '85	Model simplification techniques suggested for all steps of model development
1980		
	Ziegler, '76	The first summary of model simplification techniques
1970	Meisel & Collins, '73	Advantages of using simplified models

MA applications

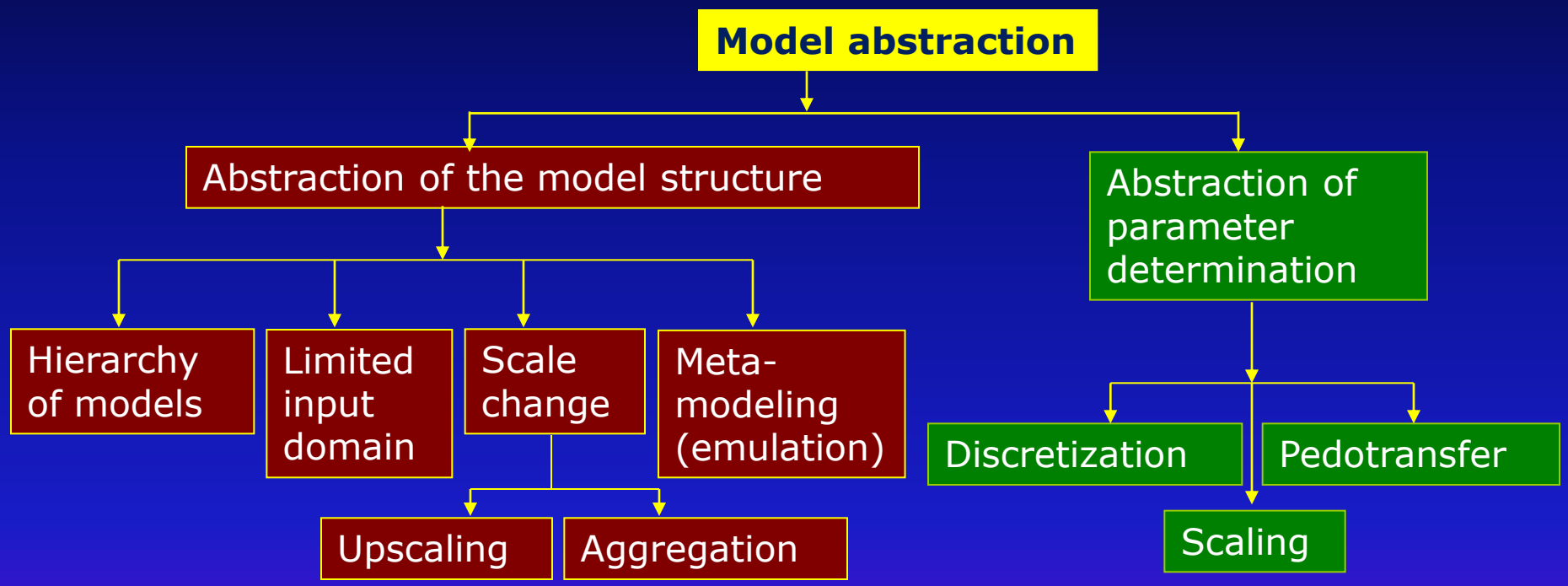
- MA results in a change in conceptual model
  or
  in a change in parameter estimation paradigm.
- MA has been applied in the large number of R&D fields.
- MA methods are R&D field-specific.
- MA is site- or case-specific.

Lessons for subsurface contaminant hydrology

A set of appropriate MA methods should be defined and characterized

A procedure for the systematic and comprehensive MA should be developed and tested.

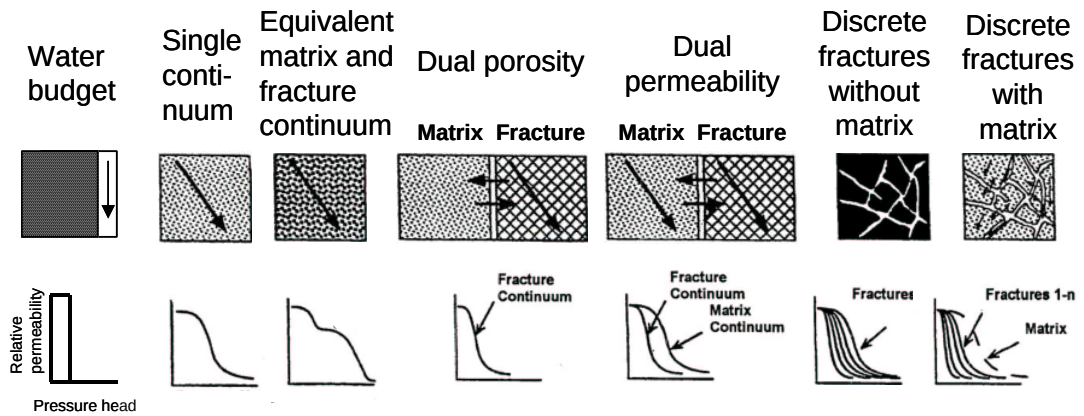
Categories of MA approaches applicable in contaminant hydrology



http://www.nrc.gov/reading-rm/doc-collections/nuregs/contract/cr6884/

Examples of process description hierarchies

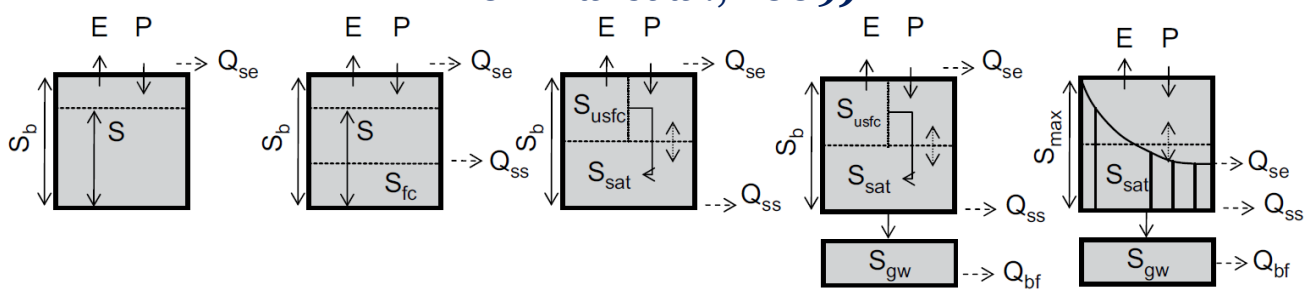
Hierarchy of models to simulate water flow and solute transport in structured soils or in unsaturated fractured rock (modified from Altman et al., 1996)



Complexity

Model abstraction

Hierarchy of models for soil water content accounting in watershed modeling (modified from Bai et al., 2009)



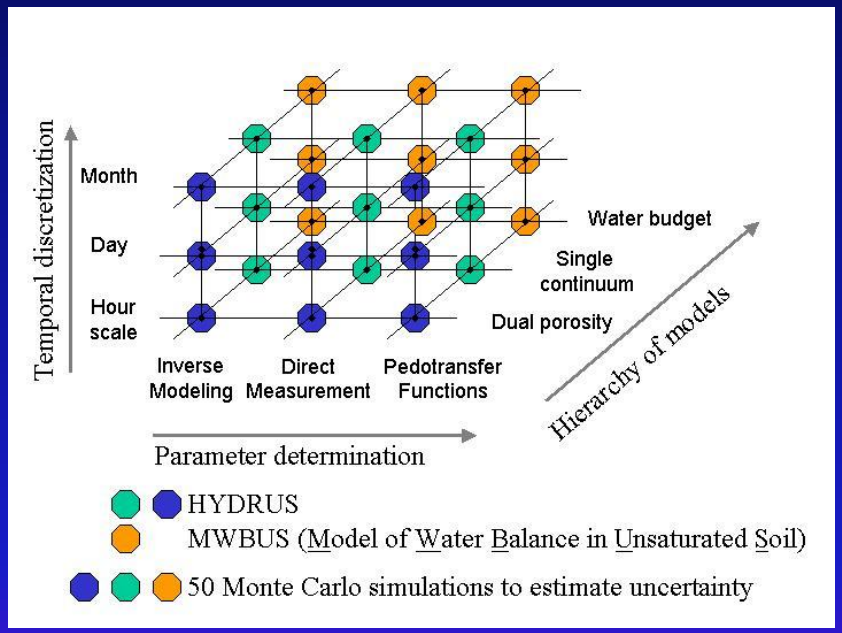
Complexity

Model abstraction

The model simplification has to be systematic and comprehensive

Suggested by
Neuman, Wierenga,
and Nicholson (2003).

Example of systematic MA via model structure and parameter determination



- ❖Justify the need for the model abstraction
- ❖Review the context of the modeling problem (FEP)
- ❖Design model abstraction with selected techniques
- ❖Perform model abstraction

Reviewing modeling context – step 1 in MA

Reviewing the model key output

- Purpose of modeling - key output use
- Key output type and scale
- Acceptable accuracy and uncertainty of the key output
- Model performance indicators

Reviewing assumptions made during development of the base model and justifications for those assumptions

- Subsurface structural units.
- Dimension of the problem.
- Simulation domain, initial and boundary conditions.
- Estimated model parameters.
- Data available for calibration.
- Calibration procedure and results.
- Software properties.
- Model documentation

Example of review points: Subsurface structural units

- Does a specific site have subsurface structural units and features that may drastically change the fate and transport of pollutants in the vadose zone along the projected trajectory of a contaminant plume?
- If a restrictive fine-material layer is expected, does it have dikes or faults; can the layer have gaps?
- If a restrictive layer is expected, can it have a topography causing flow and transport via preferential pathways along it upper surface?
- Are there natural capillary barriers (i.e., boundaries between finer material overlaying the coarse sediments)? If yes, are gaps in these barriers expected?
- Can funnel flow in coarse-textural soils develop due to presence of a layer of coarse materials between two fine-textured layers?
- Can geochemical conditions of saturated or perched zones in the vadose zone cause changes in pollutant transformations or retention?
- Can well-conducting layers contain fine-scale high-conductivity parts of the pore space that will facilitate transport through large pores during episodic infiltration events?
- Is the lateral conductivity of the capillary fringe large enough to allow substantial contribution of the capillary fringe to lateral transport above the water table?

An essential condition here is to obtain answers to these questions from an available knowledge base that is as broad as possible.

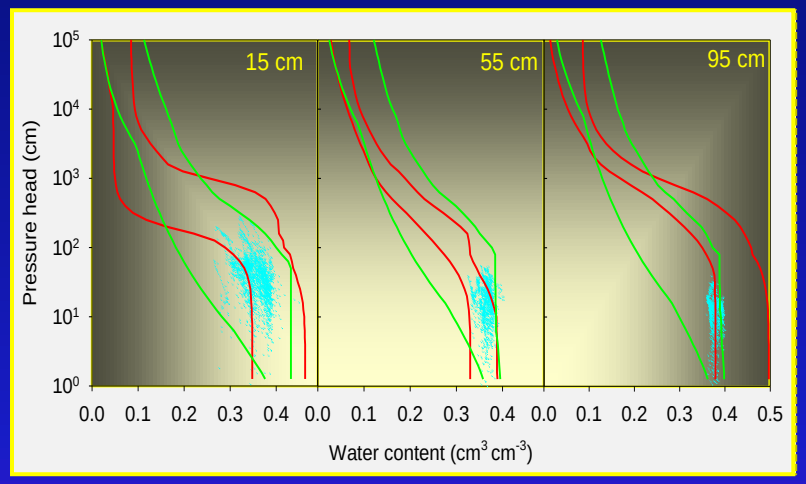
The geological, hydrogeological, and hydrogeophysical assessment can gain benefit greatly from complementary sources such as types of stream hydrographs, the presence and hydrology of springs, the presence of paleosoils, documented fragipans, experience during well construction, occurrence and concentrations of agricultural chemicals in well water, crop yield variability in dry years., etc.

MA of parameter determination with pedotransfer functions

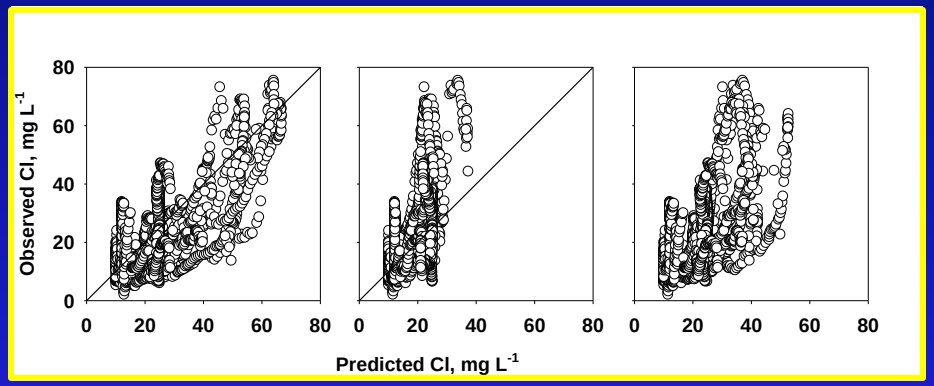
Ensemble modeling or multimodeling

PTF ensembles work well for water retention in variable saturated soils and weathered rocks

PTF ensembles do not work well for saturated hydraulic conductivity ; this abstraction needs to be coupled with scaling.



Calibration PTF PTF+scaling



Measured in the field

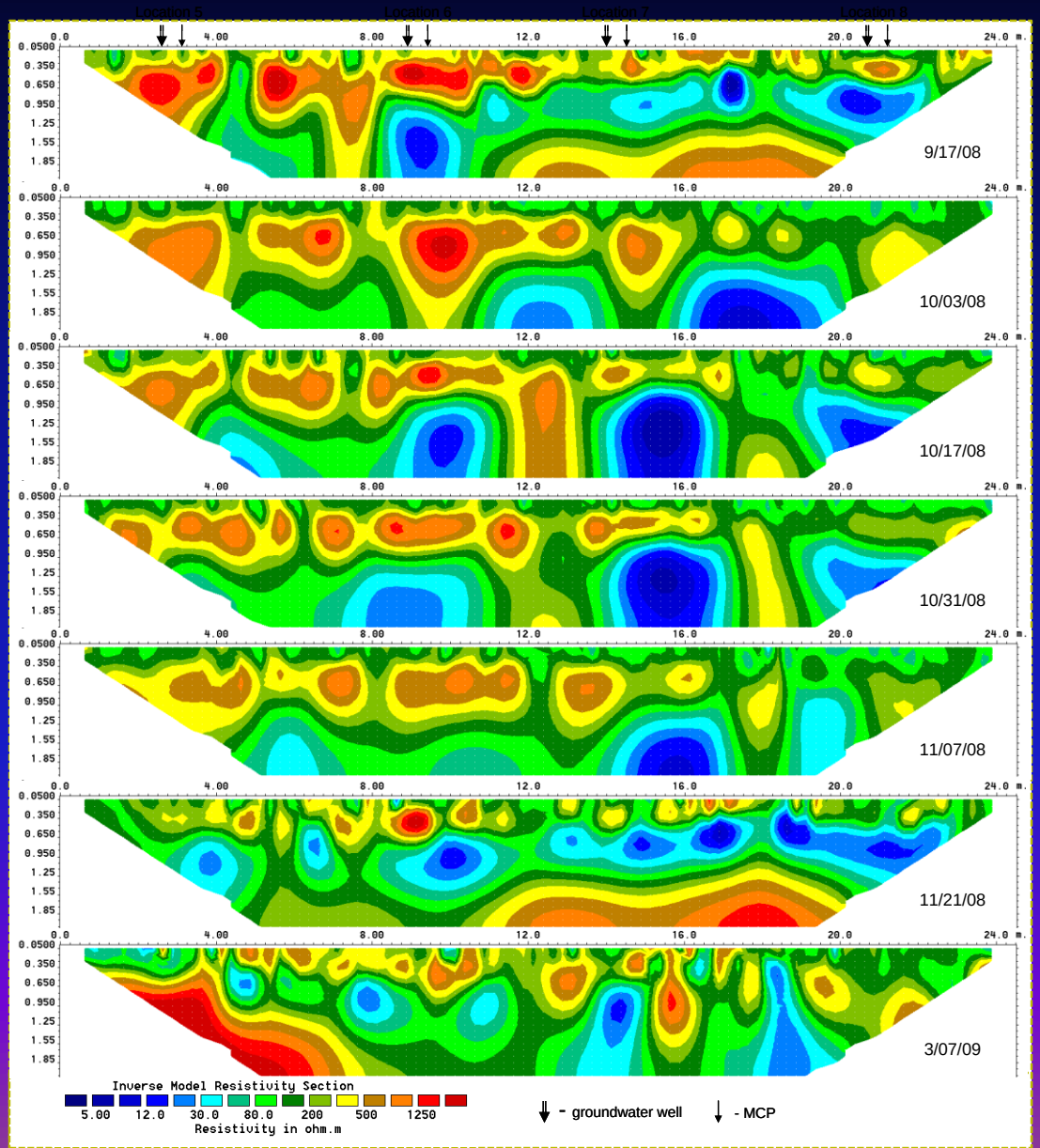
Laboratory water retention - 95% tolerance interval

PTF ensemble-estimated water retention – 95% tolerance interval

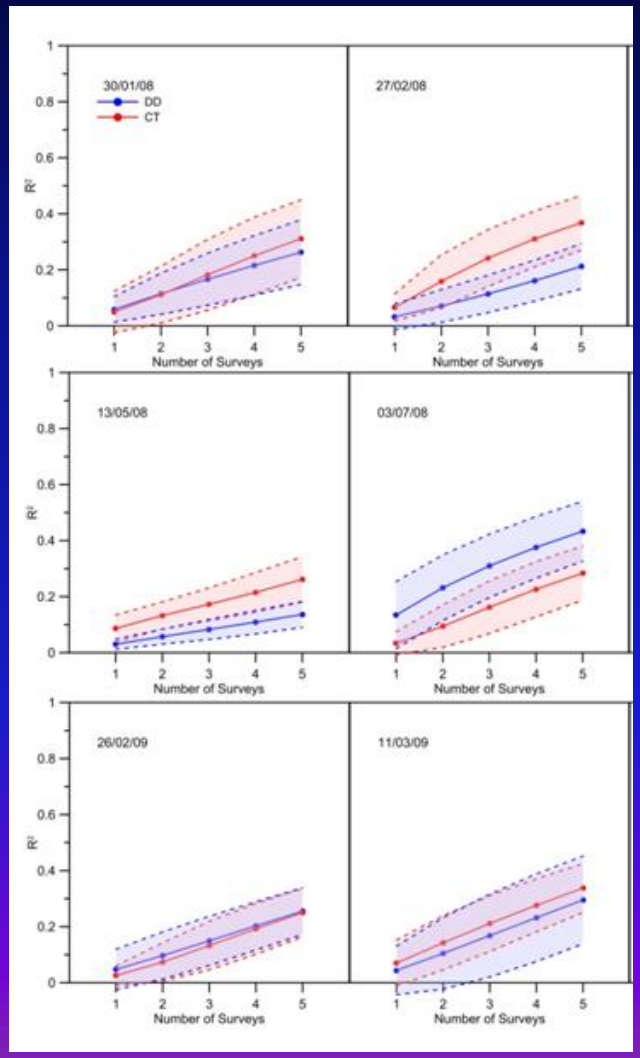
MA of parameter determination with discretization

Time-lapse or multiple surveys

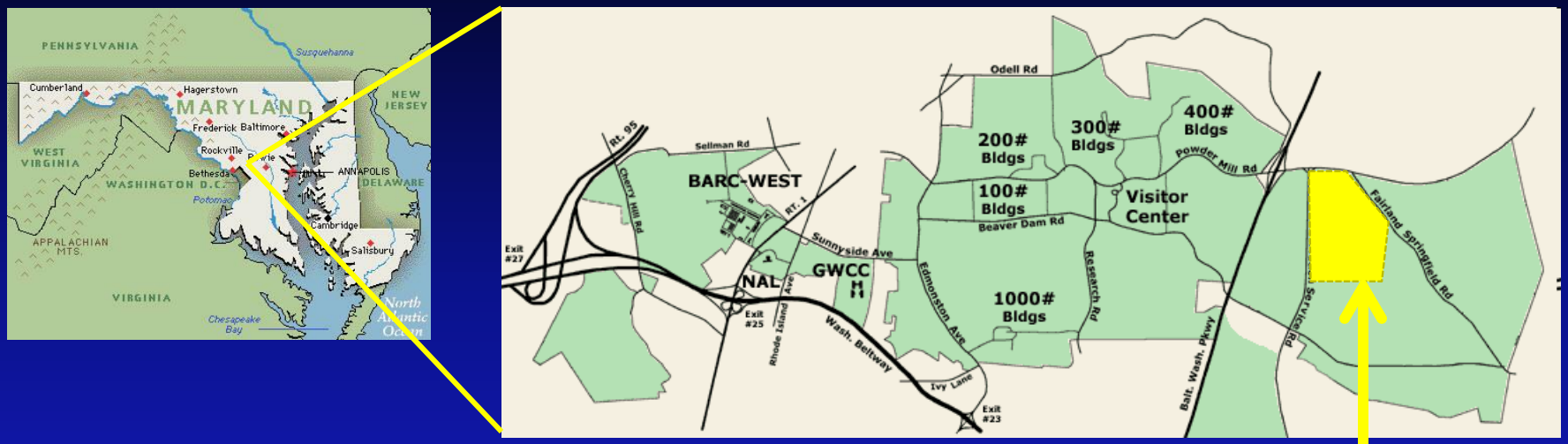
OPE3 ER Tomography (Beltsville, MD)



EC as soil water contents predictor (Sevilla, Spain)



MA case studies at the USDA-ARS Beltsville OPE3 site



- Centennial anniversary in 2010
- 11 miles to the White House
- 7000 acres
- 800 employees
- 4 Institutes (plant sciences, animal and natural resources, human nutrition, U. S. National arboretum)

The OPE3 site

Densely instrumented to:

- ✓ **Determine fluxes of water, nutrients, and ag-chemicals from crop production systems.**
- ✓ **Determine behavior and impact of water, nutrients, and agricultural chemicals on a wooded, riparian wetland and first-order stream.**
- ✓ **Develop remotely sensed data products and techniques for measuring and managing spatial variability of crops and soils.**
- ✓ **Determine long-term economic and environmental impacts of 3 crop production systems and evaluate their tradeoffs.**

USDA-ARS MA case studies

1. Water flow in variably saturated soils.
   Abstraction provided the explanation for inexplicable results obtained with the complex model. The conceptual model had to be corrected. NUREG 6884.

2. Solute flux measurements in soils.
   Abstraction proved that the fast tracer appearance in sampling wells could not be considered as the evidence of the preferential flow in soils. The abstracted model provided the alternative plausible conceptual model. NUREG 7026.

3. Tracer transport in variable saturated soils.
   The 3D->2D abstraction process showed that the assumption of part of the soil not significantly participating in the solute transport process created a better representation of the solute breakthrough curves. The 2D->1D abstraction step suggested the location of preferential flow pathways. NUREG 7026.

4. Search for groundwater monitoring locations to decrease prediction uncertainty and provide discrimination between conceptual models.
   The pedotransfer abstraction appeared to be efficient in sensitivity and uncertainty estimation. NUREG (in preparation).

Implications of the multiplicity of models for software design and implementation: a user view

- The advent of multimodeling and model abstraction presents both challenges and opportunities for software system design and implementation for environmental modeling.
- Need to have the same domain and the same discretization.
- Need to handle nonlinearities and coexistence of different types of equations.
- Need to incorporate hydrogeophysical data.
- Need to handle soft and expert data.
- Analysis of the modeling context for model abstraction with database-supported model population.
- Ensemble modeling and multimodeling.
- Options for data assimilation.
- Additional flexibility is required that may be well compensated by the improved insights into systems behavior and predictions reliability.

Conclusions

- Model abstraction is a fast developing modeling methodology which has recently established itself in contaminant hydrology.

- Studies demonstrated the usefulness of model abstraction in simulations of flow and transport in a 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 allows for the explicit treatment of structural (conceptual) uncertainties in modeling.

- Diagnostics, monitoring and modeling of contaminant transport are all based on conceptual models. Developments in model abstraction support progress in all these types of activitites.