Quantifying Vadose Zone Flow and Transport Uncertainties using a Unified, Hierarchical Approach

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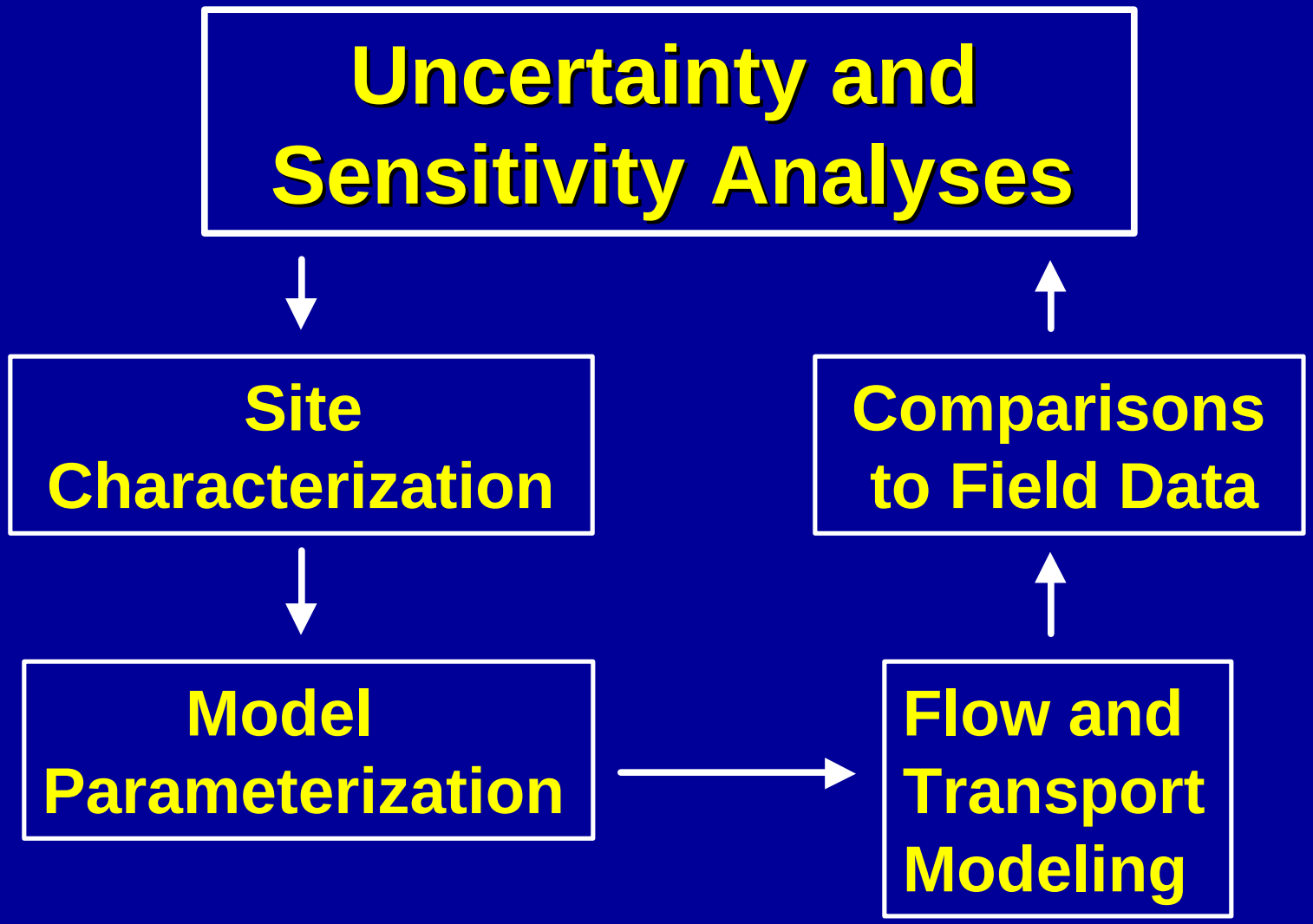

Uncertainty and Sensitivity Analyses
Site Characterization
Model Parameterization
Flow and Transport Modeling
Comparisons to Field Data

Key Question:

What are the appropriate measurement and modeling scales, and methods required to accurately represent flow and transport processes in heterogeneous, unsaturated porous media like these? →

Objectives

- Develop improved methods (*software tools*) for parameterizing water flow and solute transport models for field-scale applications in heterogeneous, variably saturated porous media

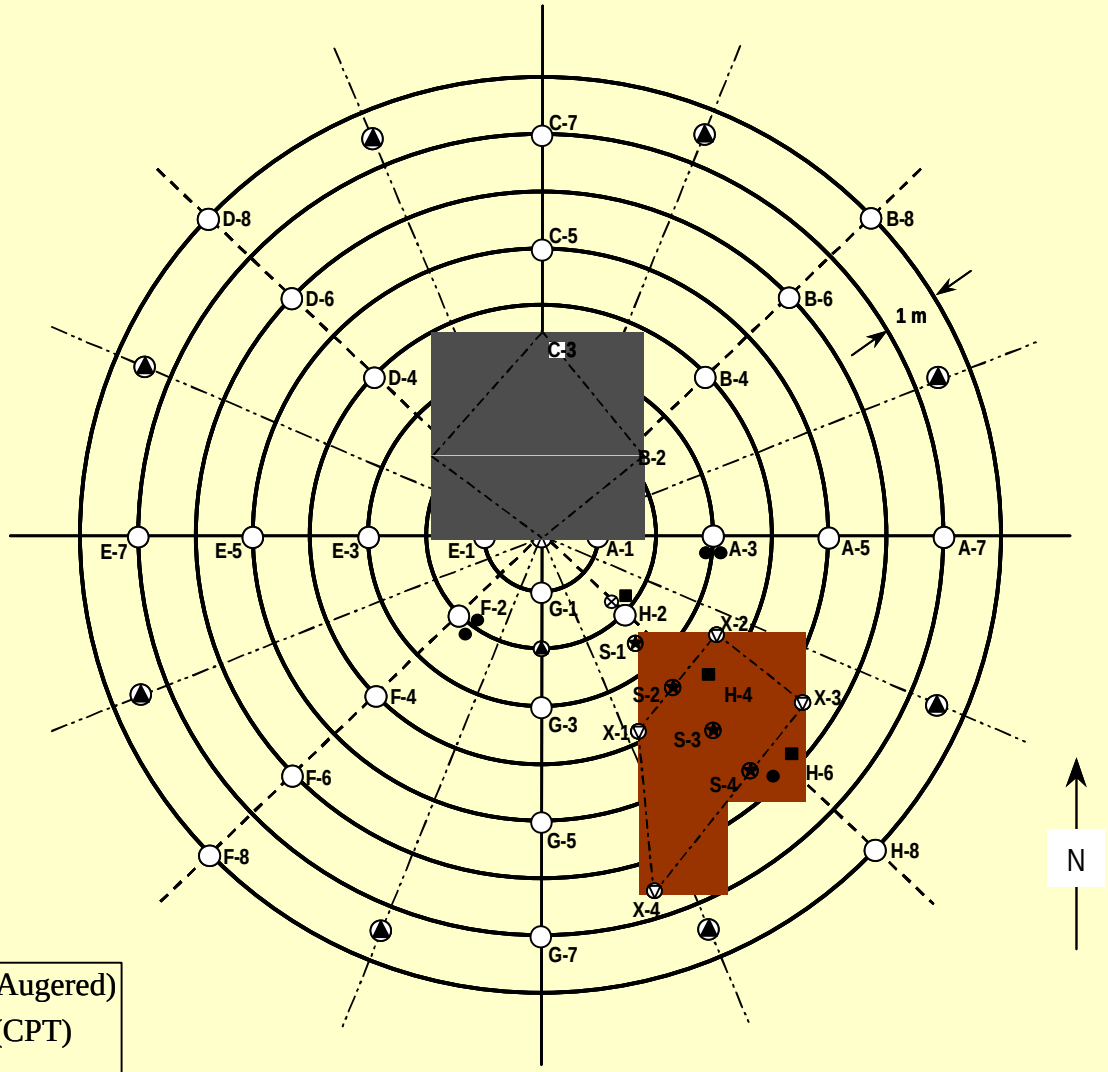
- Evaluate predictive accuracy and uncertainty associated with using different data types for model parameterization (hard and soft data), by comparing model simulations with observed data from well-controlled field experiments

Outline

- Field Experiment
- Parameterization Method
- Observed and Simulated Results

Field Experiment

- Conducted in inter-bedded sands and silts at the Hanford Site in SE Washington state in June-July 2000
- 5 weekly subsurface injections of ~4000 L of water, each applied over a period of 4 – 7 hr at depth of 4.3 m
- Bromide and other tracers added in third injection
- Water plumes monitored to depth of 18 m using neutron probe in 32 access tubes



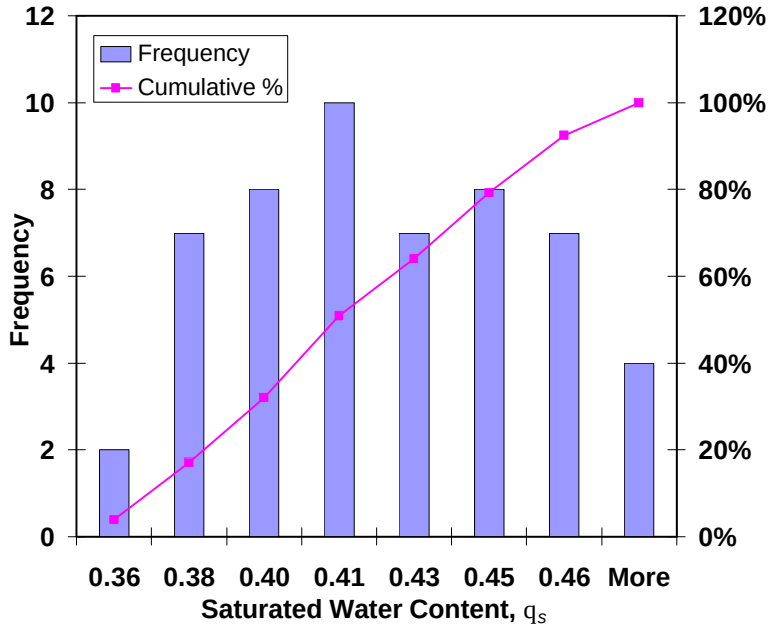
Legend

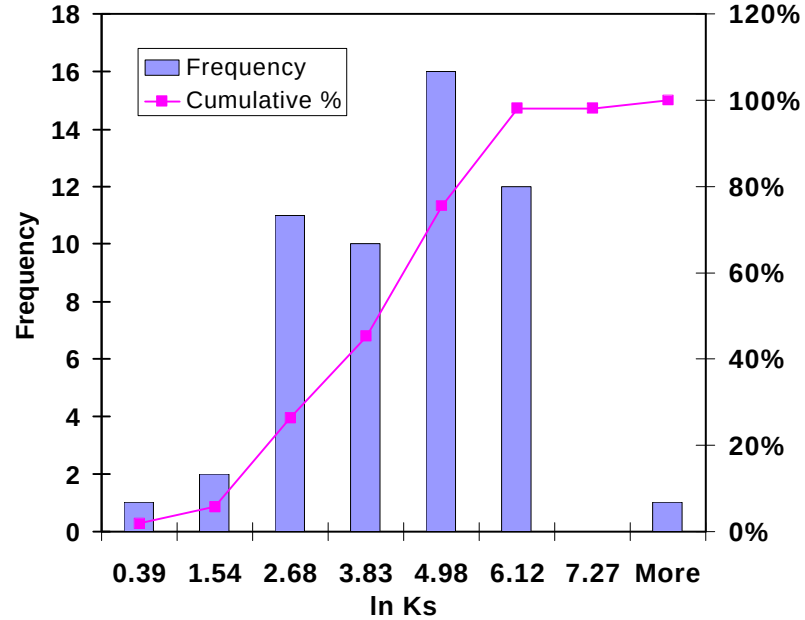
- ■ Adv.Tensiometer Nest (Augered)
- ● Adv. Tensiometer Nest (CPT)
- ▽ Cross-Borehole Access
- ▲ ERT Array
- ⊗ New Injection Point
- ◆ Subsurface Radiation Zone
- ⊛ Split-spoon Cores
- ○ Steel-cased Well

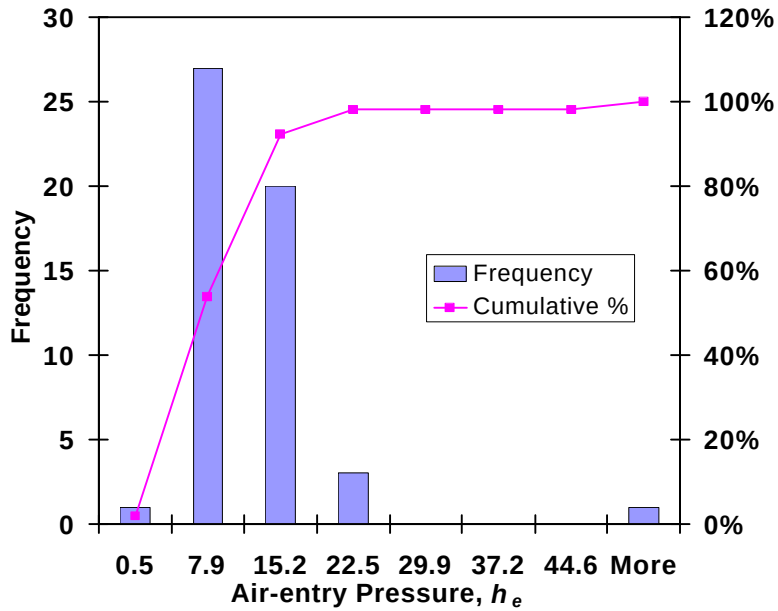
Experimental Site

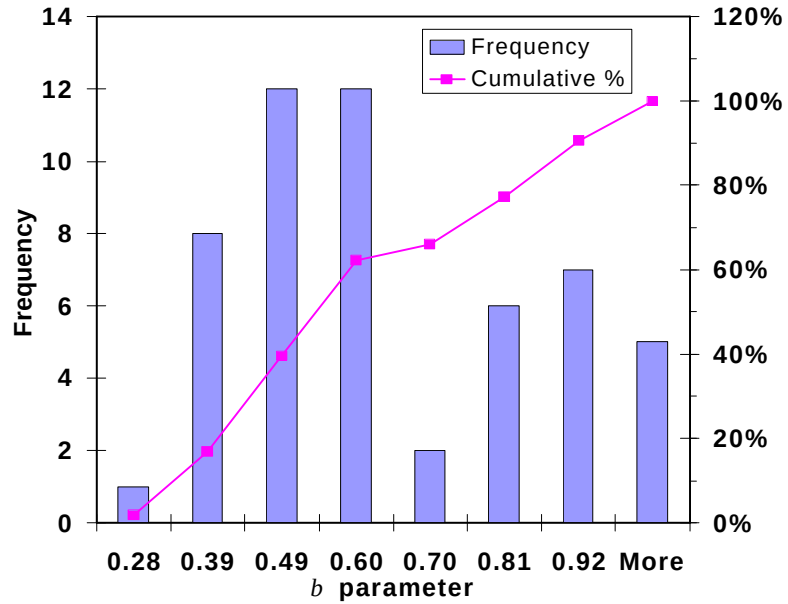
http://vadose.pnl.gov

UP


Frequency
Cumulative %
Frequency
0
2
4
6
8
10
12
0%
20%
40%
60%
80%
100%
120%
0.36
0.38
0.40
0.41
0.43
0.45
0.46
More
Saturated Water Content, q_s


Frequency
Cumulative %
Frequency
0
2
4
6
8
10
12
14
16
18
0%
20%
40%
60%
80%
100%
120%
0.39
1.54
2.68
3.83
4.98
6.12
7.27
More
ln Ks


Frequency
Cumulative %
Frequency
0
5
10
15
20
25
30
0%
20%
40%
60%
80%
100%
120%
0.5
7.9
15.2
22.5
29.9
37.2
44.6
More
Air-entry Pressure, h_e


Frequency
Cumulative %
Frequency
0
2
4
6
8
10
12
14
0%
20%
40%
60%
80%
100%
120%
0.28
0.39
0.49
0.60
0.70
0.81
0.92
More
b parameter

Parameterization Method

Step 1. Estimate scale-mean hydraulic parameters

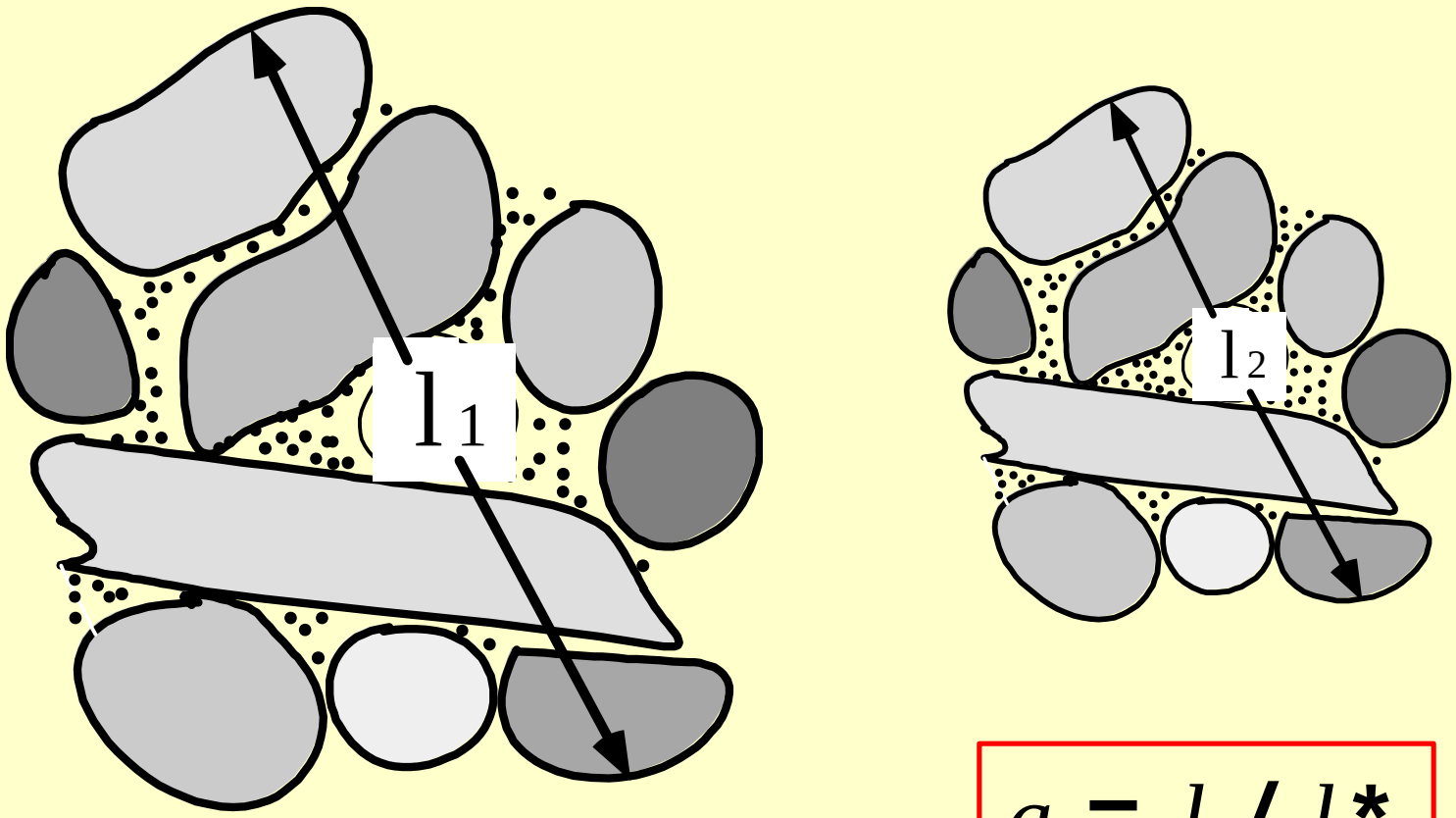
Step 2. Geostatistical analyses and conditional simulation of field-measured water content and porosity distributions on a *fine* grid

Step 3. Infer scaling factors and hydraulic parameters at fine grid scale from the saturation distribution and scale-mean parameters

Step 4. Generate upscaled, effective model parameters for a *coarse* numerical model grid

Similar Media Scaling

(adapted from Miller & Miller, 1956, *J. Appl. Phys*.)



$$a = l / l^*$$

Step 1. Estimate scale-mean parameters

Miller & Miller

- $h^*(q) = a\, h(q)$
- $K^*(q) = K(q) / a^2$

Generalized

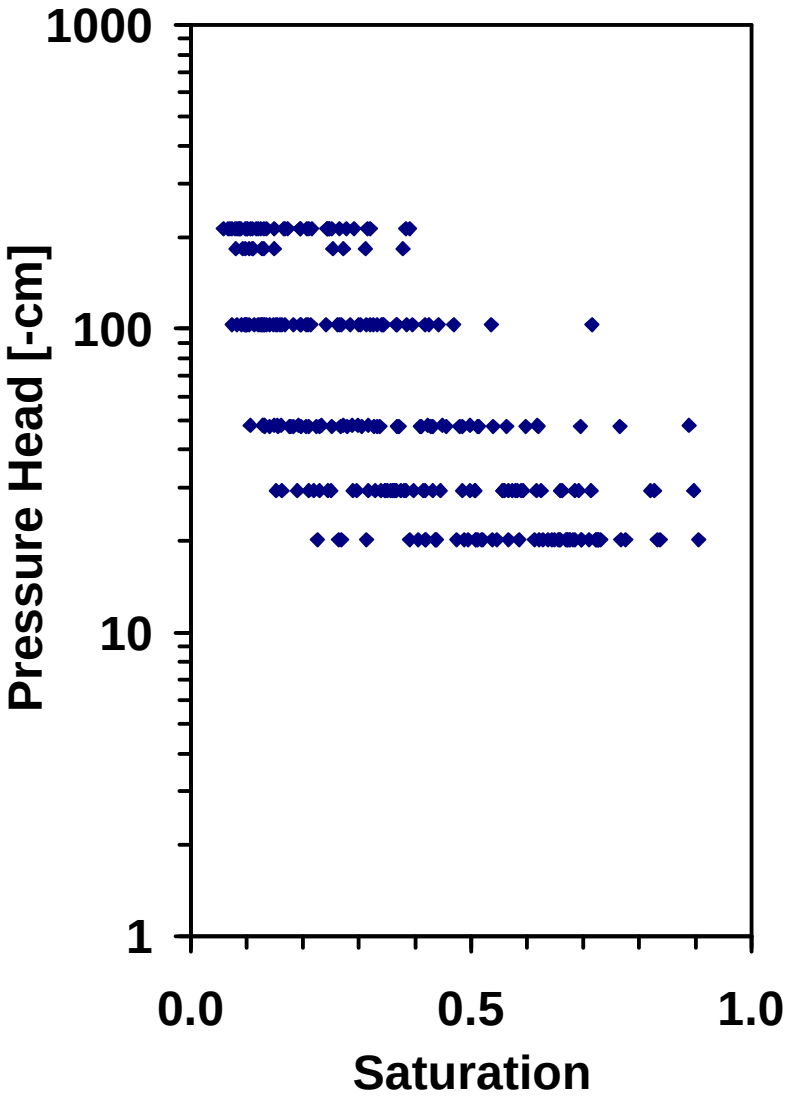
- $h^*(S) = a_h\, h(S)$
- $K^*(S) = K(S) / a_k^2$
- $a_k = f(a_h)$

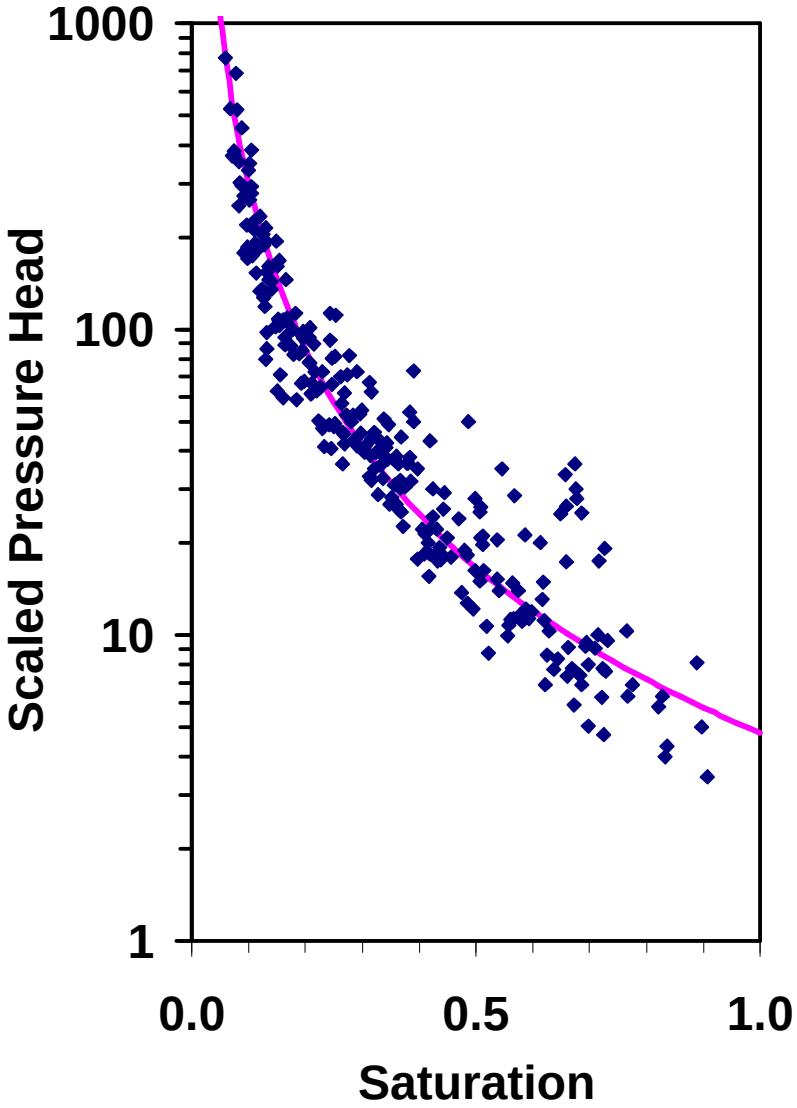
Scale-mean parameters

$$h^*(S) = n\left[\sum_{i=1}^{n} \frac{1}{h_i(S)}\right]^{-1}$$

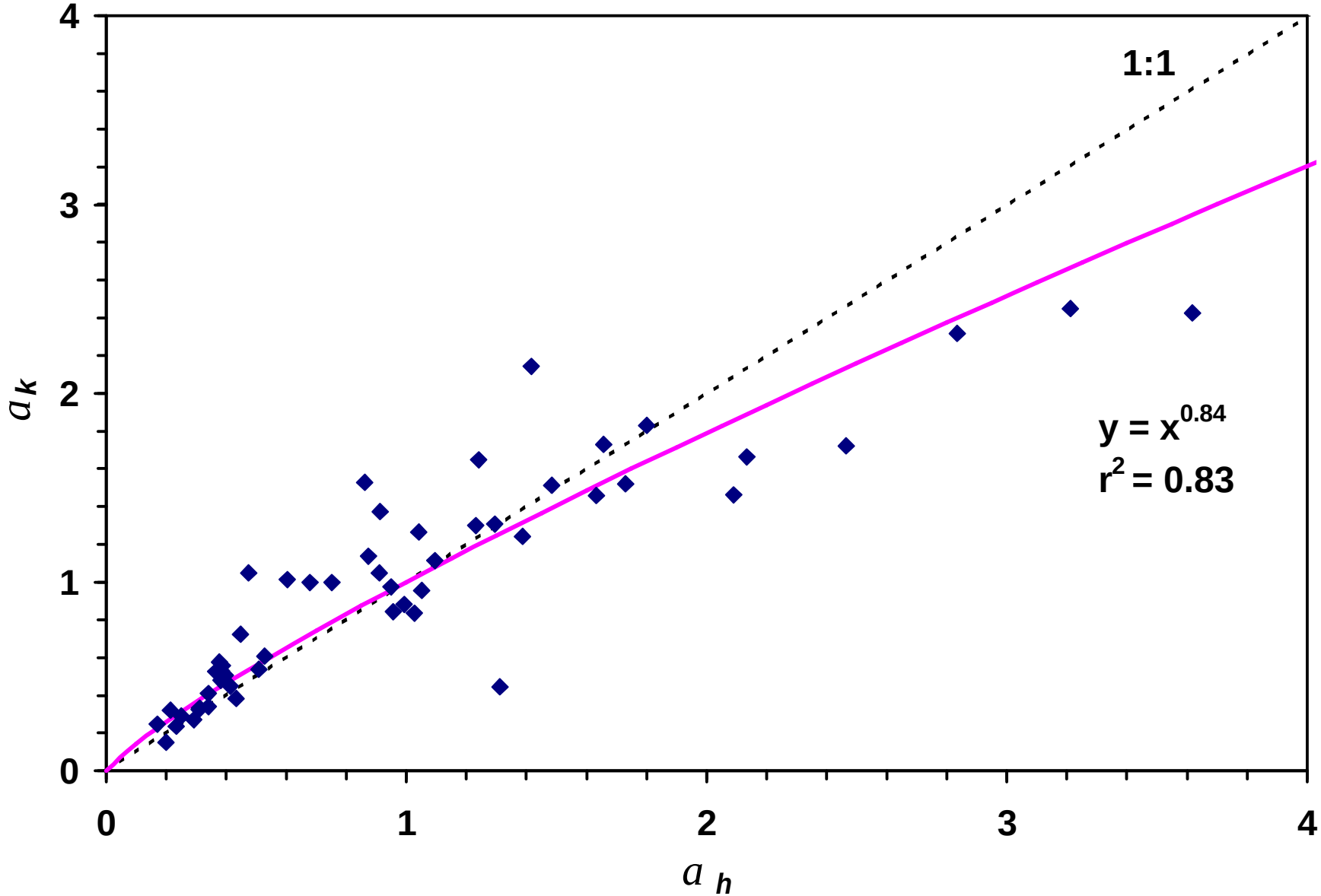
$$K^*(S) = \left\{\frac{1}{n}\sum_{i=1}^{n}\left[K_i(S)^{1/2}\right]\right\}^2$$

Unscaled and scaled pressure-saturation data



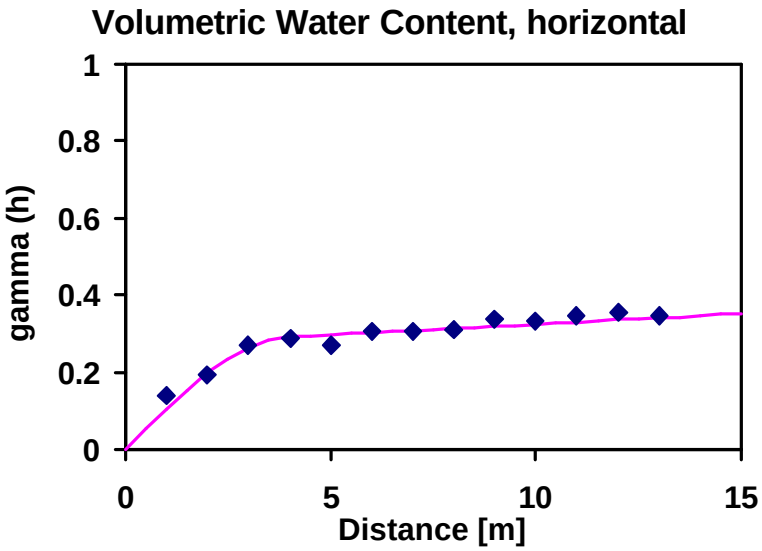


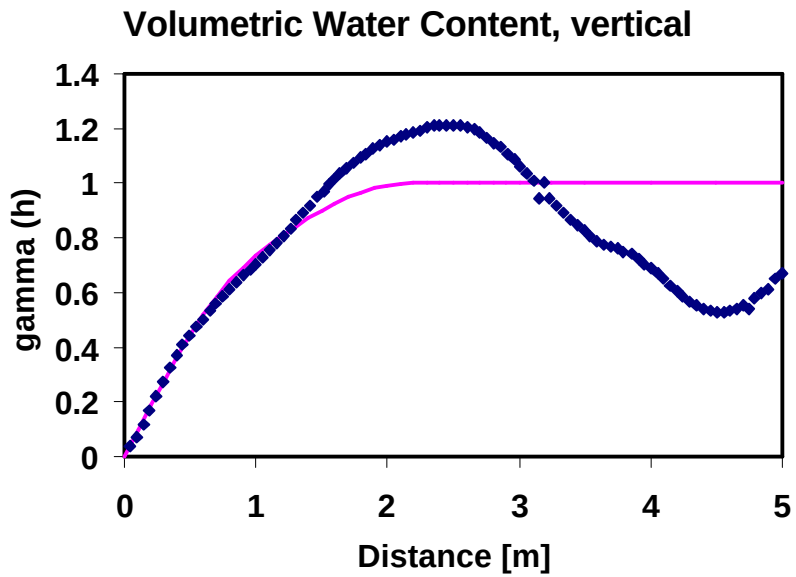
Relationship between a_h and a_k scaling factors

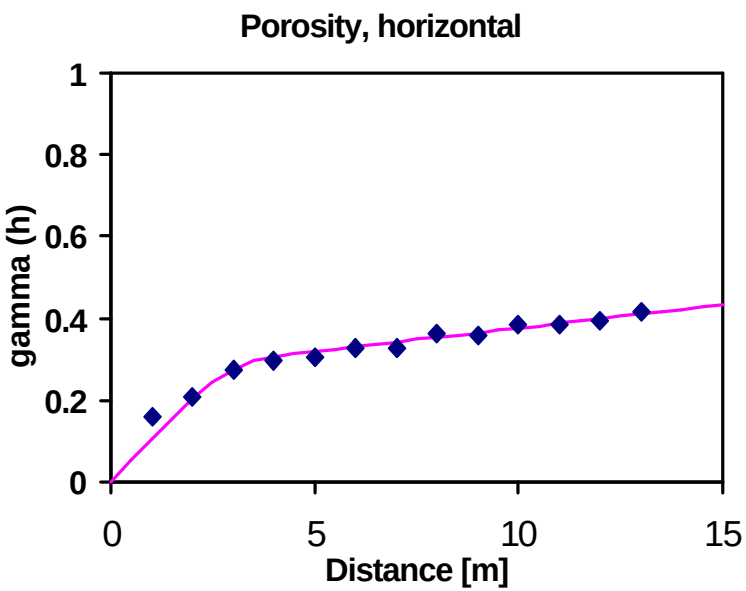


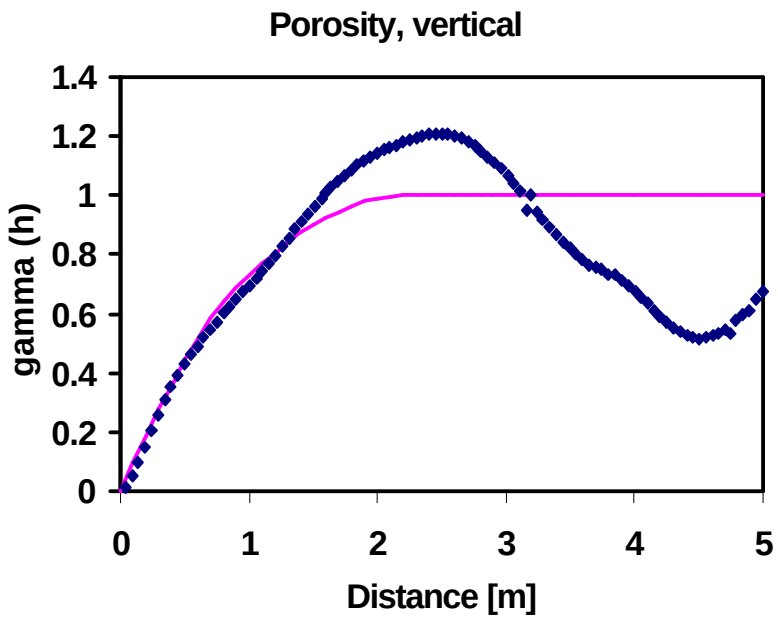
Step 2. Geostatistics and Conditional Simulation

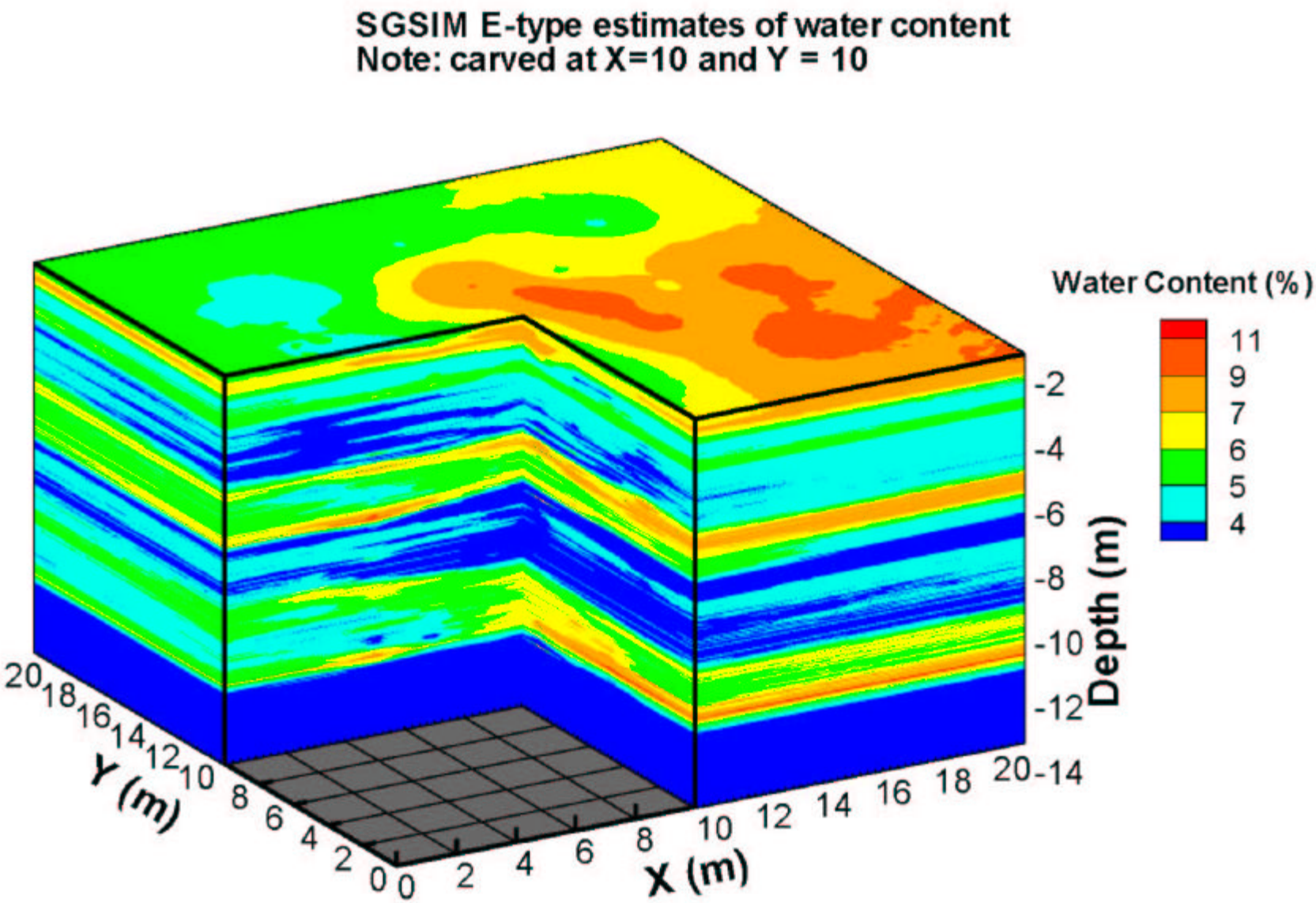
- Spherical variogram models with 2 nested structures were fit to field-measured water content and porosity data
- 30 realizations generated on 3.4 million node grid for a 20 m x 20 m x 12 m domain using SGSIM (conditioned on measured values)
- E-type (expected value) estimates used for parameterization on 22,000 node model grid


Volumetric Water Content, horizontal
gamma (h)
Distance [m]
0
0.2
0.4
0.6
0.8
1
0
5
10
15

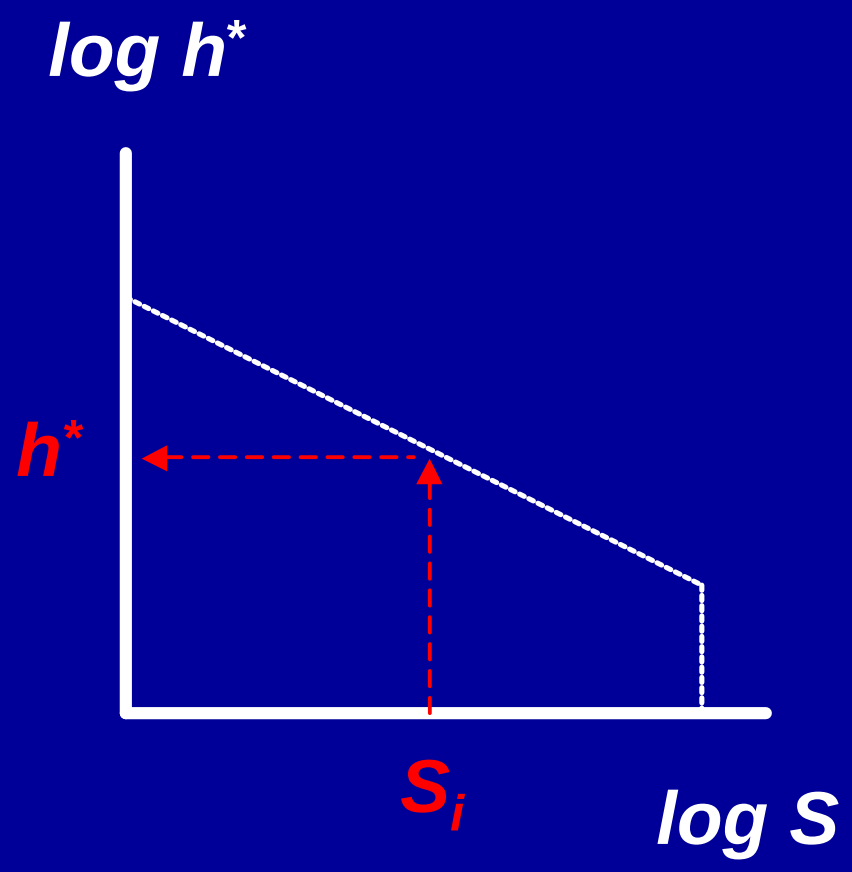

Volumetric Water Content, vertical
gamma (h)
Distance [m]
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
1
2
3
4
5


Porosity, horizontal
gamma (h)
Distance [m]
0
0.2
0.4
0.6
0.8
1
0
5
10
15


Porosity, vertical
gamma (h)
Distance [m]
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
1
2
3
4
5


SGSIM E-type estimates of water content
Note: carved at X=10 and Y = 10
Water Content (%)
11
9
7
6
5
4
Depth (m)
-2
-4
-6
-8
-10
-12
-14
Y (m)
20 18 16 14 12 10 8 6 4 2 0
X (m)
0 2 4 6 8 10 12 14 16 18 20

Step 3. Estimate scaling factors and hydraulic parameters



$$a_h = h^* / h_{avg}(z)$$

$$a_k = f(a_h)$$

$$h_e = h_e^* / a_h$$

$$K_s = K_s^* \, a_k^2$$

Step 4. Upscaling

- Volume averaging (initial water content and porosity) and
- Upscaling of hydraulic parameters with volume-averaged initial water contents and porosities, and weighted arithmetic and harmonic averaging of the fine grid block *K* values or
- Solve $\tilde{\mathrm{N}} \cdot K(\tilde{\mathrm{N}} H) = 0$ for each coarse grid block with the discretization and parameters for the fine grid blocks contained within each coarse grid block

Simple method

$$q_i^c = \sum_{j=1}^{n} q_j^f v_j^f \Big/ \sum_{j=1}^{n} v_j^f$$

$$\overline{K}_{sx} = \sum_{k=1}^{nz}\left[\sum_{j=1}^{ny}\left\{\left(dy_j dz_k\right)\left(\sum_{i=1}^{nx} dx_i \Big/ \sum_{i=1}^{nx}\frac{dx_i}{K_{ijk}}\right)\right\}\Big/\sum_{j=1}^{ny} dy_j dz_k\right]$$

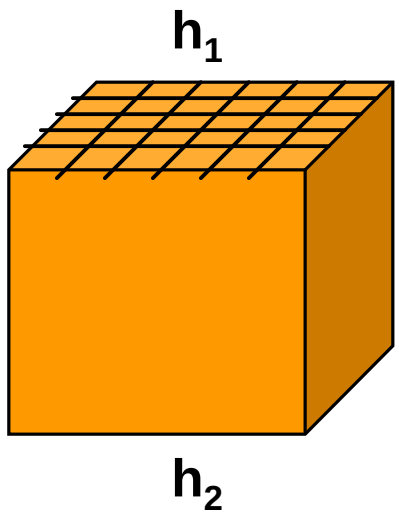
$$\overline{K}_{sy} = \sum_{k=1}^{nz}\left[\sum_{i=1}^{nx}\left\{\left(dx_i dz_k\right)\left(\sum_{j=1}^{ny} dy_j \Big/ \sum_{j=1}^{ny}\frac{dy_j}{K_{ijk}}\right)\right\}\Big/\sum_{i=1}^{nx} dx_i dz_k\right]$$

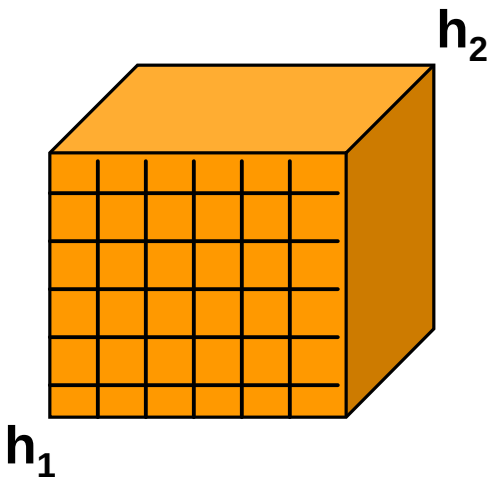
$$\overline{K}_{sz} = \sum_{i=1}^{nx}\left[\sum_{j=1}^{ny}\left\{\left(dx_i dy_j\right)\left(\sum_{k=1}^{nz} dz_k \Big/ \sum_{k=1}^{nz}\frac{dz_k}{K_{ijk}}\right)\right\}\Big/\sum_{j=1}^{ny} dx_i dy_j\right]$$

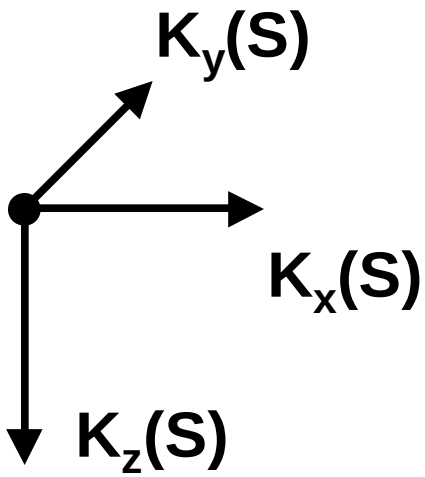
Doesn't account for <u>connectivity</u> of least-resistant flow paths !!

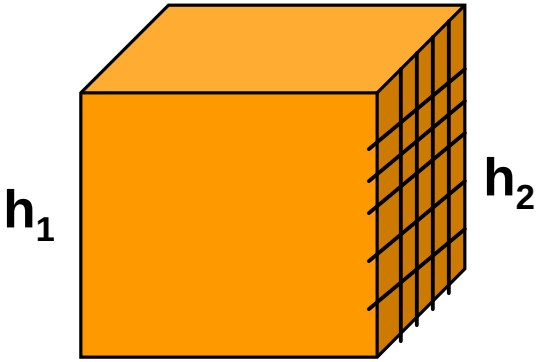
Rigorous method

$$\tilde{\nabla} \cdot K(\tilde{\nabla} H) = 0$$

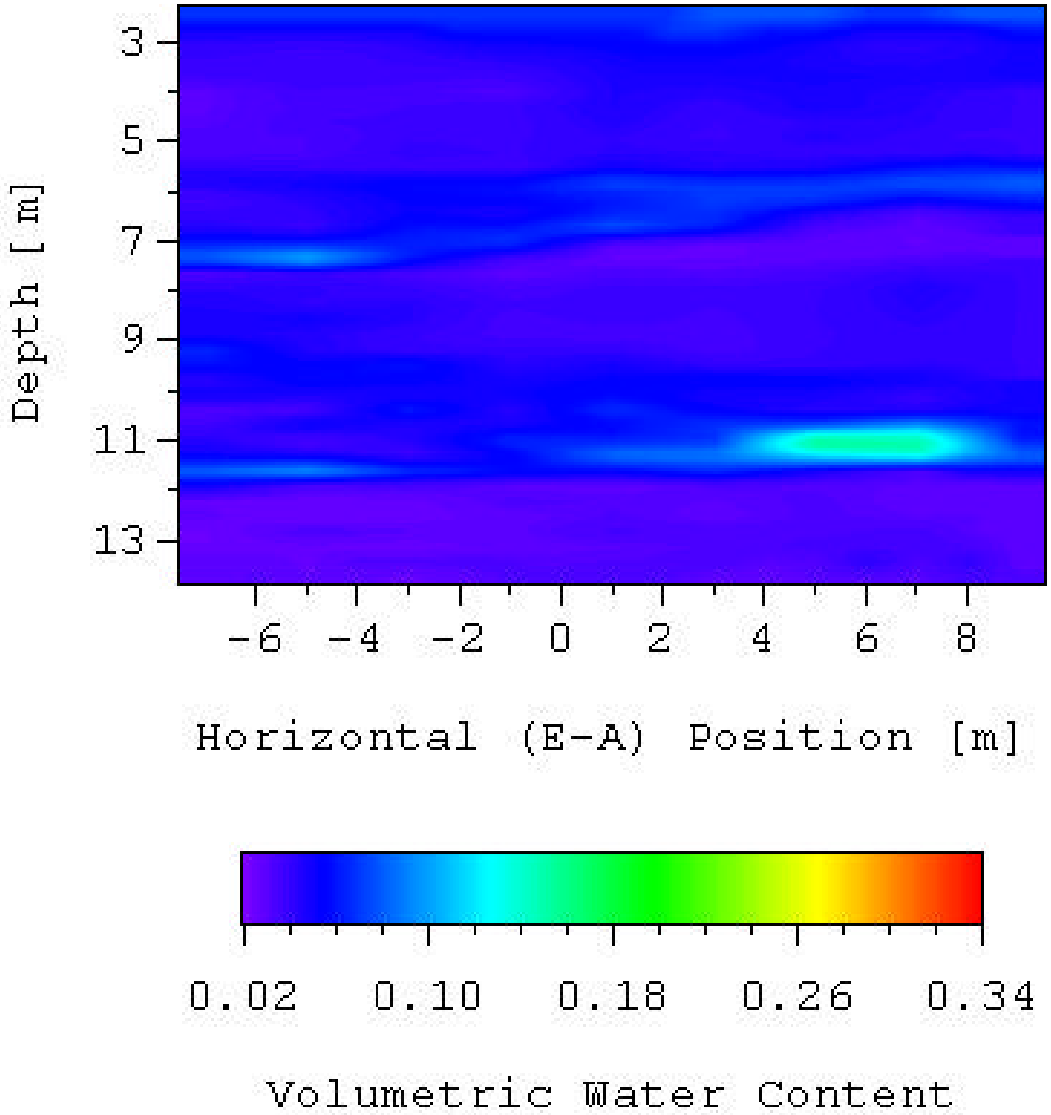




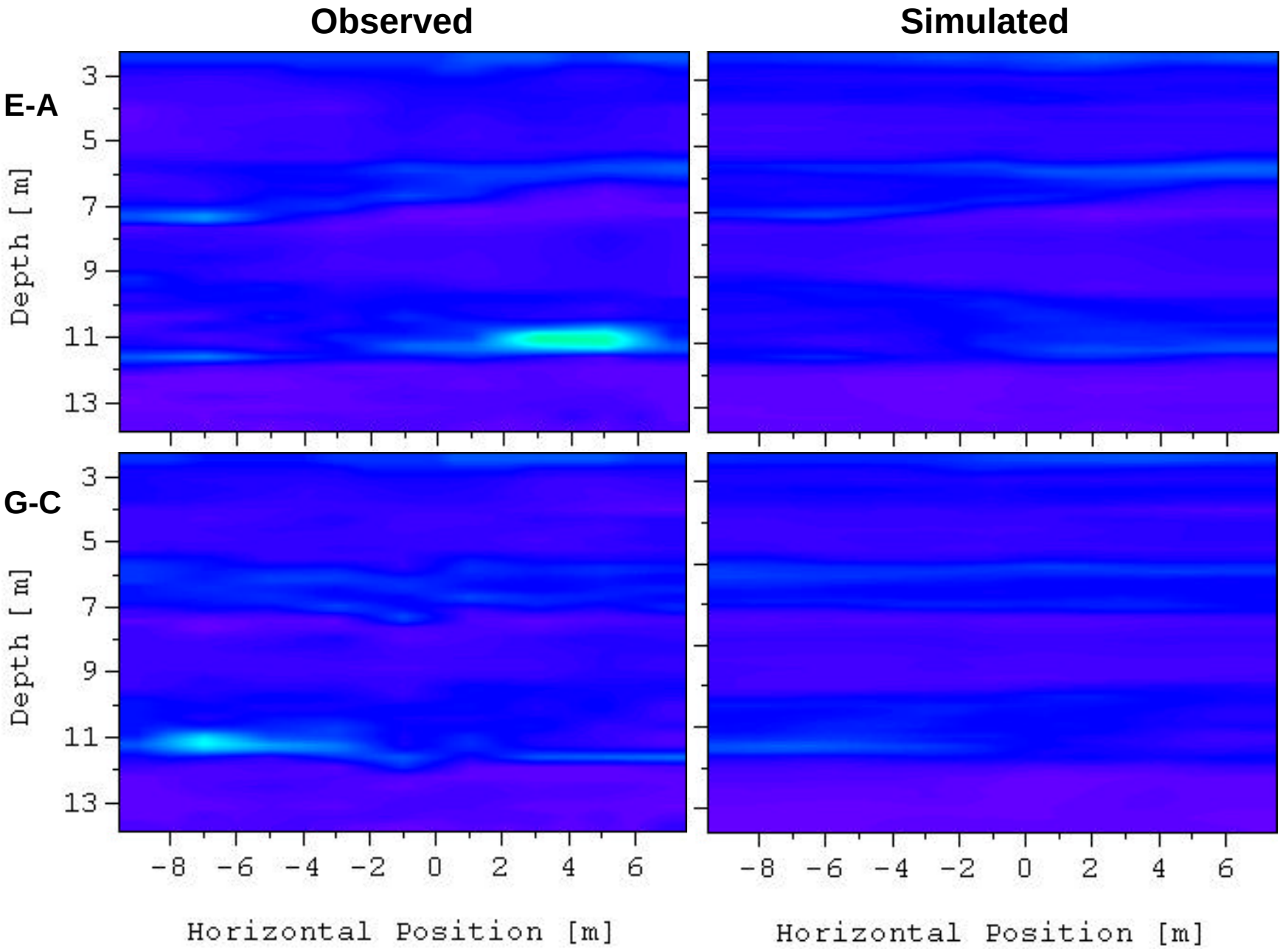




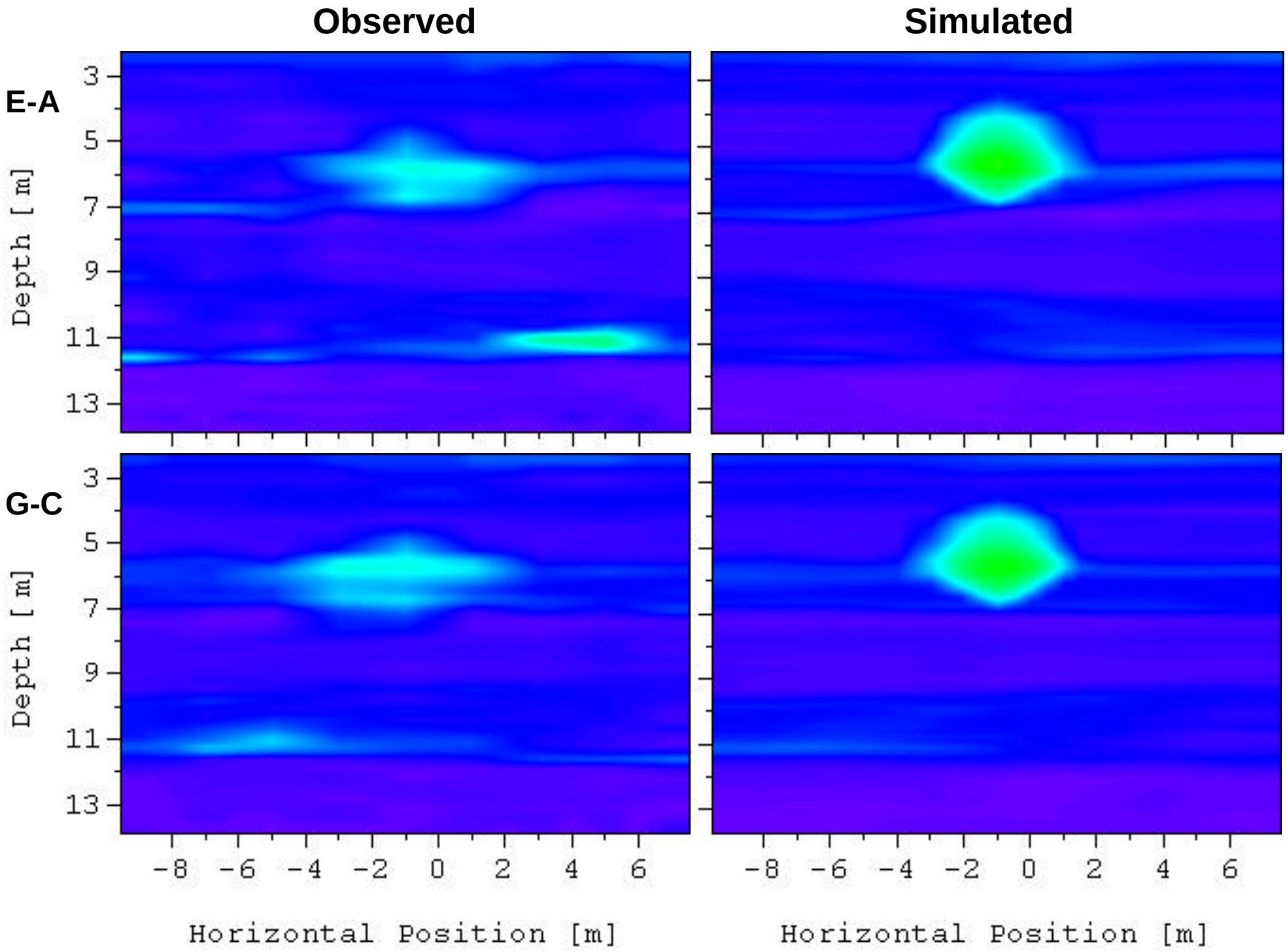
Water Content Distributions



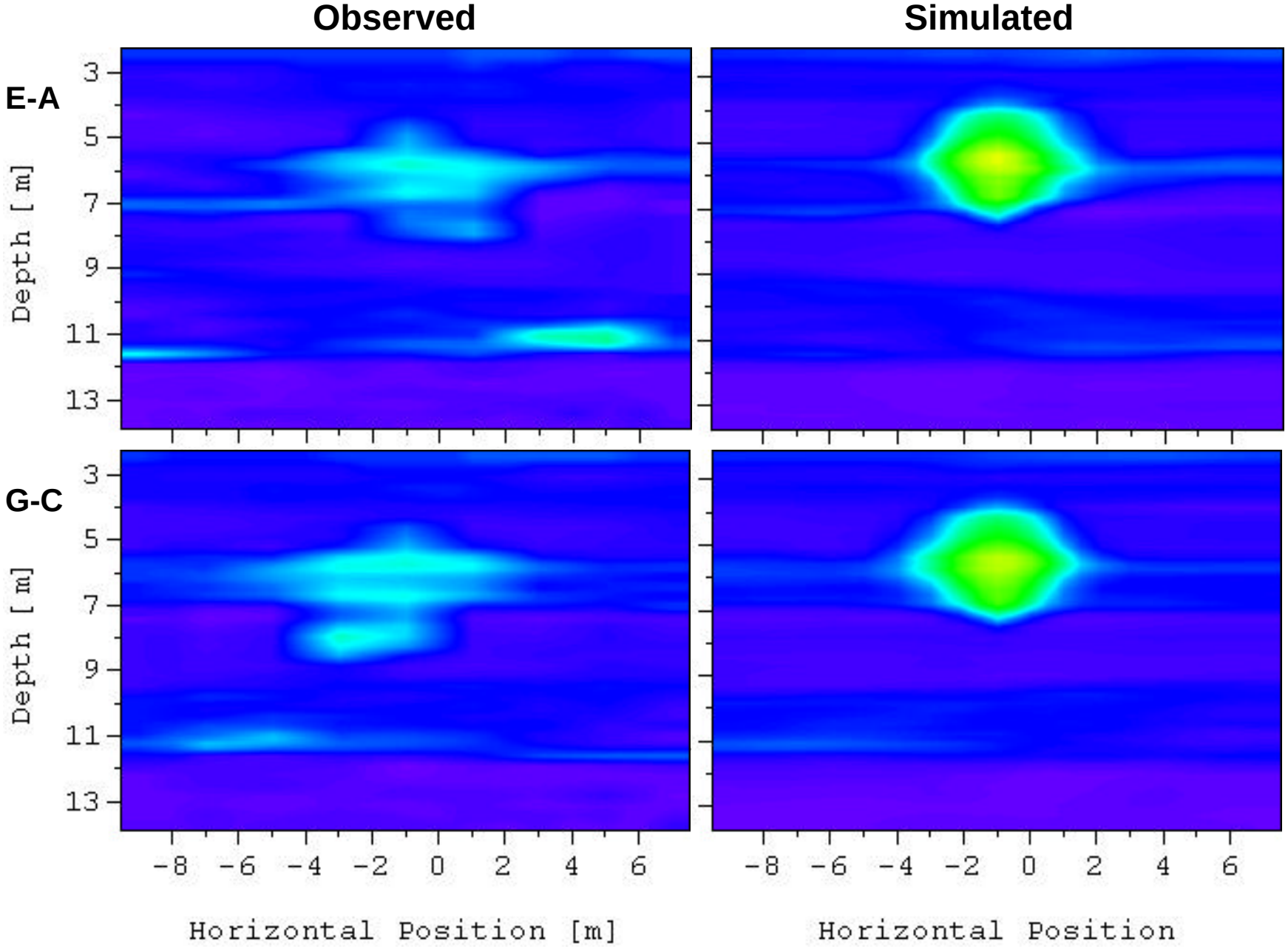
Initial water content distributions, May 5, 2000



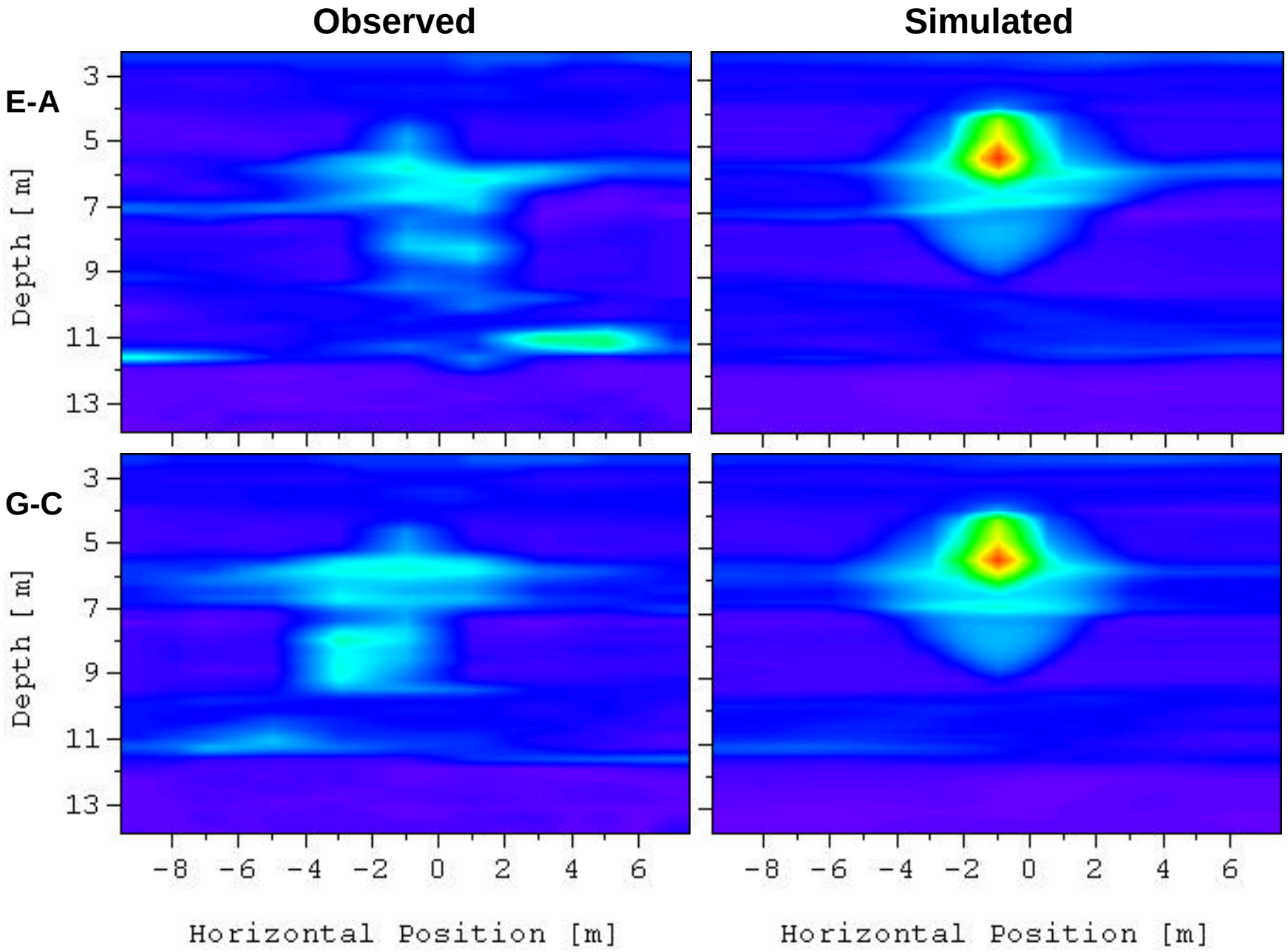
Water contents 1 day after 1st injection, June 2, 2000



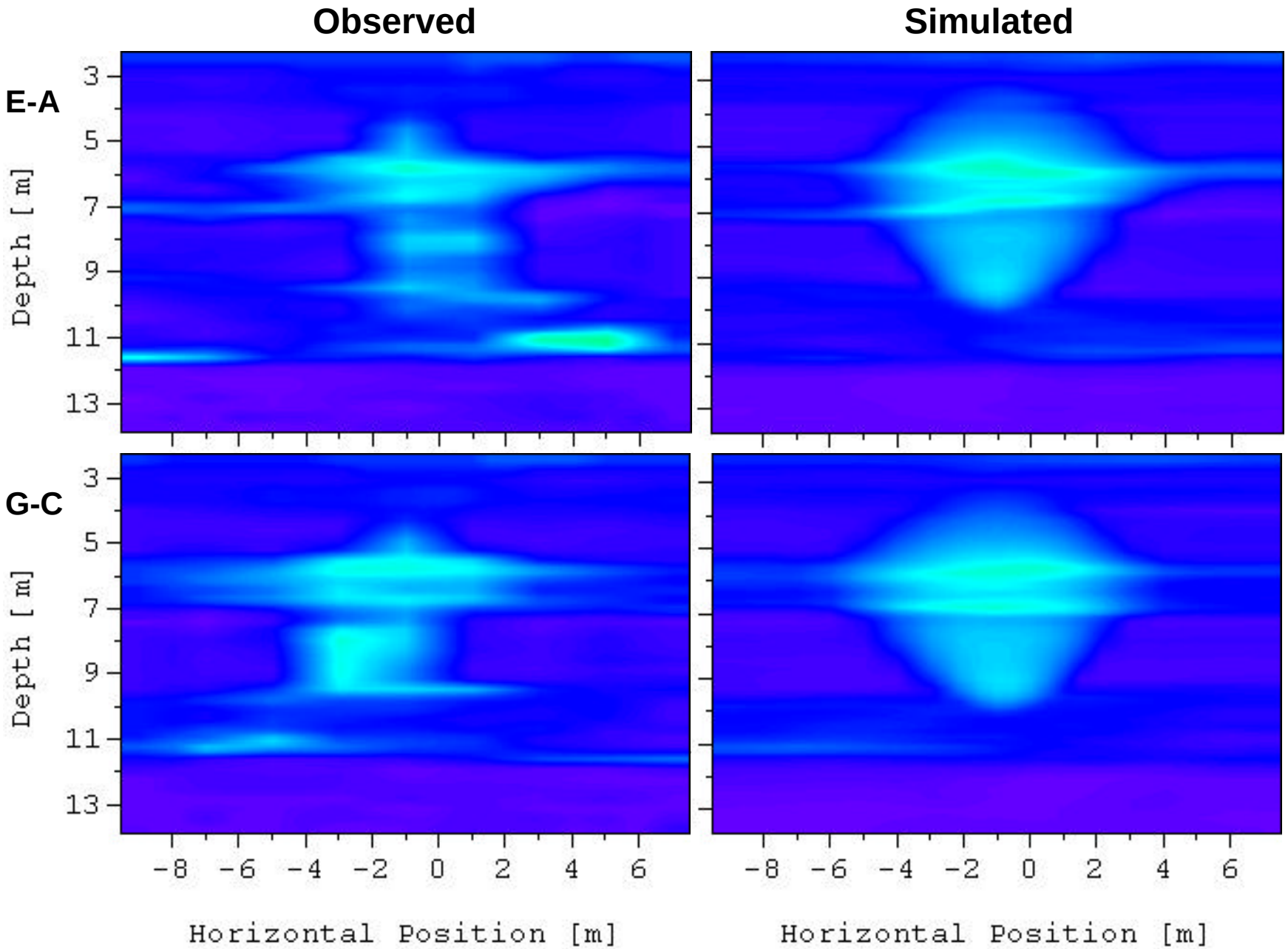
Water contents 1 day after 2nd injection, June 9, 2000



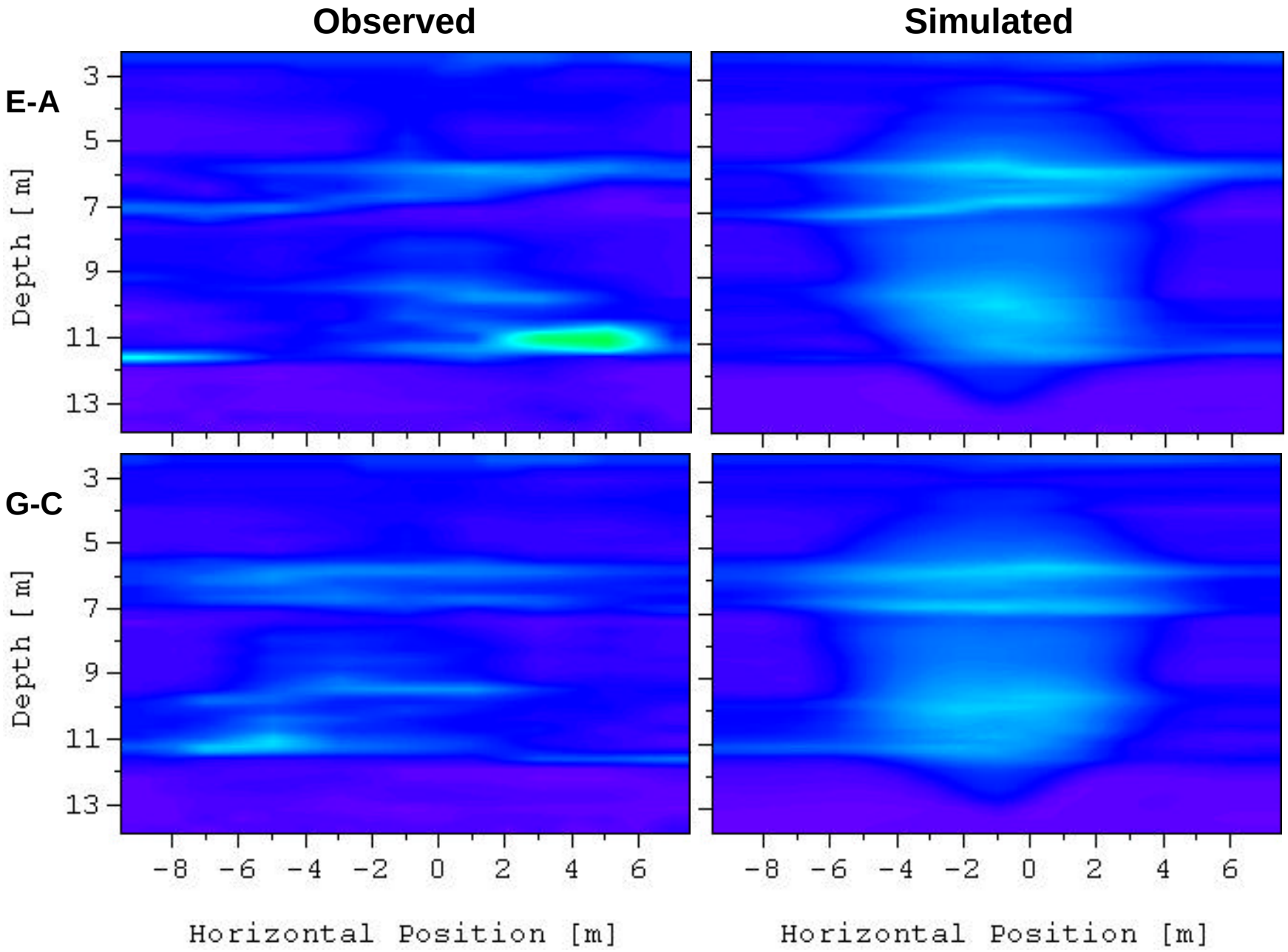
Water contents 1 day after 3rd injection, June 16, 2000



Water contents 1 day after 4th injection, June 23, 2000



Water contents 33 days after 5th injection, July 31, 2000



Preliminary Conclusions

- Both hard and soft data are needed for accurate parameterization of vadose zone flow and transport models for field-scale applications in highly heterogeneous sediments
- Parameterization methods and modeling framework described here look promising

Ongoing Work

- Implementation and testing of rigorous, saturation-dependent, K tensor upscaling scheme
- Development and evaluation of site-specific pedo-transfer functions
- Uncertainty and sensitivity analyses

Acknowledgments

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  - U.S. Salinity Laboratory, Riverside, CA
- Yi-Ju Chien, Mark White, Andy Ward, and Glendon Gee
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- U.S. Dept. of Energy, Environmental Management Science Program (DOE - EMSP)