Prototype Hanford Barrier Modeling with the STOMP Sparse Vegetation Evapotranspiration Model

Andy Ward

Pacific Northwest National Laboratory, Richland, WA

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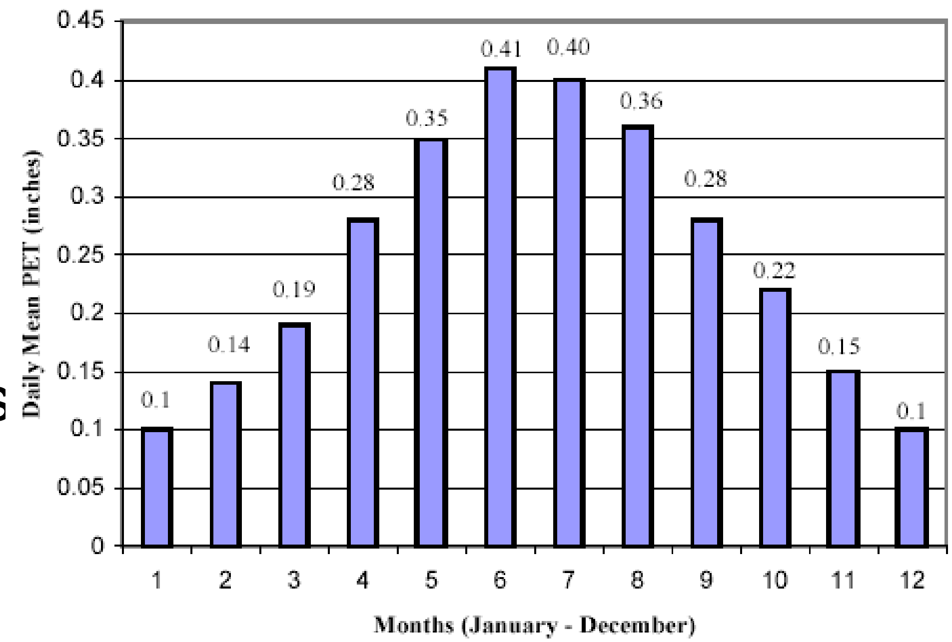
Engineered Barrier Problem

- Multidimensional
  - Raised sloped surface
  - Anisotropic
- Multiphase
  - Water, air, energy
- Spatial variability
  - Hydraulic properties
  - Thermal properties
- Temporal variability
  - Physical properties
  - Hydraulic properties
  - Ground cover
  - Vegetative properties
- Sparse canopies typical of arid environments
  - Species composition
  - Vegetative properties

Current Models

- Mostly 1D or 2D
- Isothermal
- Coupling
  - Semi-empirical climate
  - Mass and energy not coupled
- Ill-suited to sparse canopies
  - Priestly-Taylor
    - non-limiting H_2O
    - Low wind speeds
  - Penman-Monteith
    - full canopy

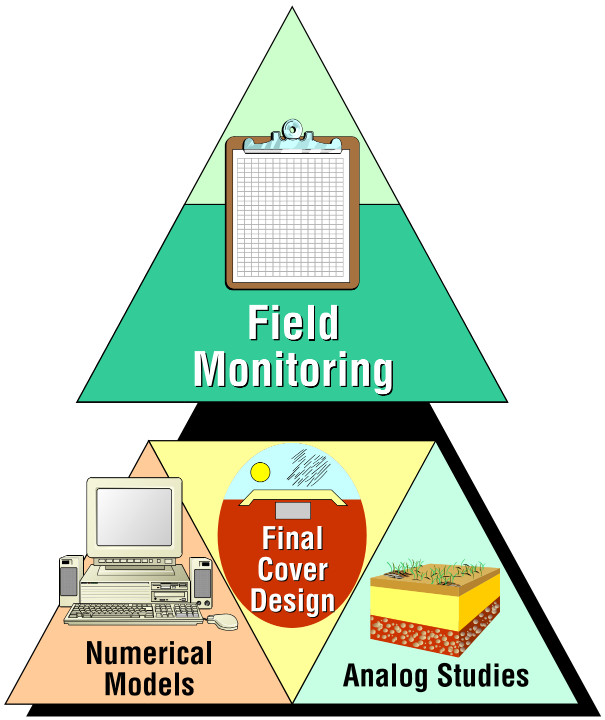


What is STOMP ?

- Subsurface Transport Over Multiple Phases
  - developed at PNNL
  - multi-fluid flow and transport
  - !-D, 2-D, or 3-D
  - sequential & parallel versions
- Phases - aqueous, gas, NAPL, ice, hydrate, …
- Modular
  - water, air, energy, oil, salt, CO_2, CH_4, reactive chemistry
- Isothermal, non-isothermal
- Hysteretic, entrapment, residual
- Grid - structured (Cartesian, cylindrical, boundary fitted)
- Solvers - banded, conjugate gradient, PETSC
- Currently used by PNNL and site contractors to investigate multifluid flow, transport, and to remedial action issues
- Website - http://stomp.pnl.gov

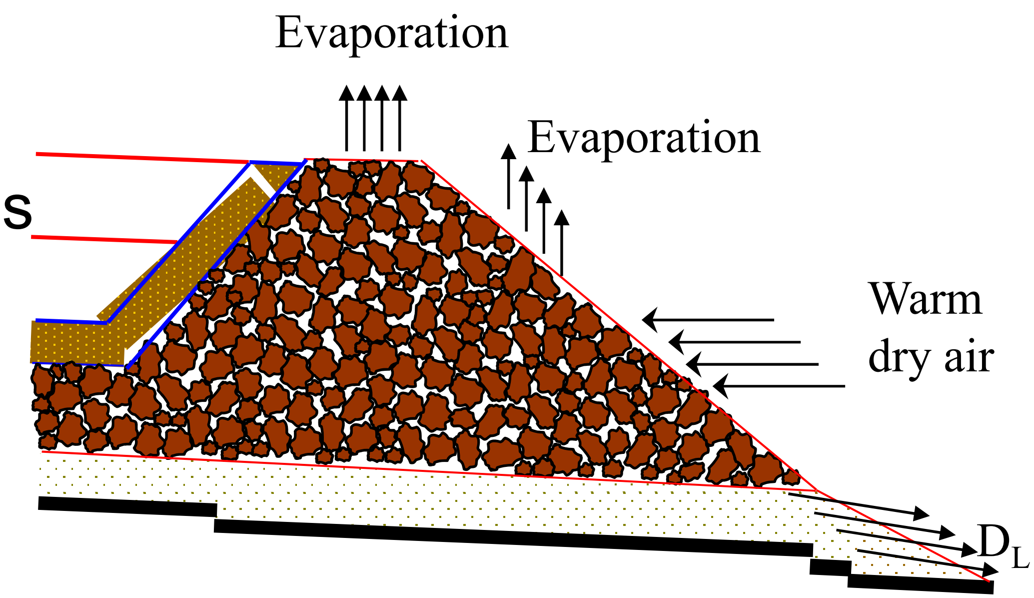
When Should Modeling be Performed?

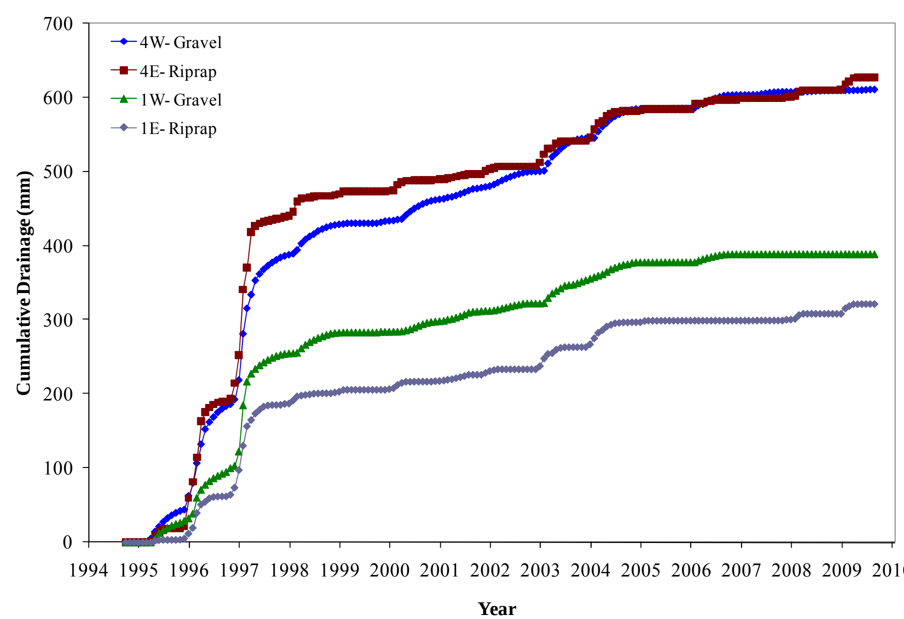
- Goal is to provide a measure of the cover's ability to prevent infiltration over long periods
- Quantify system behavior
- Assessment of data quality objectives
  - Difference between constraints and sensor resolution
  - Select monitoring system and instrumentation
- Coupled with monitoring
  - Improve identification and understanding of processes
  - Identify most sensitive state variable or surrogate



Side Slope Effects

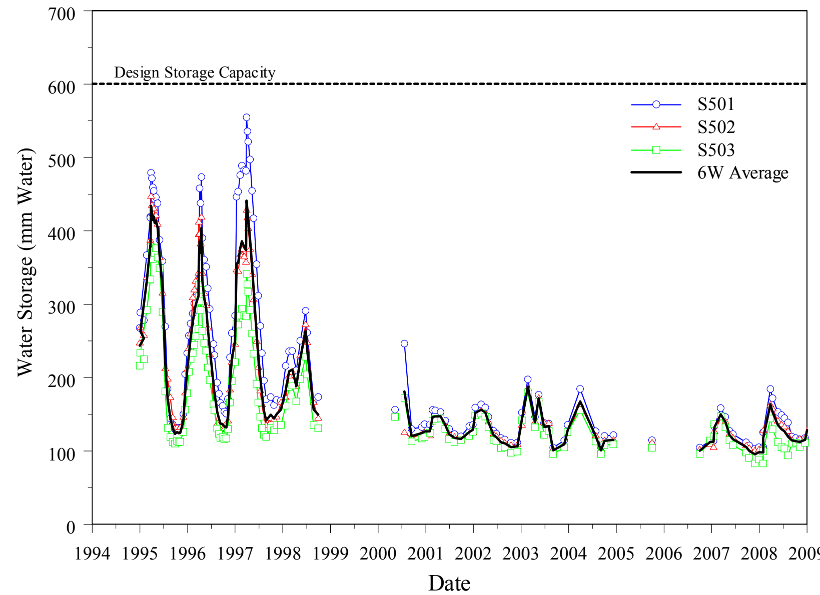
- Advective airflow (air convective embankment)
- Solves for aqueous and gas phase flow
  - wind pumping
  - advective drying
  - reduced temperature
  - reduced recharge
  - Riprap vs. gravel
- Irrigated treatments the same in long-term (18% of ppt)
- Non-irrigated treatment different in long-term (11% of ppt)





Time Periods for Simulation

- Challenging to precisely predict performance over long periods
  - Weather
  - Disturbance (e.g. fire)
  - Biointrusion
  - Change in soil properties
- Important to demonstrate acceptable performance over a range of potential conditions
  - Elevated precipitation
  - Bare surface



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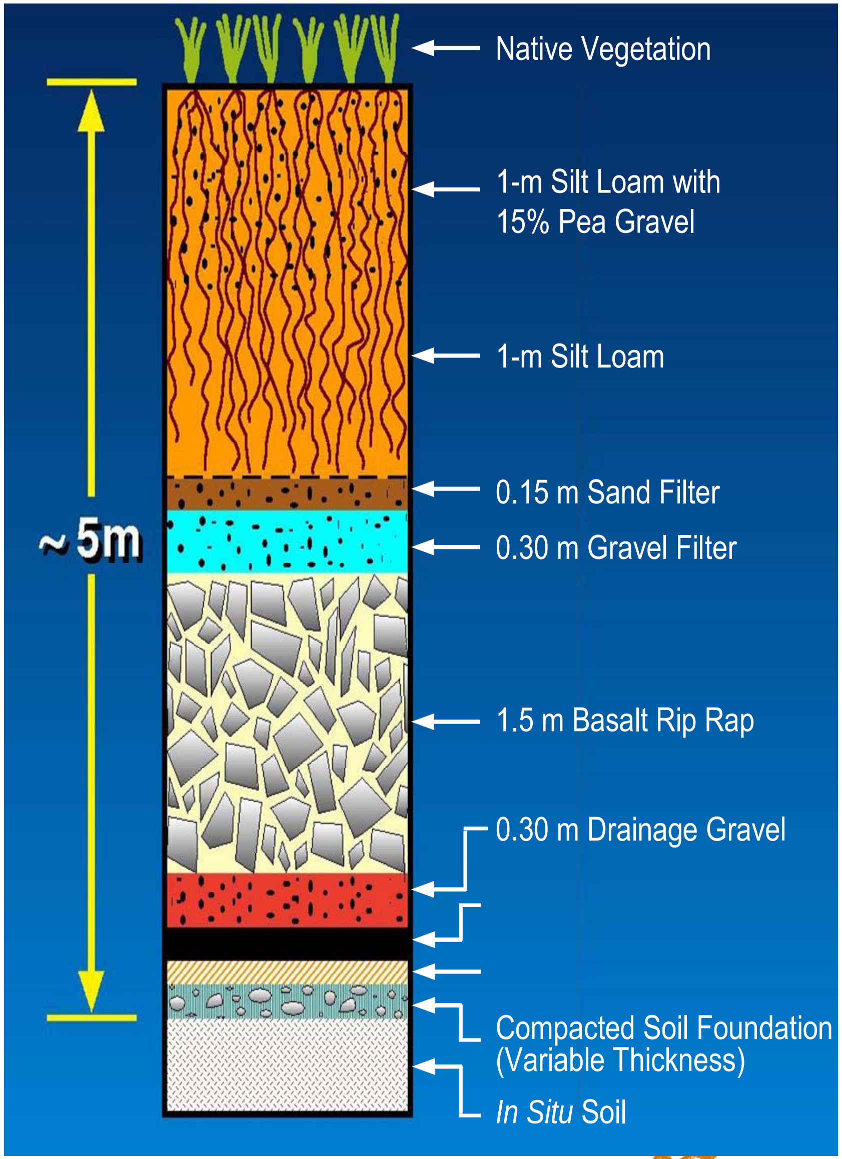
Criteria to Determine Detail of Modeling

- Barrier Type
  - Monofill
  - Composite
- Processes to be simulated
  - Flow
  - Transport
- Spatial Resolution
  - Layers from 0.05 m to 1.5 m
  - Sloped layers, 2% to 50%
  - Location of instruments
- Temporal Resolution
  - Some meteorological inputs can't be integrated
  - Comparison with Observations
- Computing resources



Evaluating Long-term Performance

- Mechanistic Model
  - Simulate variably saturated (water and air phase) flow with Richard’s equation
  - Solve the heat transport equation
- Multidimensional
  - Functional portion
  - Protective side slopes
  - Lateral flow

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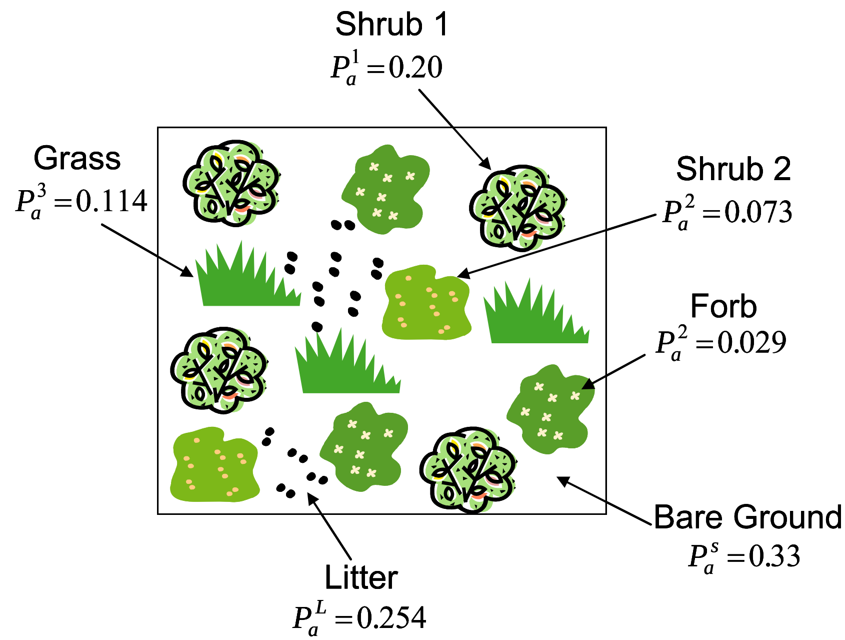
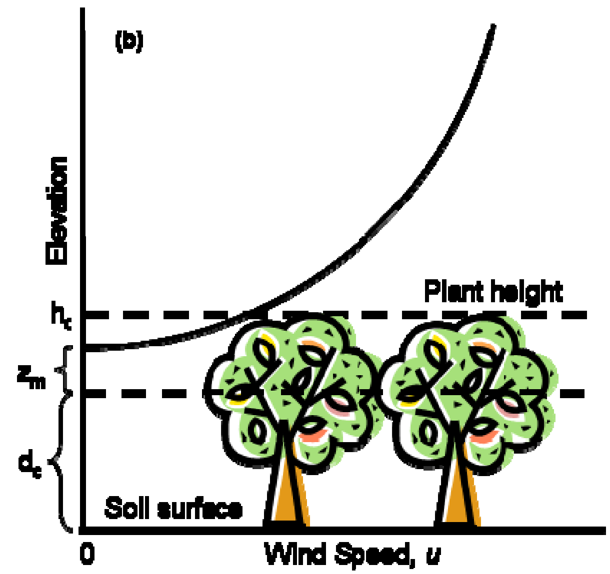
Predicting Physical and Chemical Changes in Soil Properties

- Time varying material properties
  - EkeCHEM- reactive transport
  - Precipitation/dissolution
  - Predict changes in pore size distribution
- Freeze-thaw cycles
  - Coupled mass and energy
  - Change in hydraulic properties
- Physical Deterioration ??
  - Burrowing
  - Root penetration
  - Cracking

Incorporation of Ecological & Climatological Changes

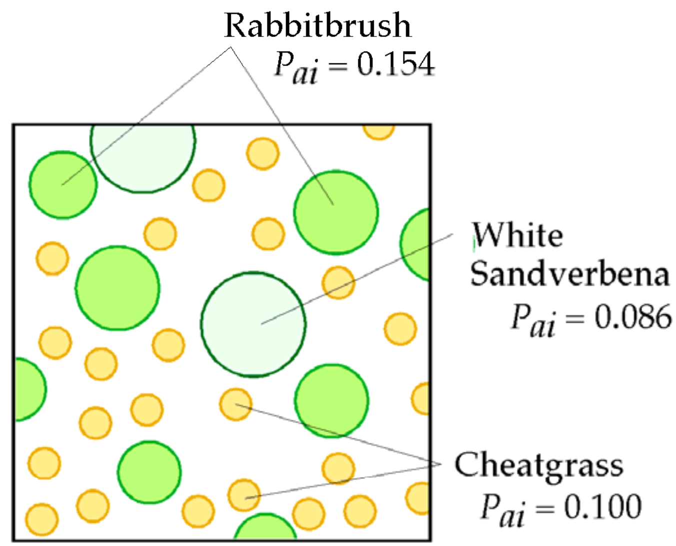
- Multispecies distribution
  - Plant Area Index
  - Sum of components = 1
  - Time dependent input
- Phenophase
  - Controlled by degree days
  - Lowest winter temperature
- Roughness length and zero-plane displacement can vary over time
  - bare surface
  - vegetated surface
- Metrological input from global climate change models

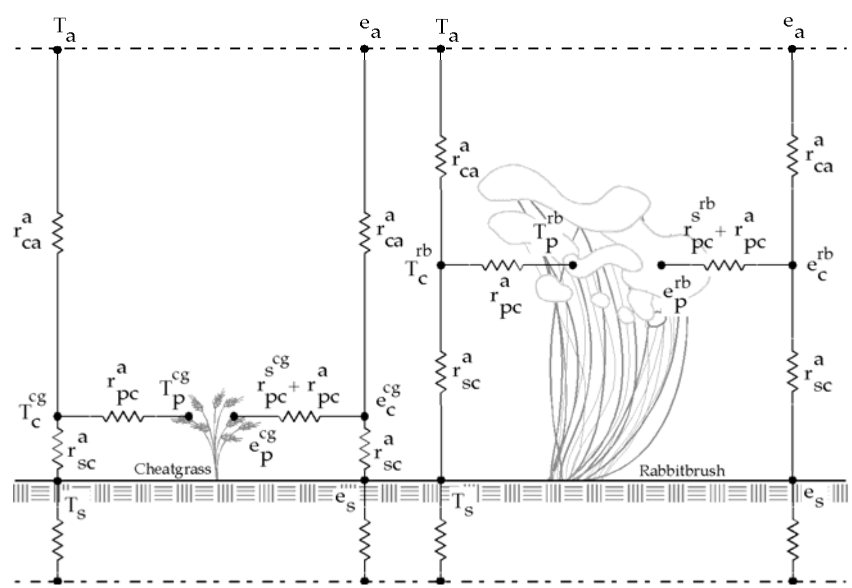




Sparse Vegetation ET Model

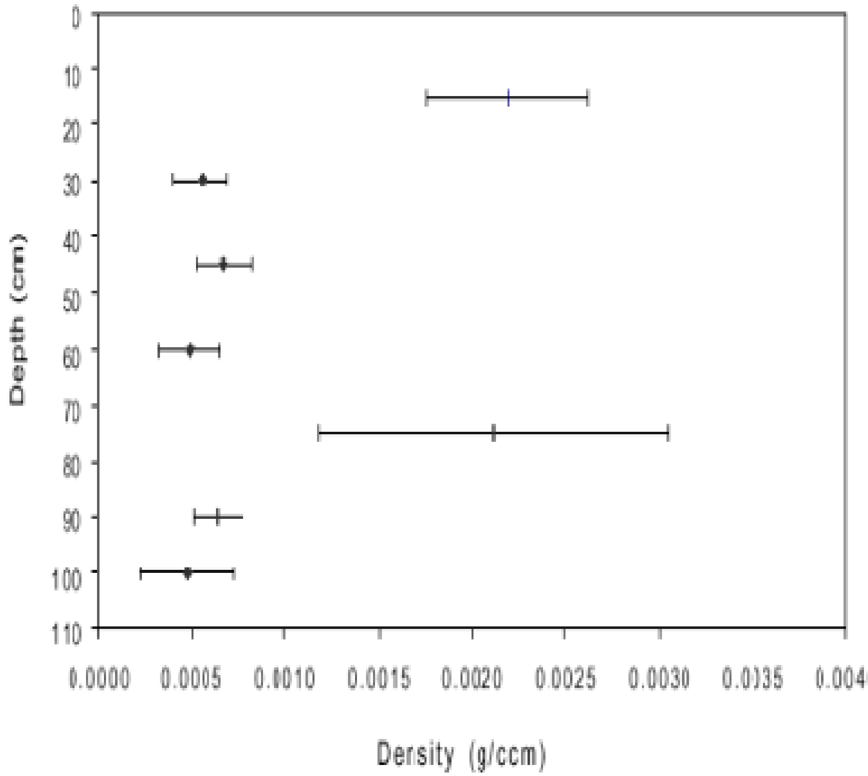
- Sparse vegetation
- Non-overlapping canopies
- Leaf area Index for each species
  - leaf area to ground surface ratio
- Plant Area Index for each species
  - Fractional ground cover for species
- Soil-plant-atmosphere continuum model
  - Bare-surface model
  - Single plant temperature model
  - Multiple plant temperature model





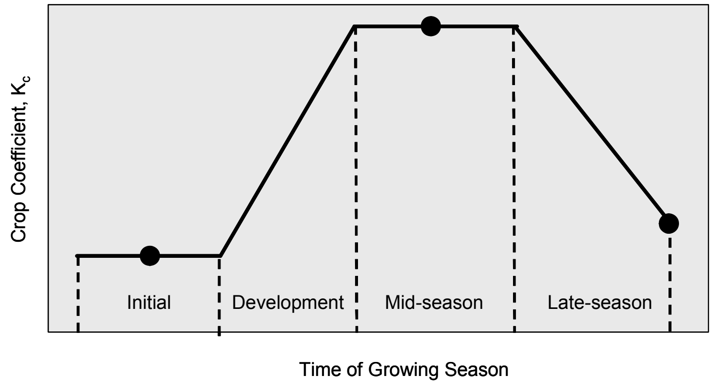
Root Water Uptake

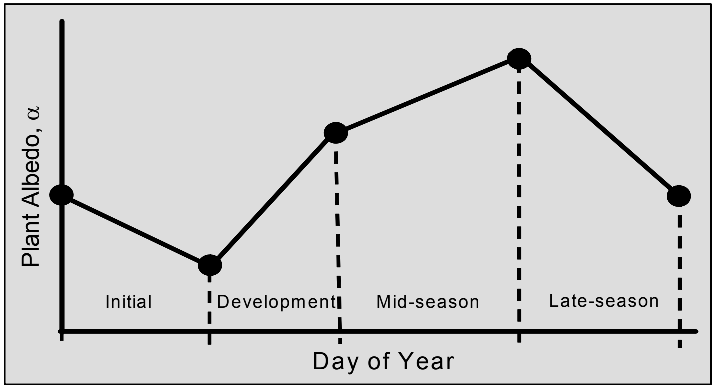
- Root water uptake based on Vrugt [2001] model
- Modified to handle multi-layered soils
  - root length density does not decrease exponentially with depth
- Water uptake depends on
  - Suction
  - max root lengths (3D)
  - Transpiration

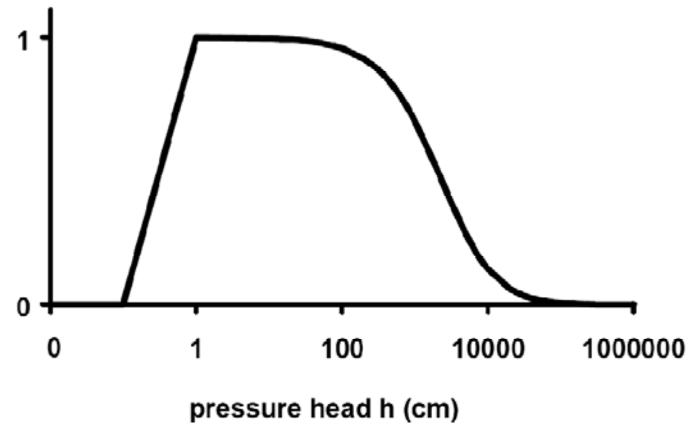


Input Data and Parameters- Biotic

- Plant parameters
  - Plant species
  - Phenophase
  - Albedo
  - Leaf area index
  - Ground cover
  - Plant height
  - Root distribution
  - Transpiration reduction function
  - Bulk stomatal resistance
  - Canopy interception
- Data package developed for species of interest

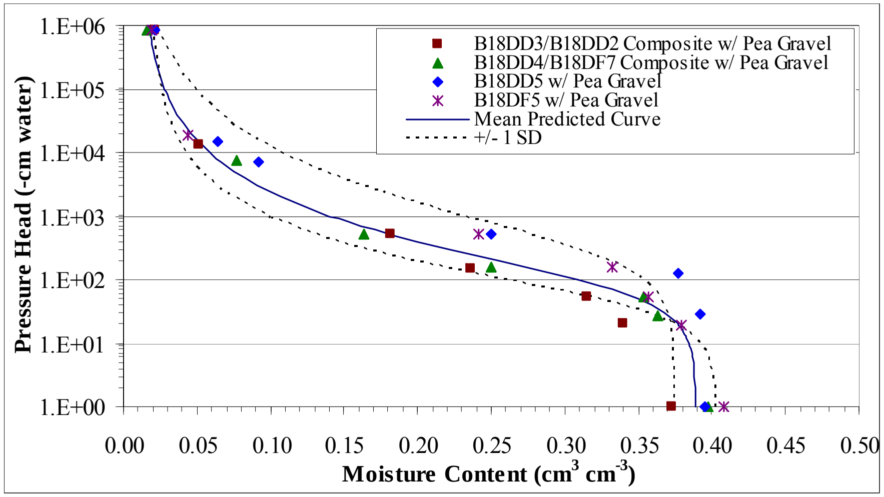




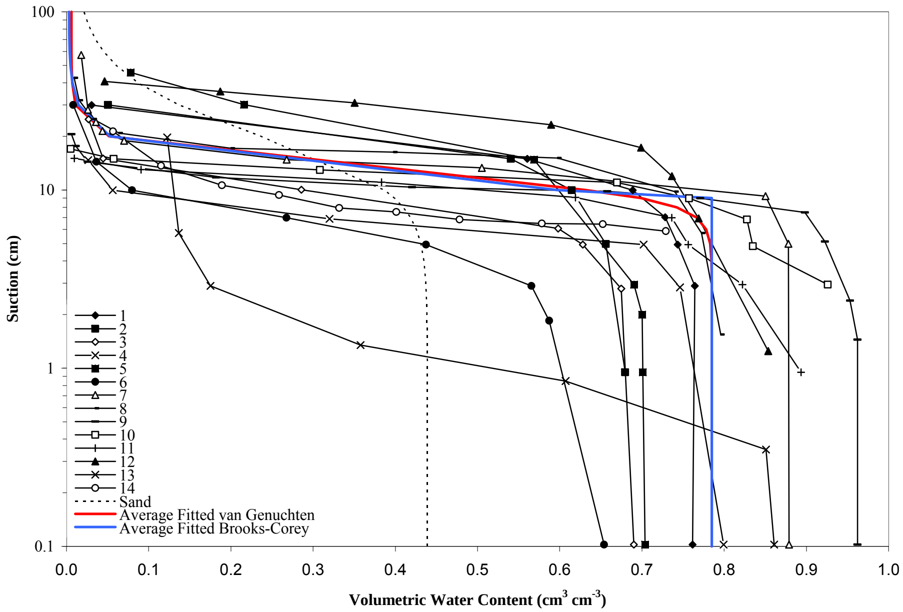


Input Data and Parameters- Abiotic

- Physical Properties
  - Porosity
  - Bulk density
  - Particle density
- Hydraulic/Pneumatic Properties
  - k_w-s_w-p relations
  - Pore connectivity
- Thermal Properties
  - Heat capacity
  - Thermal conductivity
  - Albedo
- Data package developed for materials of interest
  - Measurements
  - Pedotransfer functions



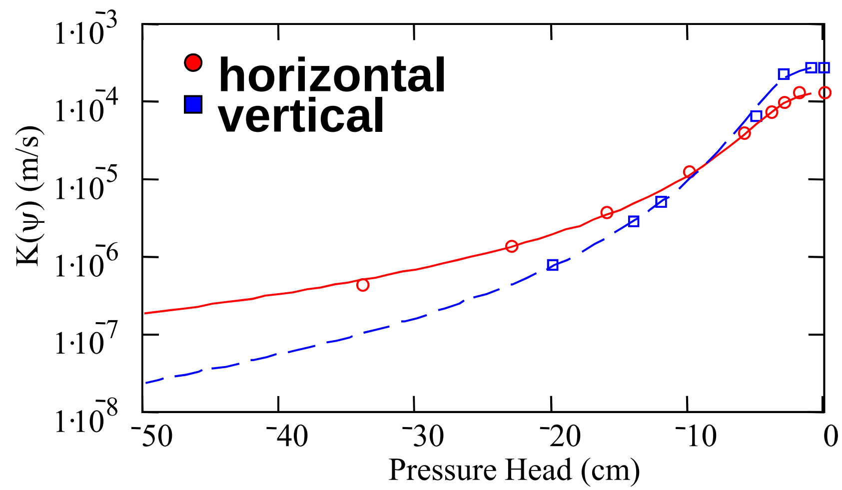
Measured and Fitted Drying Phase SMCC for Soil

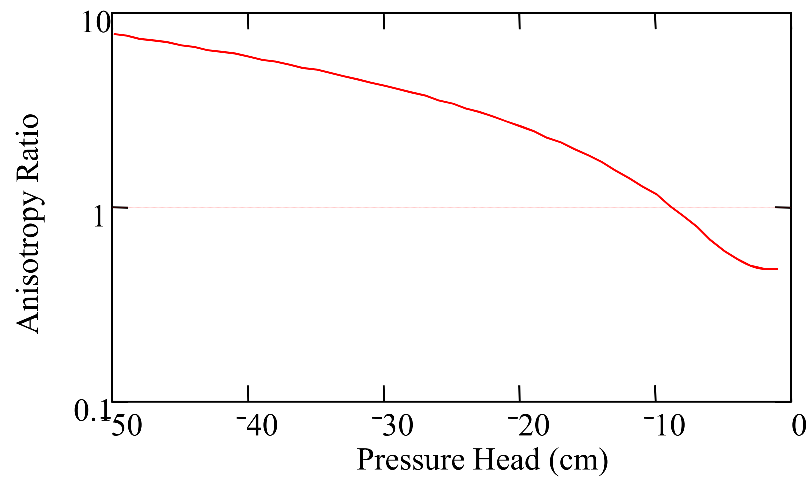


Drying Phase SMCCs for Geotextiles.

Unsaturated Hydraulic Conductivity

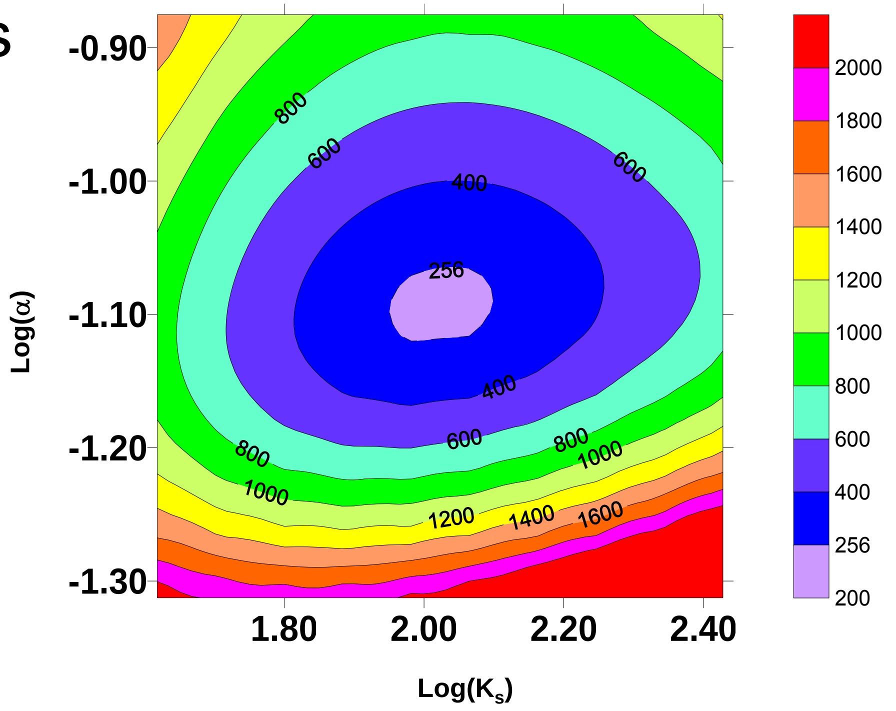
- Modified to handle saturation dependent anisotropy
- Based on concept of a pore connectivity-tortuosity tensor
- “ℓ” parameter
  - Direction dependent
  - Soil dependent
  - < 0 for fine-textured, laminated soils
  - 0.5 for sands
  - > 0.5 for coarse sands and gravels



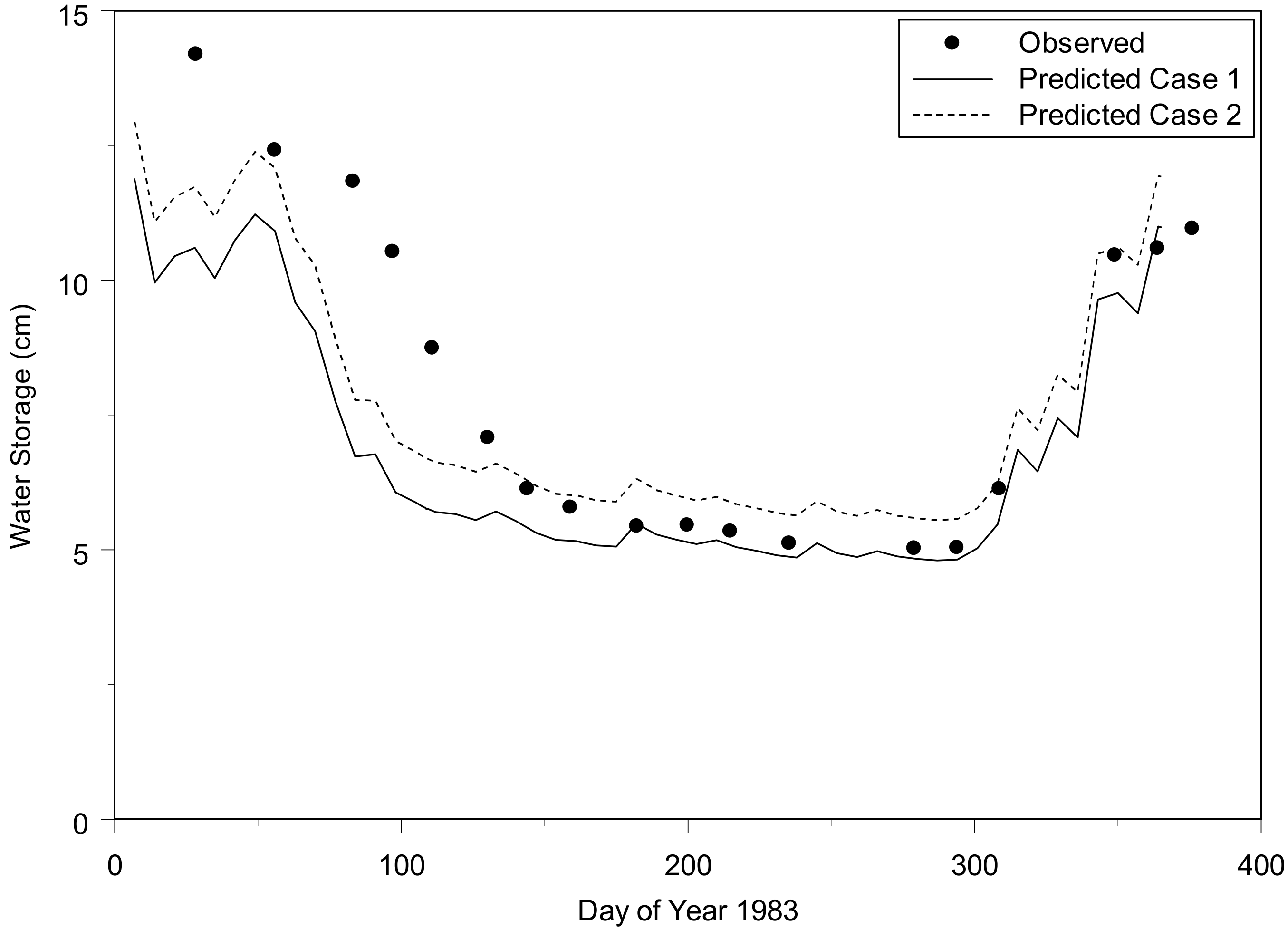


Input Parameters- Inverse Modeling

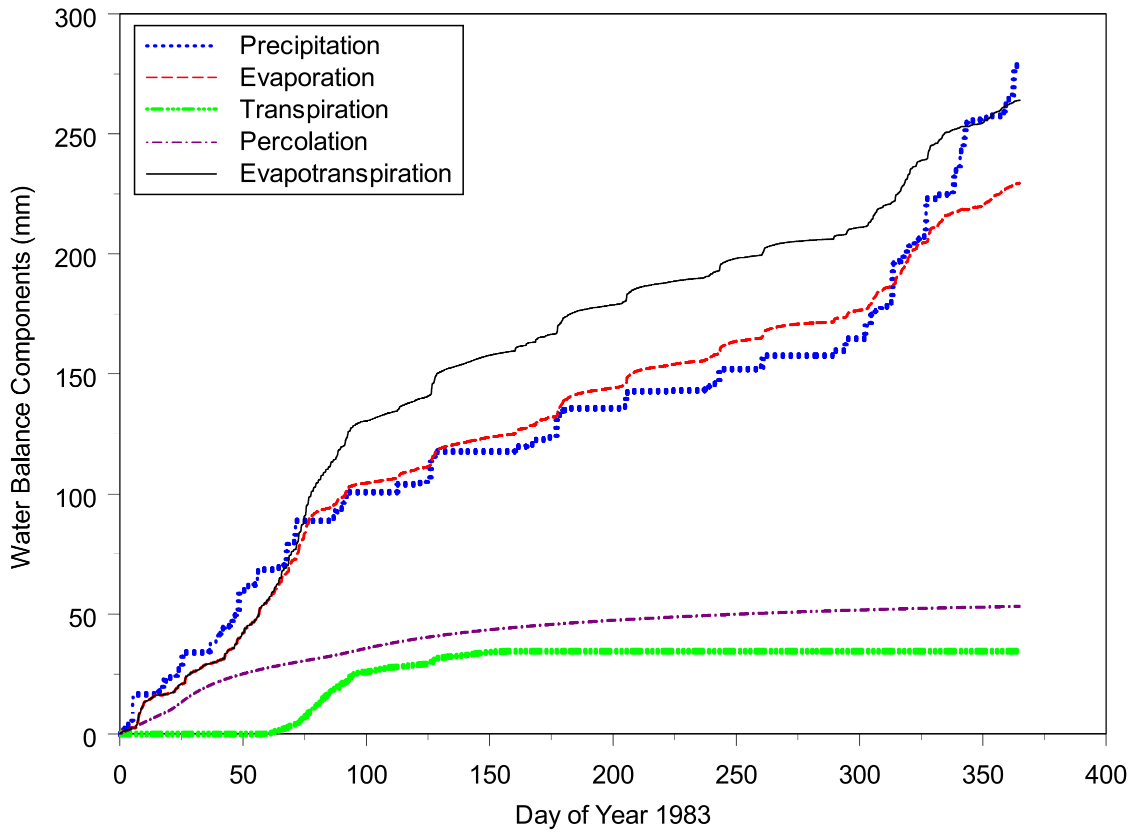
- STOMP
  - PEST
  - SCEM-UA
- Unique to STOMP for Barriers
- Parameter Estimation
  - Run STOMP with initial parameter values
  - Minimize objective function
  - Update parameter values
  - Continues until convergence criterion is met
- Field-scale parameters
  - Upscaling
  - downscaling



Simulated Soil Water Storage in the 0-1 m 300 A Grass Site



Simulated Water Balance at 300A Grass Site



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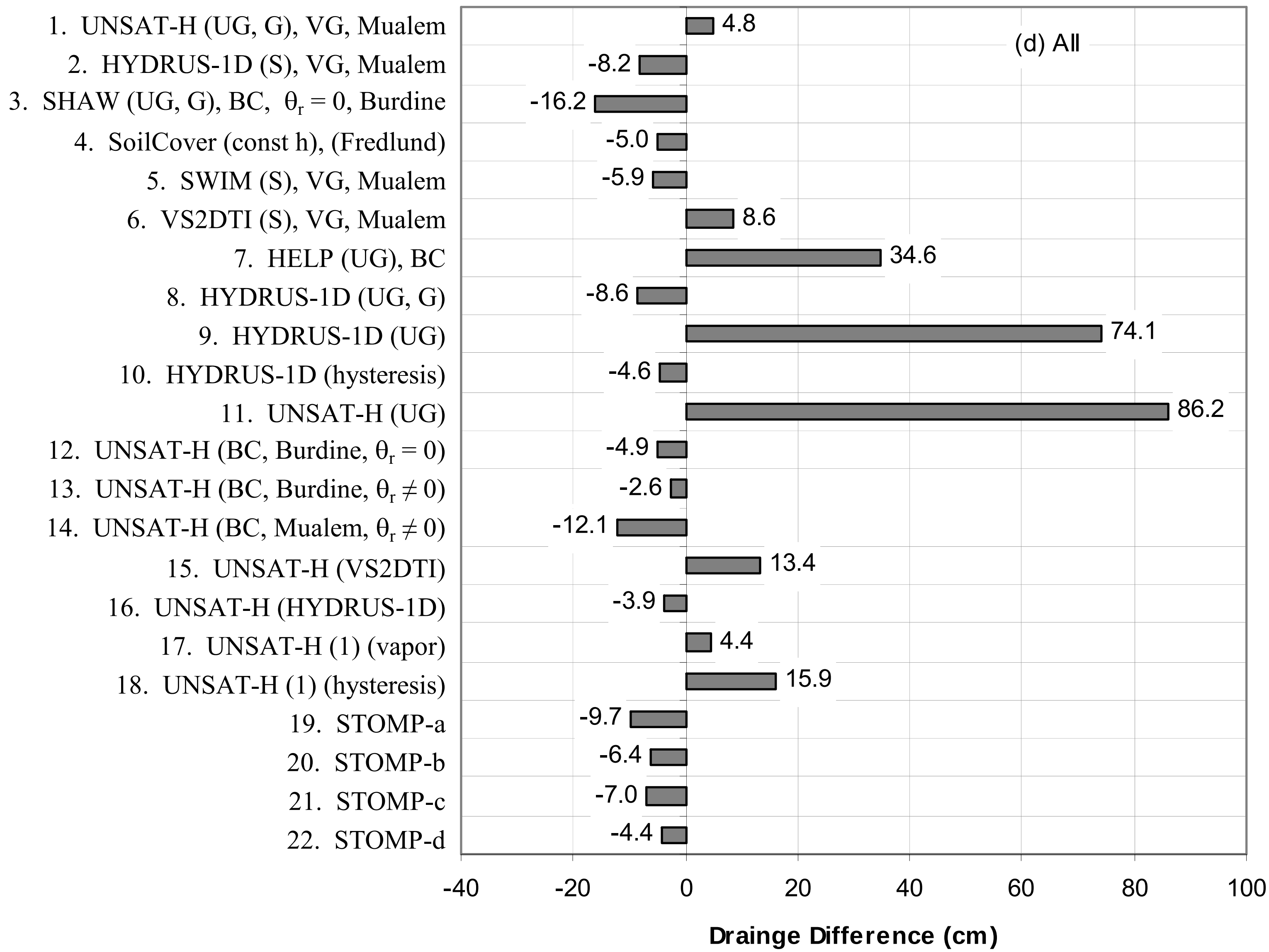
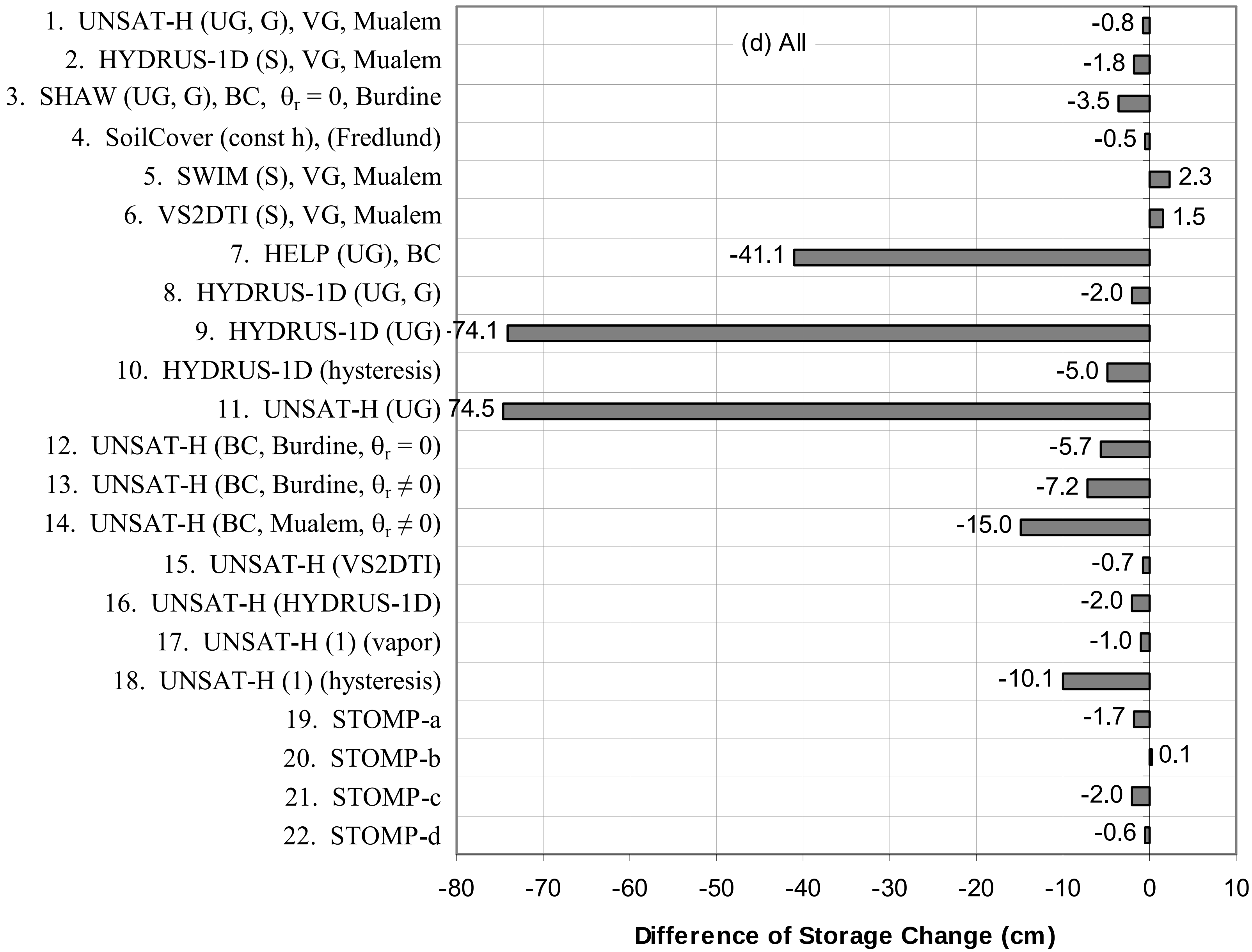
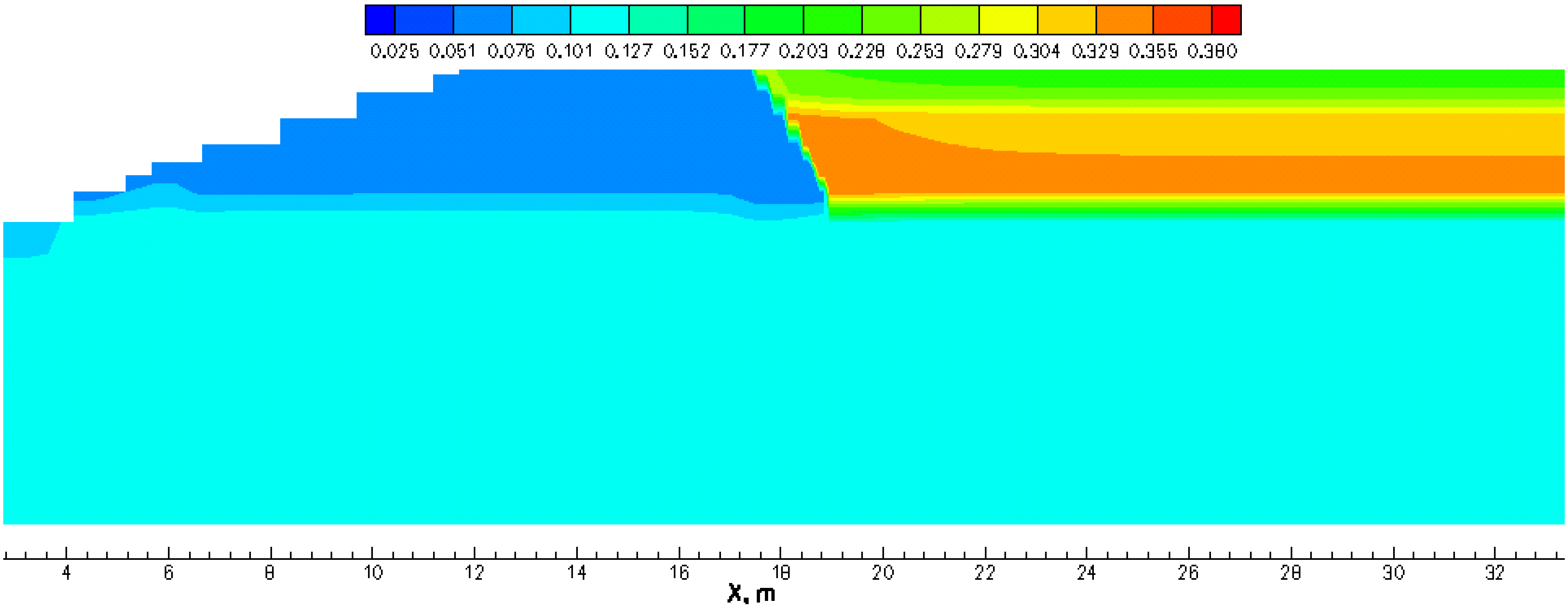
Scanlon's Intercode Comparison- Drainage (FY97-99)



Scanlon's Intercode Comparison- Simulated Storage Drainage (WY97-99)



Hypothetical Monolithic Cover Jan - Dec 1995



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Summary

- Barrier simulation is a multidimensional, multiphase problem
- Performance controlled by tightly coupled processes
- Available tools for barrier design not always applicable
- STOMP used extensively at DOE sites for subsurface flow and Transport
- Soil-Plant-Atmosphere Continuum
  - physically based
  - full climate coupling
  - fully coupled mass and energy
  - well suited to sparse canopies typical of arid environments