The Catchment Isoscape:
A Meta-Model for Stable Isotope Tracers at the Shale Hills Critical Zone Observatory

Christopher Duffy

2007-2013 NSF CZO Program
2013-2016 NSF INSPIRE CREATIV
2013-2017 EPA, Center for Integrated Multi-scale Nutrient Pollution Solutions,

In this paper:

- Describe a 5 year experiment for water isotopes at Shale Hills CZO

- Present a theory for "age" and "residence time" of mobile-immobile water flow in soils and regolith

- Compare theory and experiment to test for the existence of macropore-matrix flow at Shale Hills

"The Catchment Isoscape"

National CZO Program

Advancing interdisciplinary studies of earth surface processes

The Susquehanna/Shale Hills Critical Zone Observatory

PENNSTATE 1855

NSF

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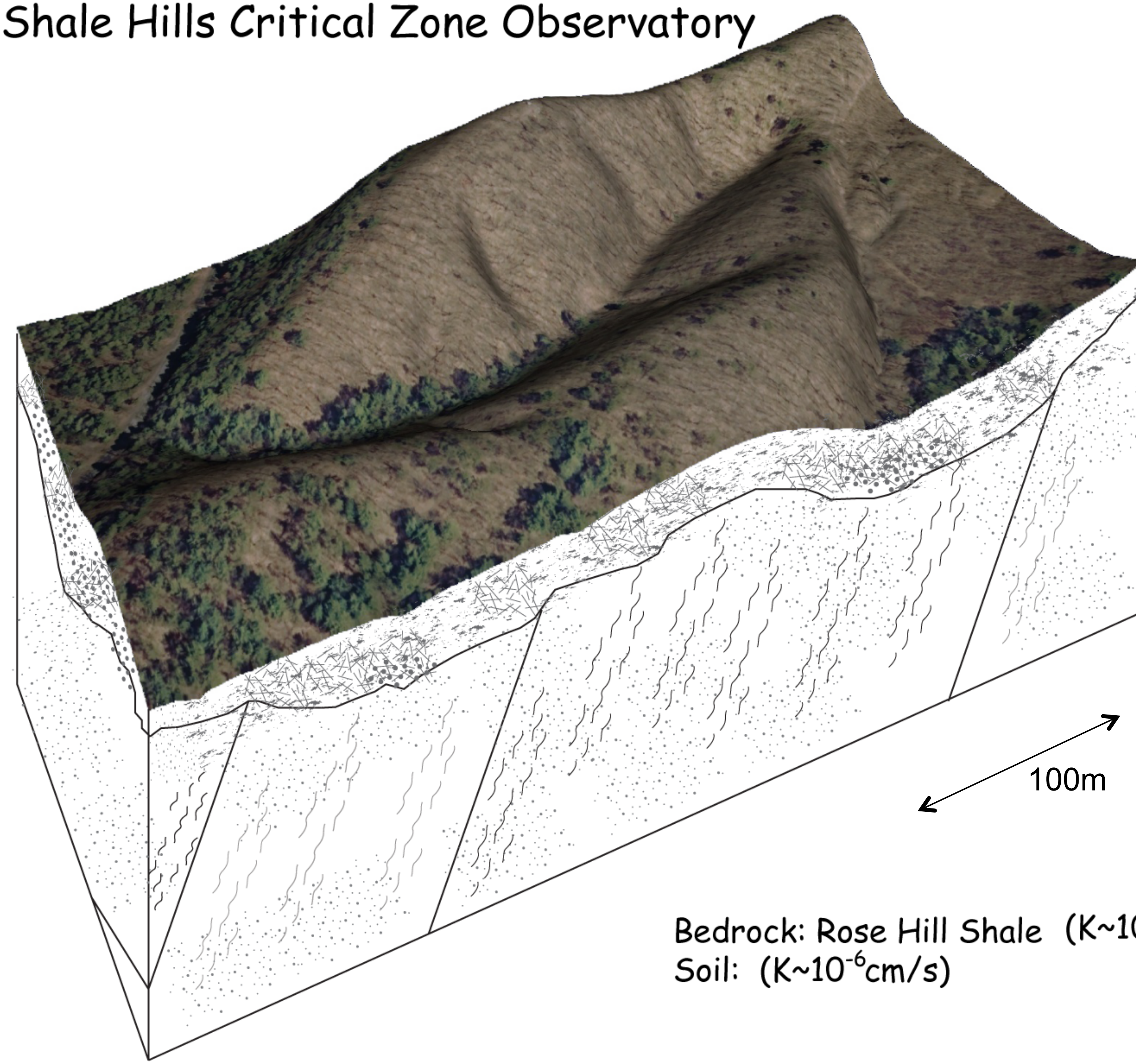
CZEN

CUAHSI
universities allied for water research

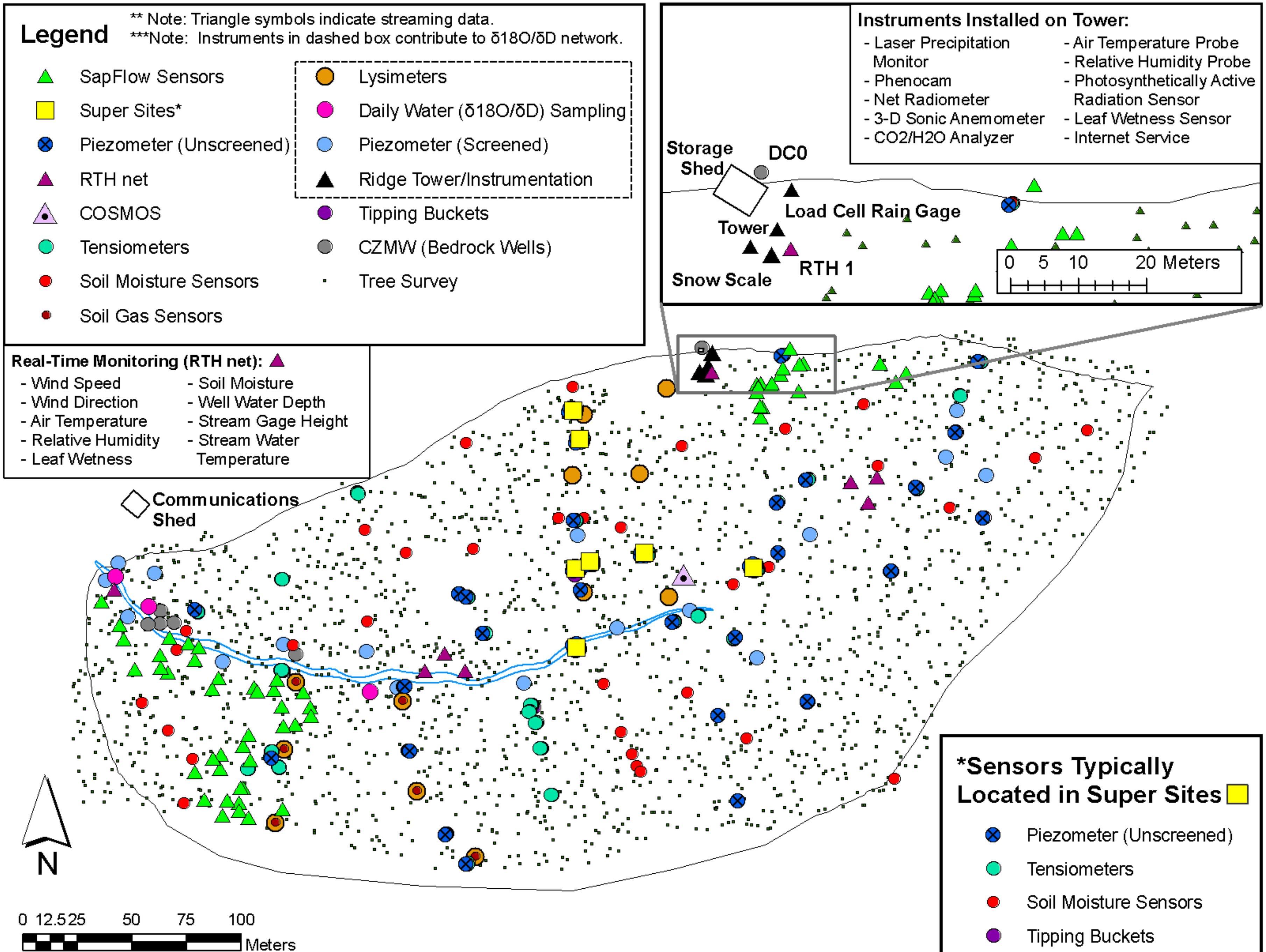
CSDMS
COMMUNITY SURFACE DYNAMICS MODELING SYSTEM

Shale Hills Observations & Experiments to Support Earth System Models & Prediction

The Shale Hills Critical Zone Observatory



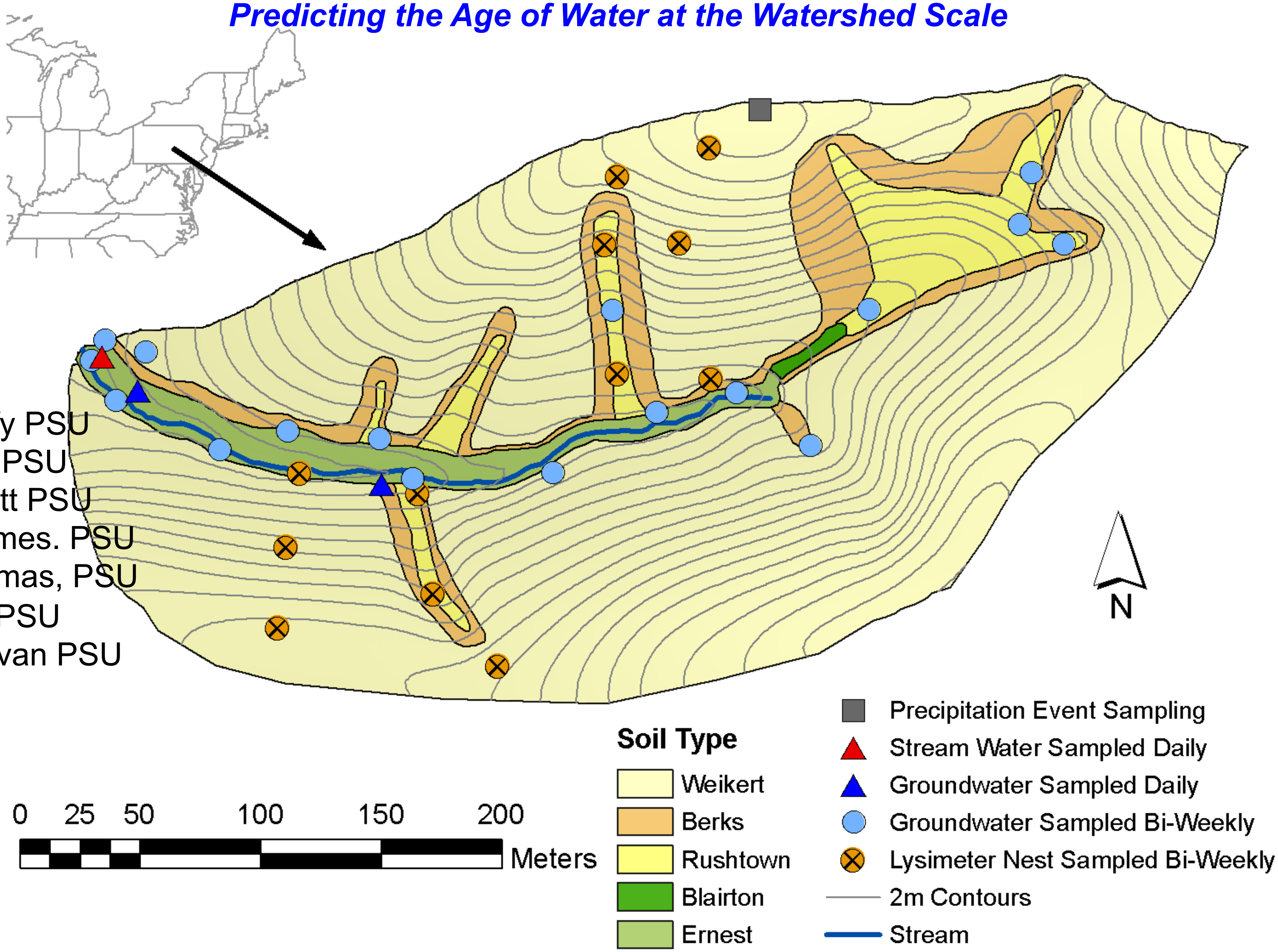
Bedrock: Rose Hill Shale ($K \sim 10^{-15}$ cm/s)
Soil: ($K \sim 10^{-6}$ cm/s)



Legend
** Note: Triangle symbols indicate streaming data.
***Note: Instruments in dashed box contribute to δ18O/δD network.
SapFlow Sensors
Super Sites*
Piezometer (Unscreened)
RTH net
COSMOS
Tensiometers
Soil Moisture Sensors
Soil Gas Sensors
Lysimeters
Daily Water (δ18O/δD) Sampling
Piezometer (Screened)
Ridge Tower/Instrumentation
Tipping Buckets
CZMW (Bedrock Wells)
Tree Survey
Real-Time Monitoring (RTH net):
- Wind Speed
- Wind Direction
- Air Temperature
- Relative Humidity
- Leaf Wetness
- Soil Moisture
- Well Water Depth
- Stream Gage Height
- Stream Water Temperature
Instruments Installed on Tower:
- Laser Precipitation Monitor
- Phenocam
- Net Radiometer
- 3-D Sonic Anemometer
- CO2/H2O Analyzer
- Air Temperature Probe
- Relative Humidity Probe
- Photosynthetically Active Radiation Sensor
- Leaf Wetness Sensor
- Internet Service
Storage Shed
DC0
Load Cell Rain Gage
Tower
Snow Scale
RTH 1
0 5 10 20 Meters
Communications Shed
N
0 12.5 25 50 75 100
Meters
*Sensors Typically Located in Super Sites
Piezometer (Unscreened)
Tensiometers
Soil Moisture Sensors
Tipping Buckets

CZO Isotope Network

Predicting the Age of Water at the Watershed Scale



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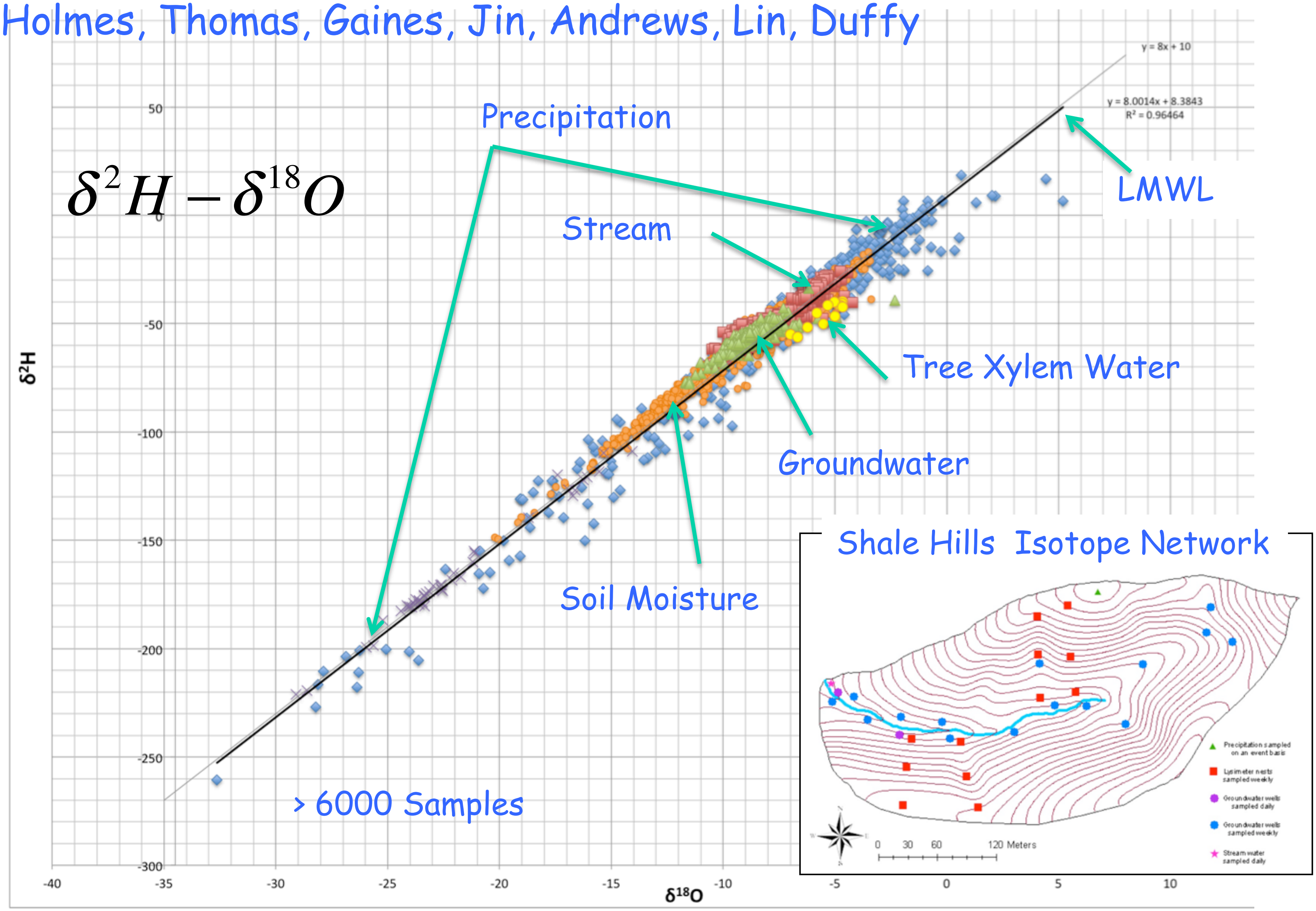
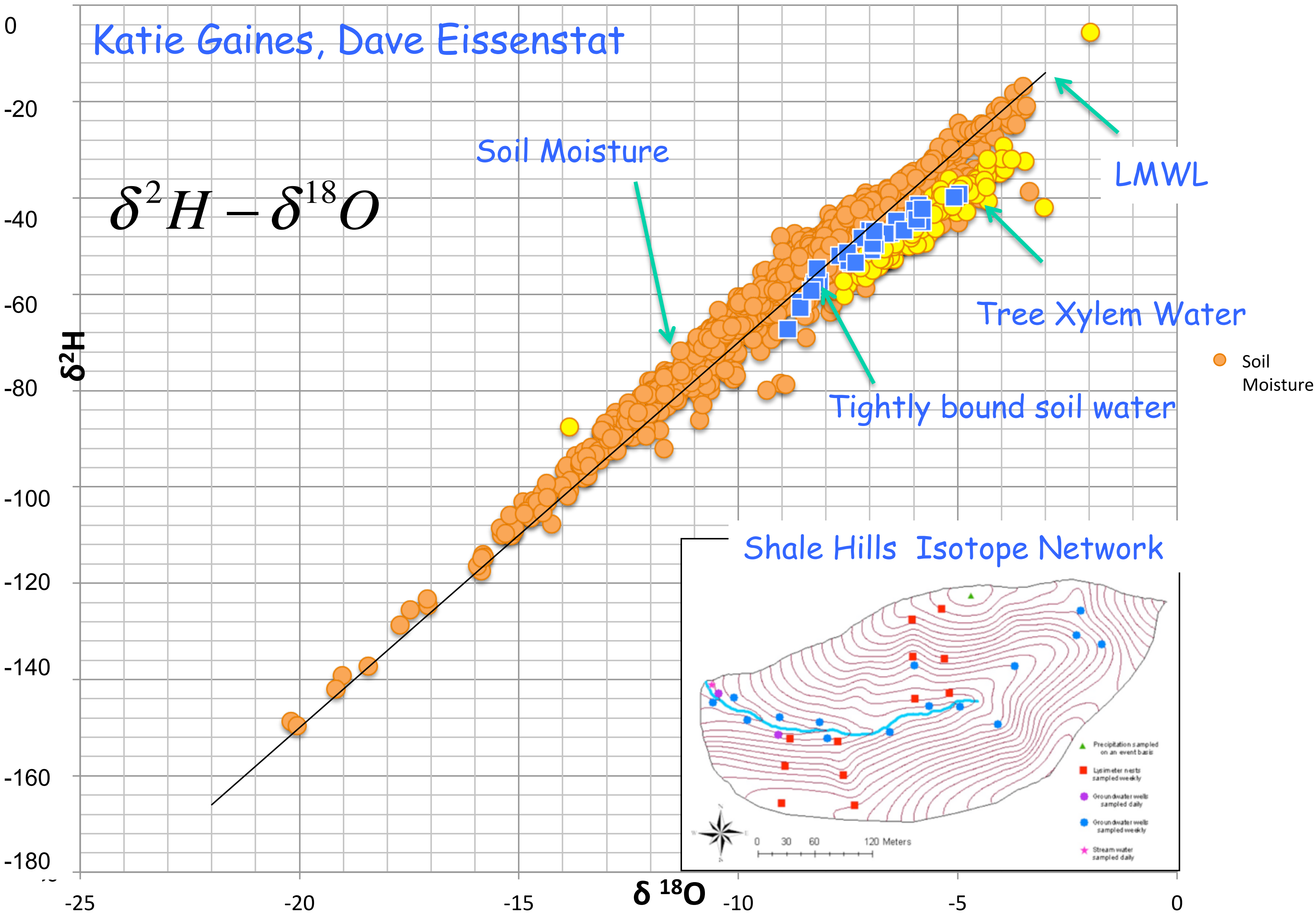
Instrumentation for Iso.Net

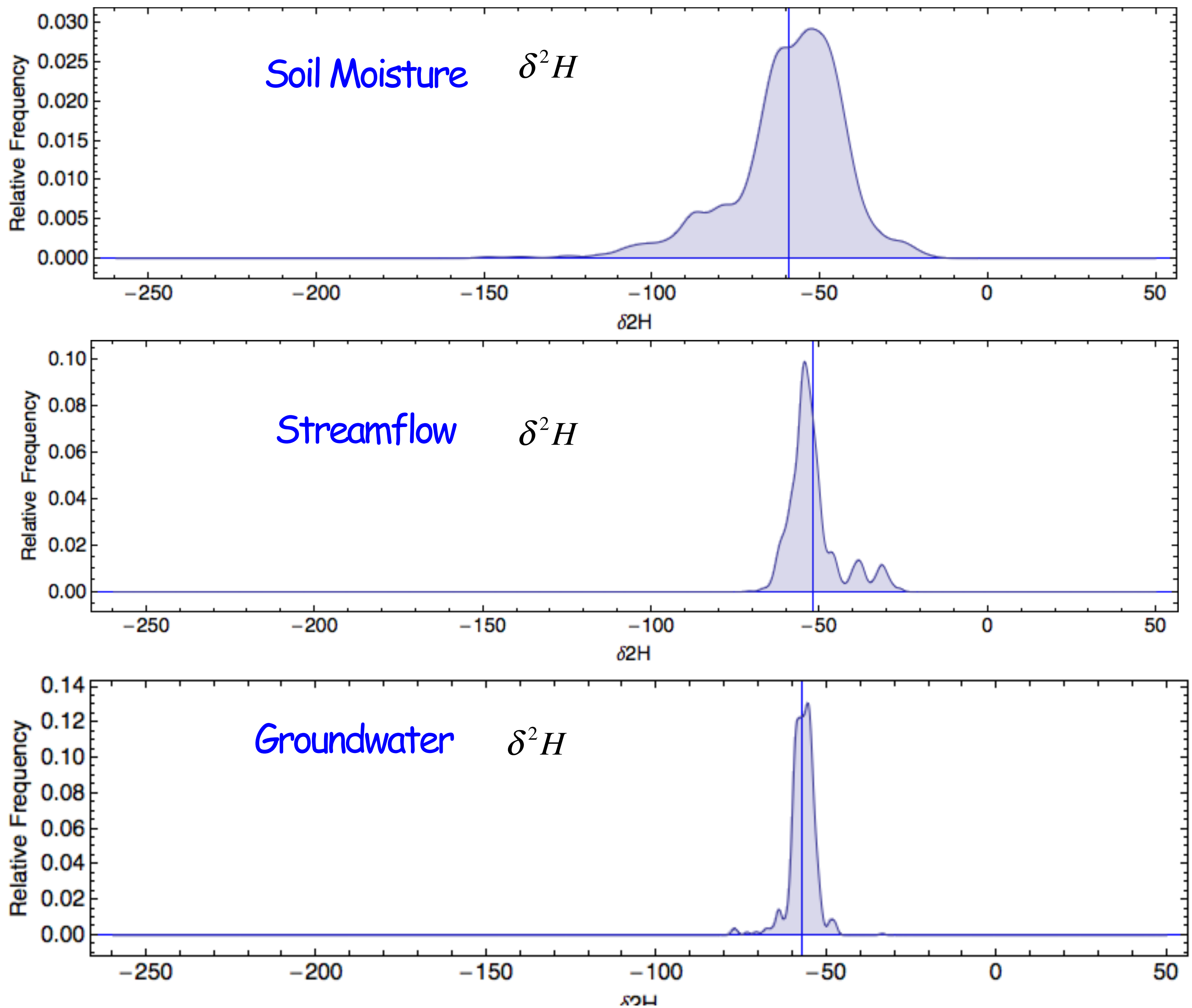
Stable Isotope Experiment 2008-20012

Holmes, Thomas, Gaines, Jin, Andrews, Lin, Duffy



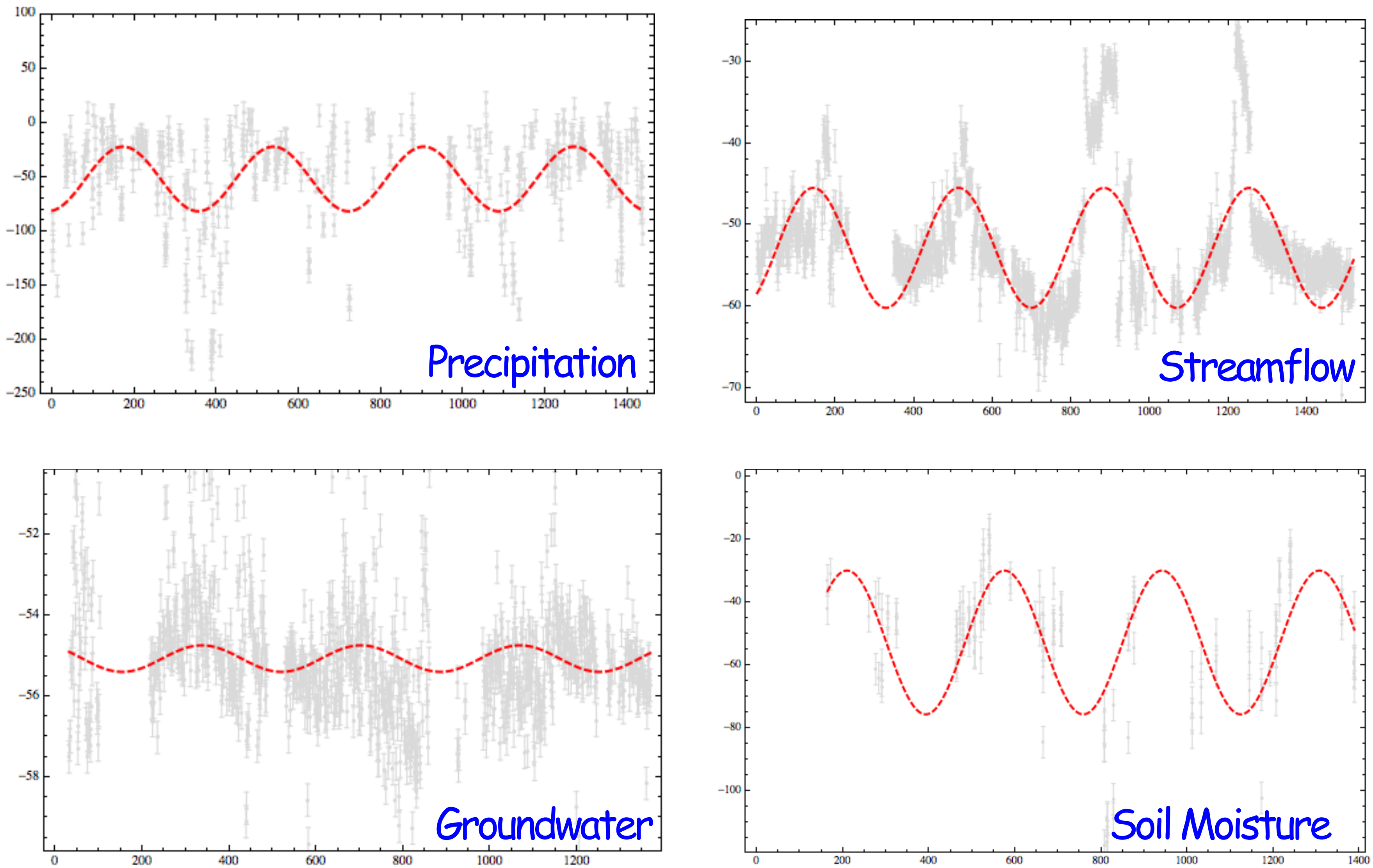
Soil Moisture - Xylem Water Experiment





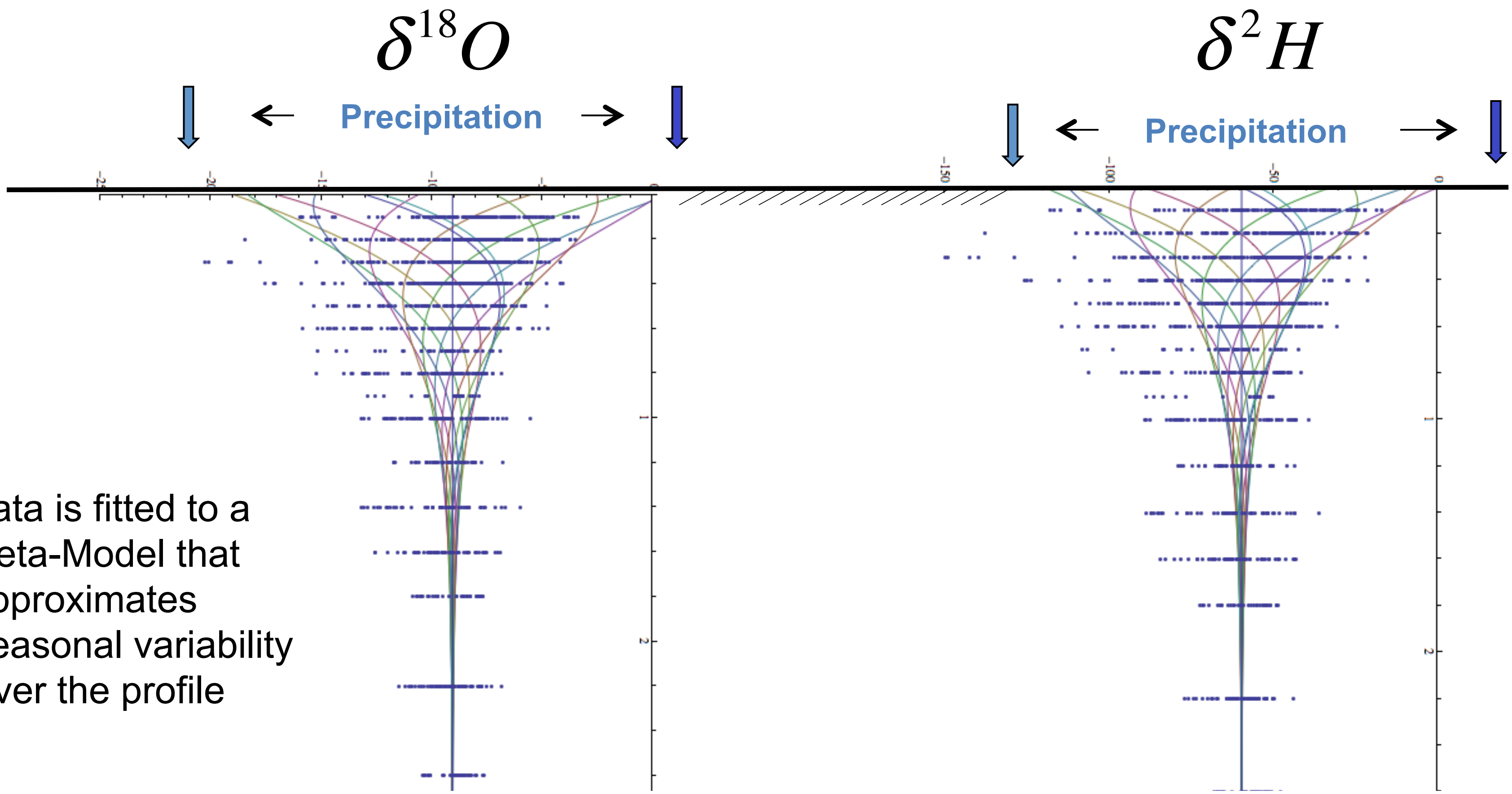
Soil Moisture
$\delta^2 H$
Relative Frequency
δ2H
Streamflow
$\delta^2 H$
Relative Frequency
δ2H
Groundwater
$\delta^2 H$
Relative Frequency

Catchment δ^2H Signature From Time Series



A Single Dominant Period: 360 < T < 370 days

Seasonal Variability over the Soil Profile



Data is fitted to a
Meta-Model that
Approximates
Seasonal variability
Over the profile

Seasonal Cycle Attenuates over Profile

The Catchment Isoscape & The Age of Water

The term "isoscape " was coined by ecologists to describe the spatial and temporal patterns of isotope ratios over a landscape (Bowen, 2010)

In this paper we explore an "isoscape" for water isotopes of $\delta^2 H - \delta^{18} O$ in soil and regolith

The goal is to develop a meta-model for space-time isotopic patterns over the catchment as a step towards predicting:

"The Distributed Age and Residence Time of Water Isotopes at the Shale Hills CZO"

Properties of the Age Distribution

$$\mu_n(x,t) = \int_0^\infty \tau^n c(x,\tau,t) d\tau$$

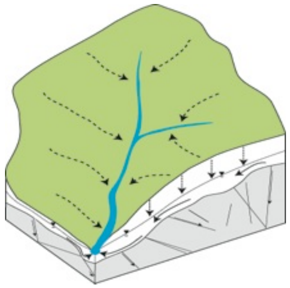
$$\mu_o(x,t) \Rightarrow \quad C(x,t) = \int_0^\infty c(x,t,\tau) d\tau$$

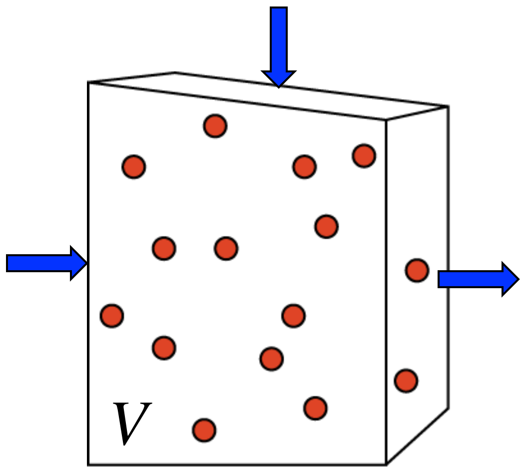
$$\mu_1(x,t) \Rightarrow \quad \alpha(x,t) = \int_0^\infty \tau c(x,t,\tau) d\tau$$

$$A(x,t) = \frac{\mu_1(x,t)}{\mu_o(x,t)} = Mean\ Age\ of\ water$$

A Model for Age Distribution

Rotenberg 1972, J, of Theoretical Biology, 37, 291-305





$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial \tau} = \Gamma_c + L(c)$$

$$L(c) \rightarrow D\frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x}$$

or

$$L(c) \Rightarrow \frac{Q_i}{V}(c_i - c)$$

$$\mathrm{D}M(t,\tau)\frac{1}{V} = \left(\frac{\partial M}{\partial t} + \frac{\partial M}{\partial \tau}\right)\frac{1}{V}$$

Transport Model in Terms of Moments

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial \tau} = \Gamma_c + L(c)$$

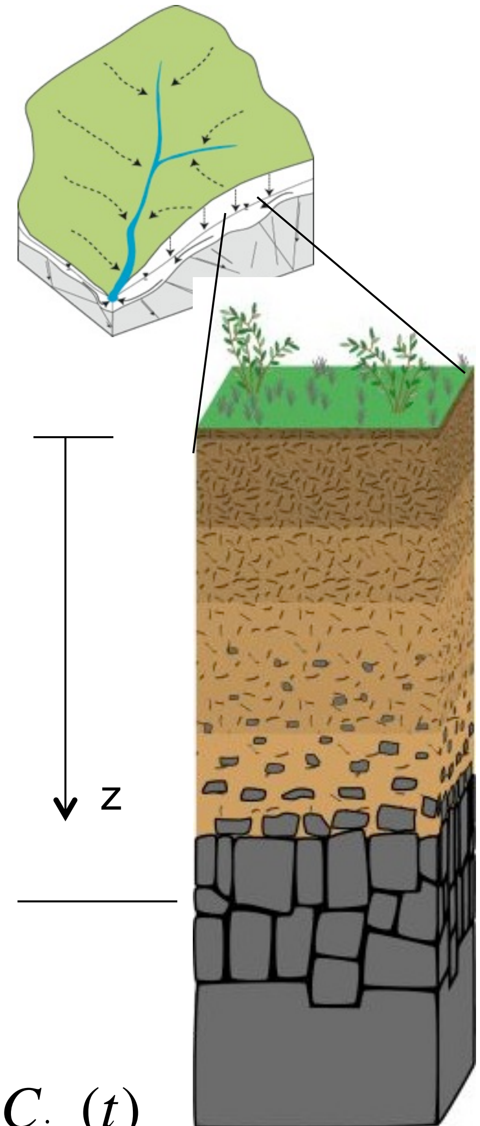
Coupling Moment

Transport operator for the nth moment

$$\frac{\partial \mu_n}{\partial t} = n\mu_{n-1} + \Gamma_{\mu_n} + L(\mu_n)$$

Source terms for the nth moment

A Theory for Concentration-Age For Mobile-Immobile Transport Over the Soil Profile



$$\frac{\partial C_m}{\partial t} = D_m \frac{\partial^2 C_m}{\partial z^2} - u_m \frac{\partial C_m}{\partial z} - \frac{k}{\theta_m}(C_m - C_{im})$$

$$\frac{\partial C_{im}}{\partial t} = \frac{k}{\theta_m}(C_m - C_{im})$$

$$\frac{d\alpha_m}{dt} = C_m + D_m \frac{\partial^2 \alpha_m}{\partial z^2} - u_m \frac{\partial \alpha_m}{\partial z} - \frac{k}{\theta_{im}}(\alpha_m - \alpha_{im})$$

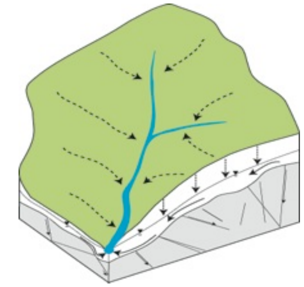
$$\frac{d\alpha_{im}}{dt} = C_{im} + \frac{k}{\theta_{im}}(\alpha_m - \alpha_{im})$$

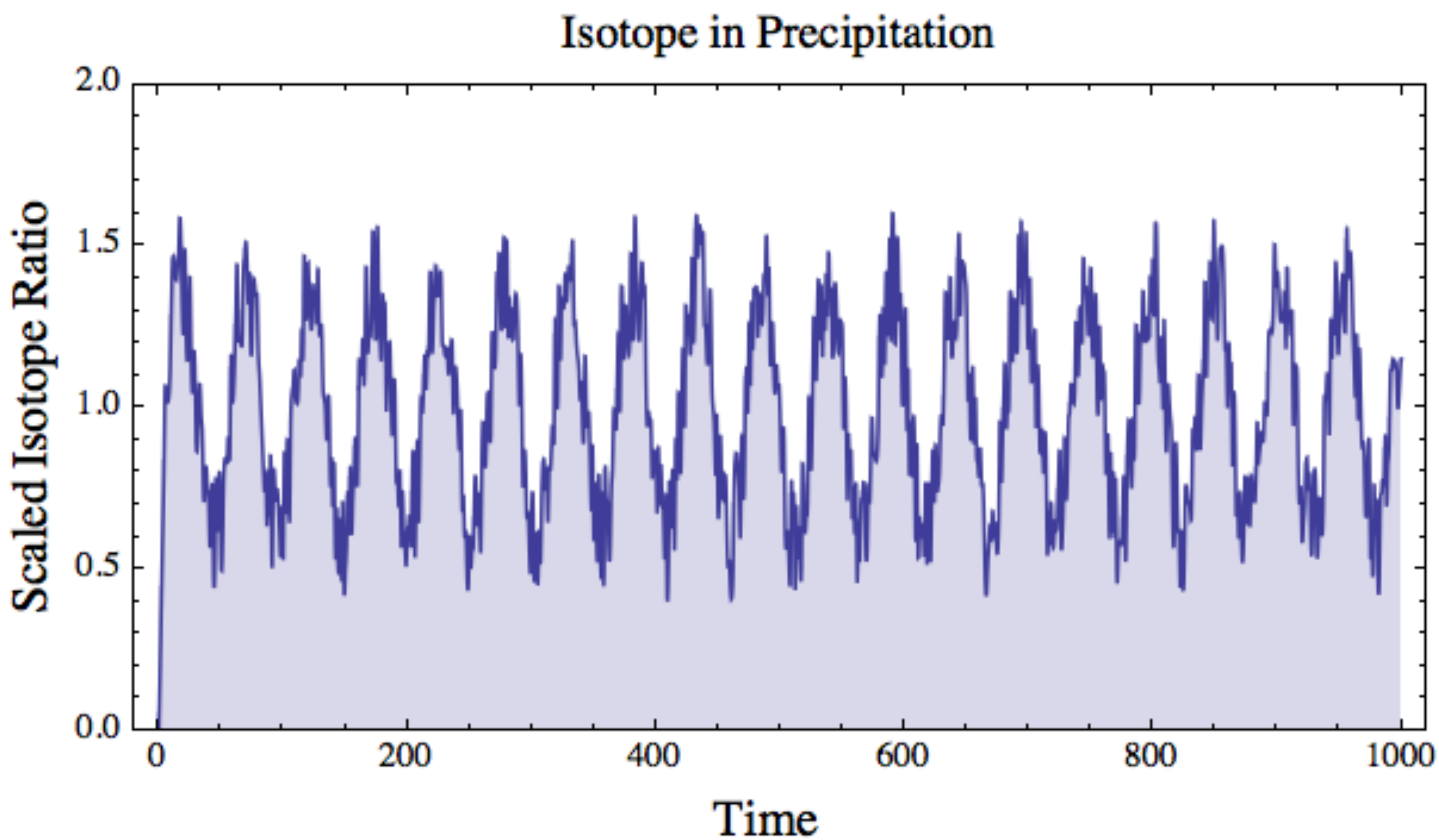
$$A_m(t) = \alpha_m(t) / C_m(t); \qquad A_{im}(t) = \alpha_{im}(t) / C_{im}(t)$$

$$C_m(0,t) = C_i(t);\; C'_m(d,t) = 0; \qquad \alpha_m(0,t) = \alpha_{im}(0,t) = \alpha'_m(d,t) = 0$$

$$C_m(z,0) = C_{im}(z,0) = 0; \qquad \alpha_m(z,0) = \alpha_{im}(z,0) = 0$$

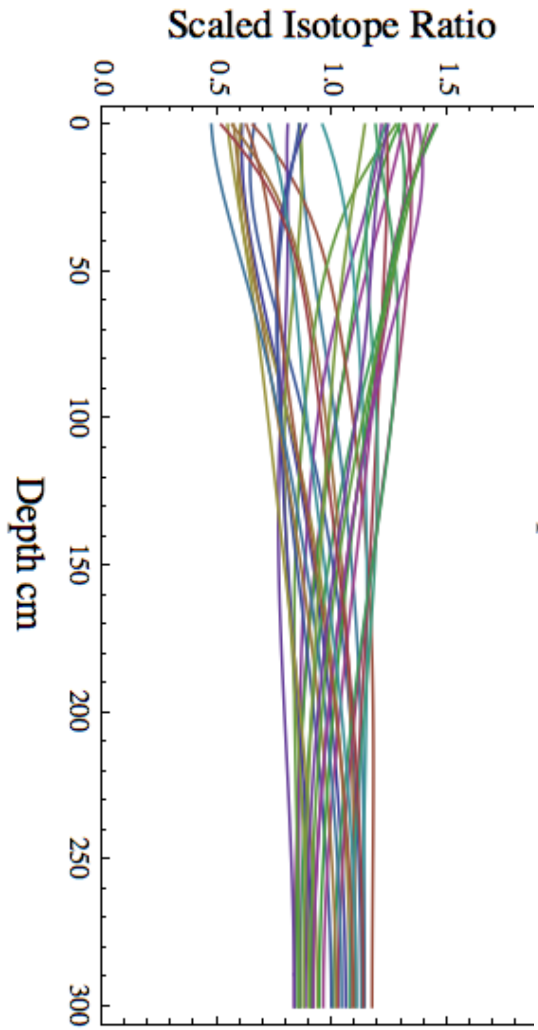
Simulated Seasonal Input C_i (scaled)



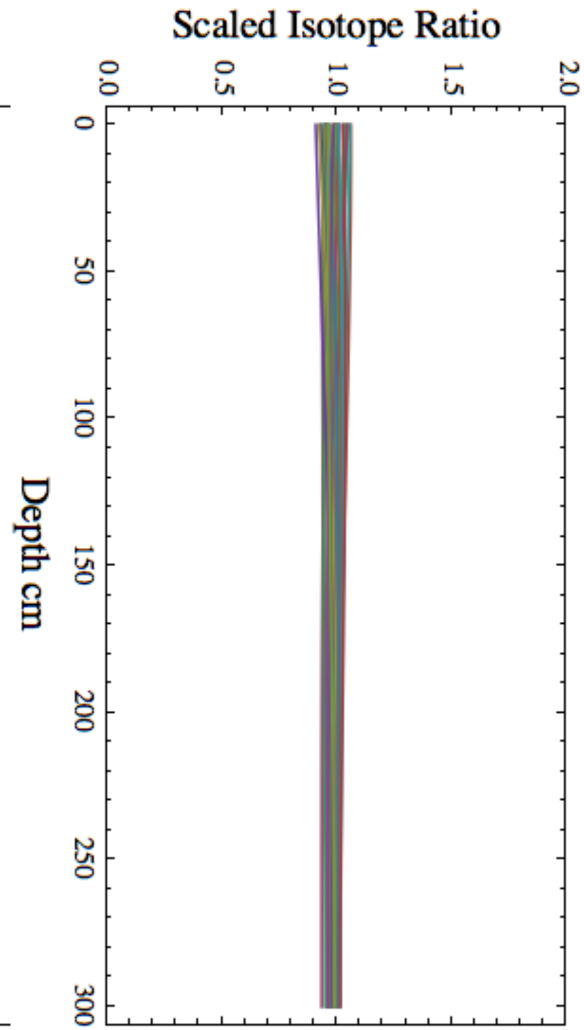


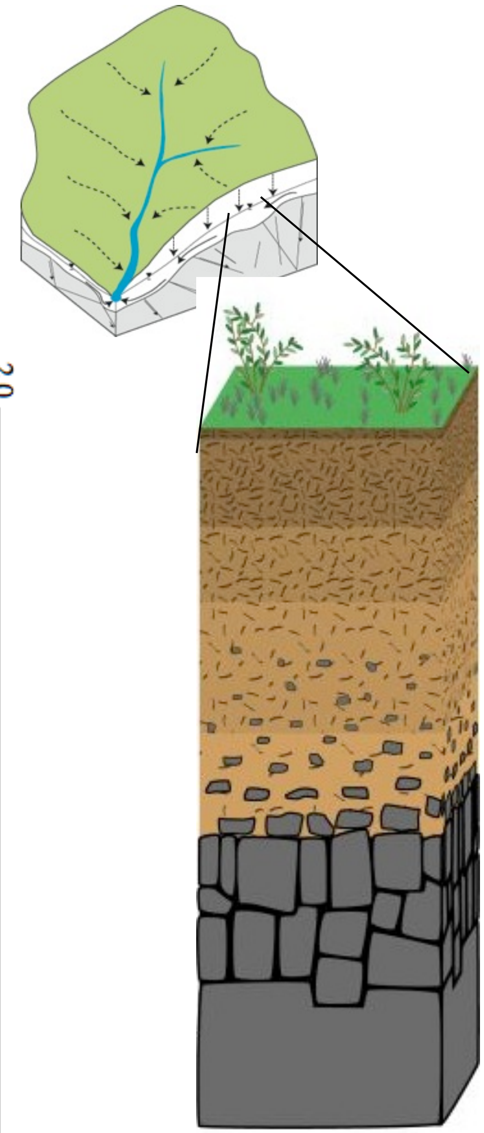
Simulated Profile C_i

mobile

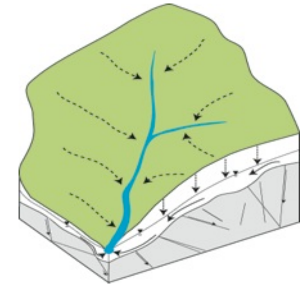


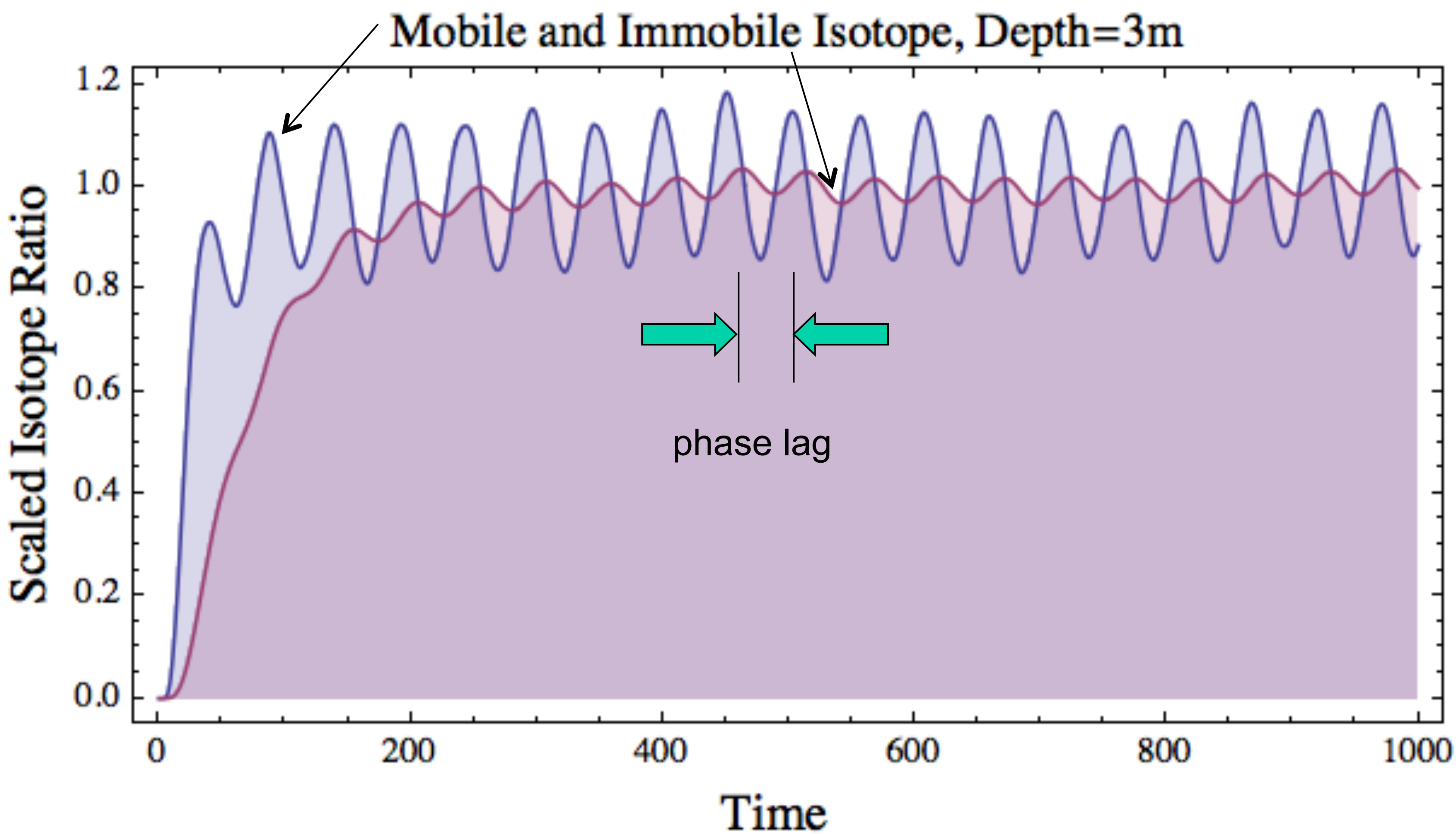
immobile



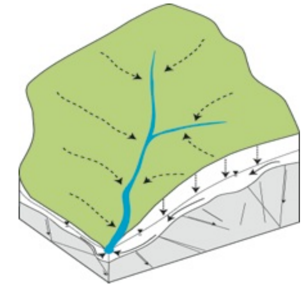


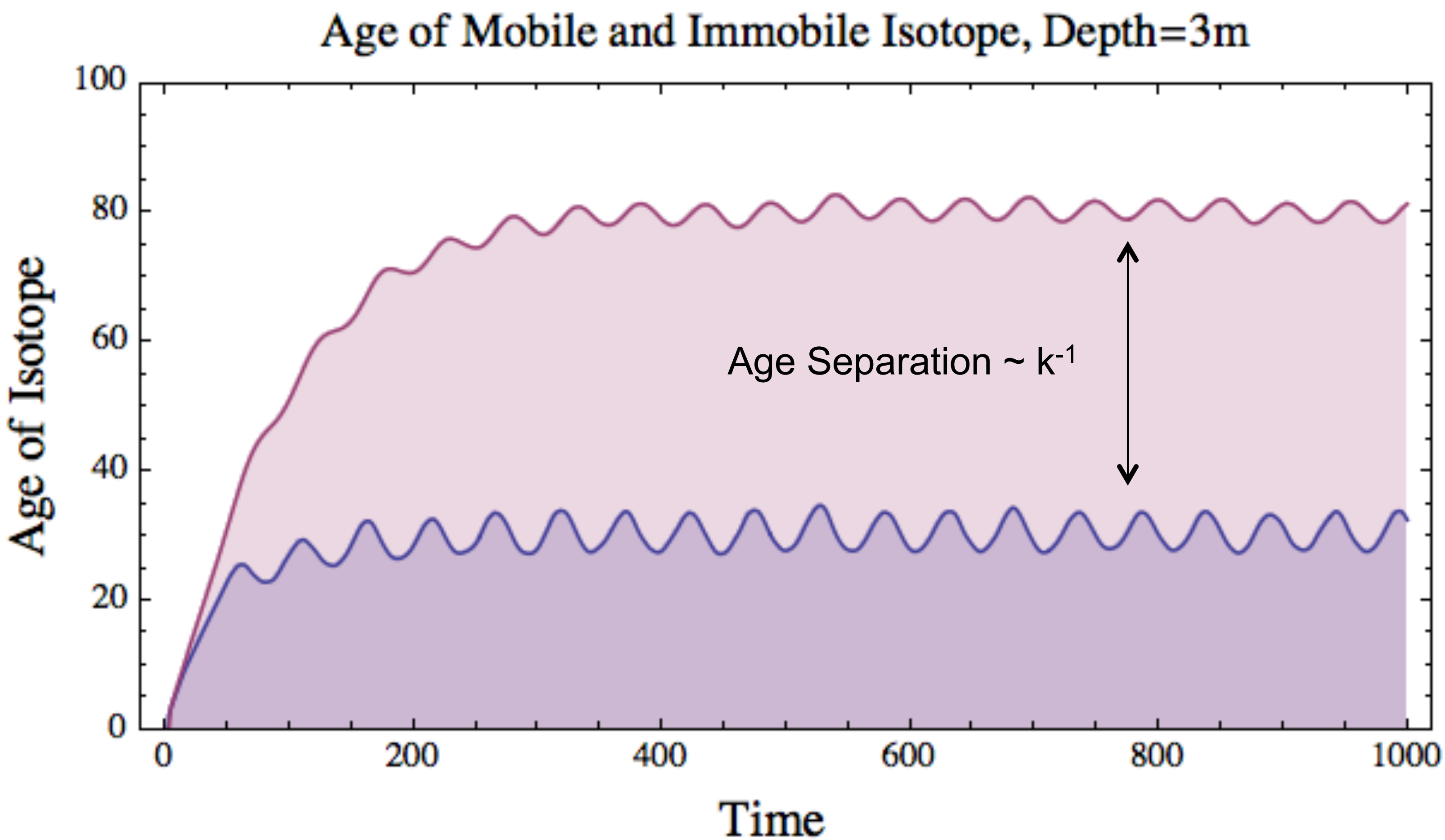
Simulated Isotope Ratio





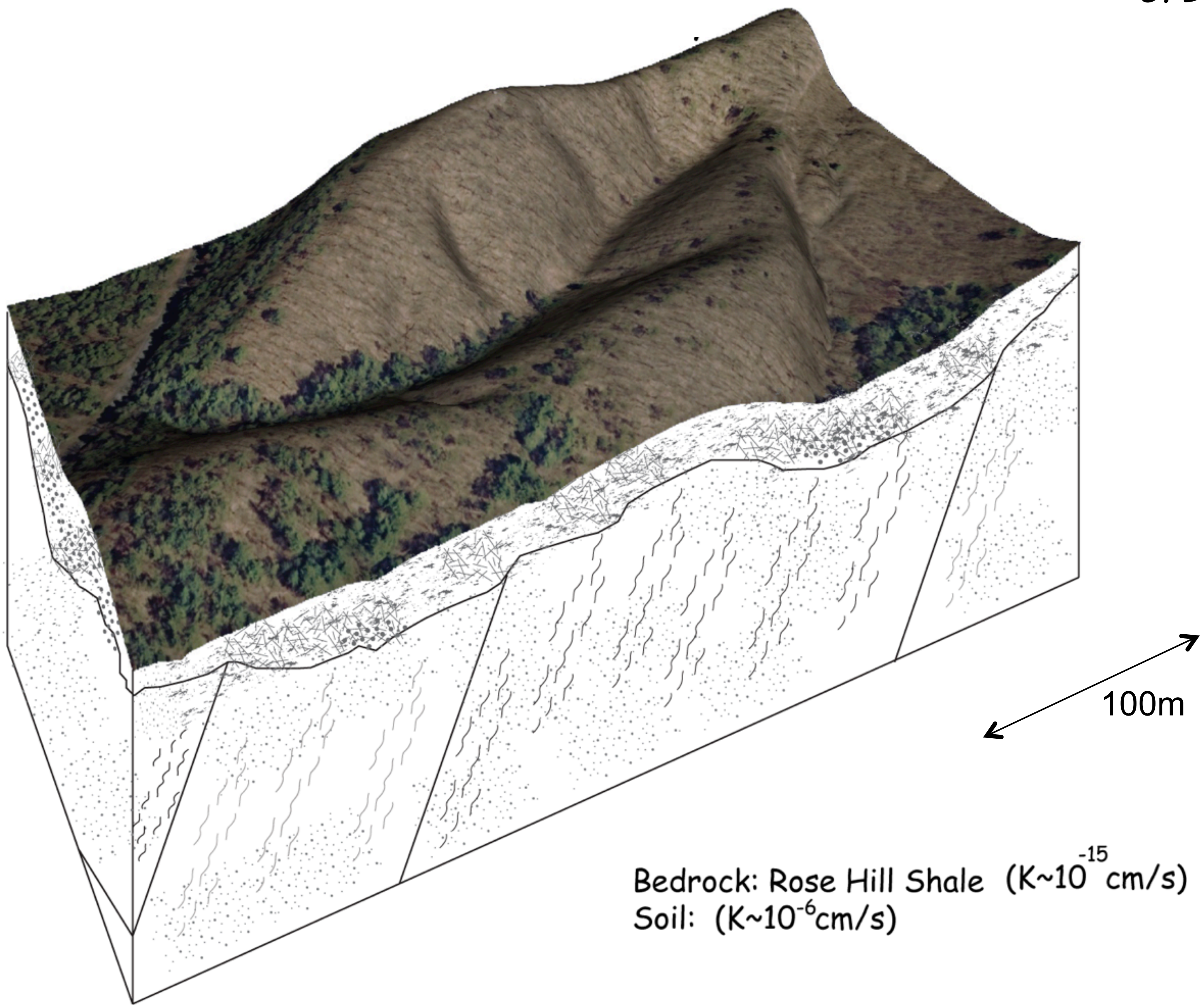
Simulated Age of





Modeling the Catchment Isoscape for Shale Hills

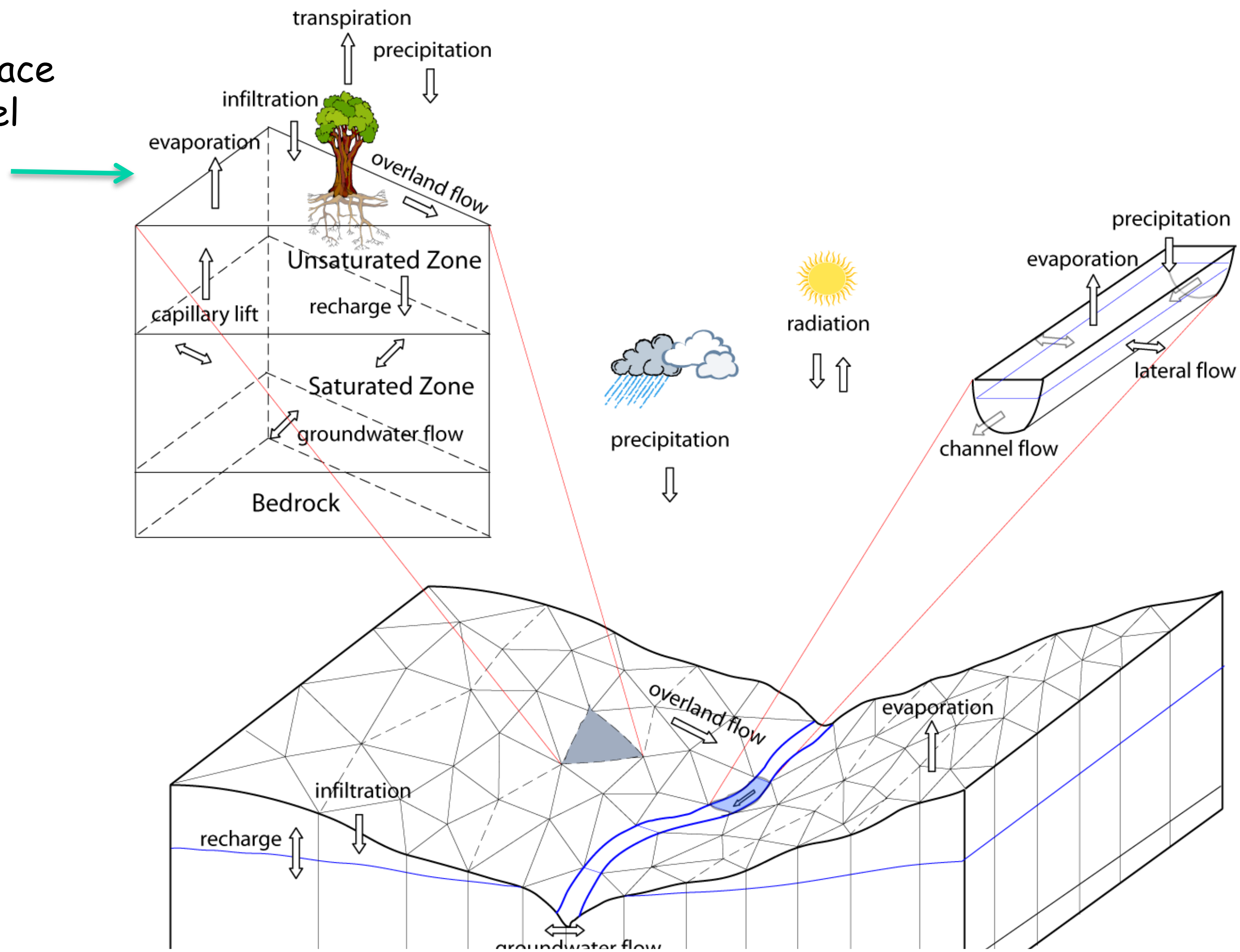
G. Bhatt 2012



Bedrock: Rose Hill Shale ($K \sim 10^{-15}$ cm/s)
Soil: ($K \sim 10^{-6}$ cm/s)

Penn State Integrated Hydrologic Model (PIHM)

Land Surface Model



M. Kumar, G. Bhatt, Duffy 2009, Y. Shi

Semi-Discrete Approach: PIHM

Process	Governing equation/model	Original governing equations	Semi-discrete form
Channel Flow	St. Venant Equation	$\frac{\partial h}{\partial t}+\frac{\partial (uh)}{\partial x}=q$	$\left(\frac{d\varsigma}{dt}=P_c-\sum Q_{gc}+\sum Q_{oc}+Q_{in}-Q_{out}-E_c\right)_i$ [1]
Overland Flow		$\frac{\partial h}{\partial t}+\frac{\partial (uh)}{\partial x}+\frac{\partial (vh)}{\partial y}=q$	$\left(\frac{\partial h}{\partial t}=P_o-I-E_o-Q_{oc}+\sum_{j=1}^{3}Q_s{}^{ij}\right)_i$ [1]
Unsaturated Flow	Richard Equation	$C(\psi)\frac{\partial \psi}{\partial t}=\nabla\cdot(K(\psi)\nabla(\psi+Z))$	$\left(\frac{d\xi}{dt}=I-q^0-ET_s\right)_i$ [2]
Groundwater Flow		$C(\psi)\frac{\partial \psi}{\partial t}=\nabla\cdot(K(\psi)\nabla(\psi+Z))$	$\left(\frac{d\zeta}{dt}=q^0+\sum_{j=1}^{3}Q_g{}^{ij}-Q_l+Q_{gc}\right)_i$ [3]
Interception	Bucket Model	$\frac{dS_I}{dt}=P-E_I-P_o$	$\left(\frac{dS_I}{dt}=P-E_I-P_o\right)_i$
Snowmelt	Temperature Index Model	$\frac{dS_{snow}}{dt}=P-E_{snow}-\Delta w$	$\left(\frac{dS_{snow}}{dt}=P-E_{snow}-\Delta w\right)_i$
Evapotranspiration	Pennman-Monteith Method	$ET_0=\frac{\Delta(R_n-G)+\rho_a C_p\frac{(e_s-e_a)}{r_a}}{\Delta+\gamma(1+\frac{r_s}{r_a})}$	$\left(ET_0=\frac{\Delta(R_n-G)+\rho_a C_p\frac{(e_s-e_a)}{r_a}}{\Delta+\gamma(1+\frac{r_s}{r_a})}\right)_i$

Distributed IsotopeTransport (Bhatt, 2012)

Transport Equation

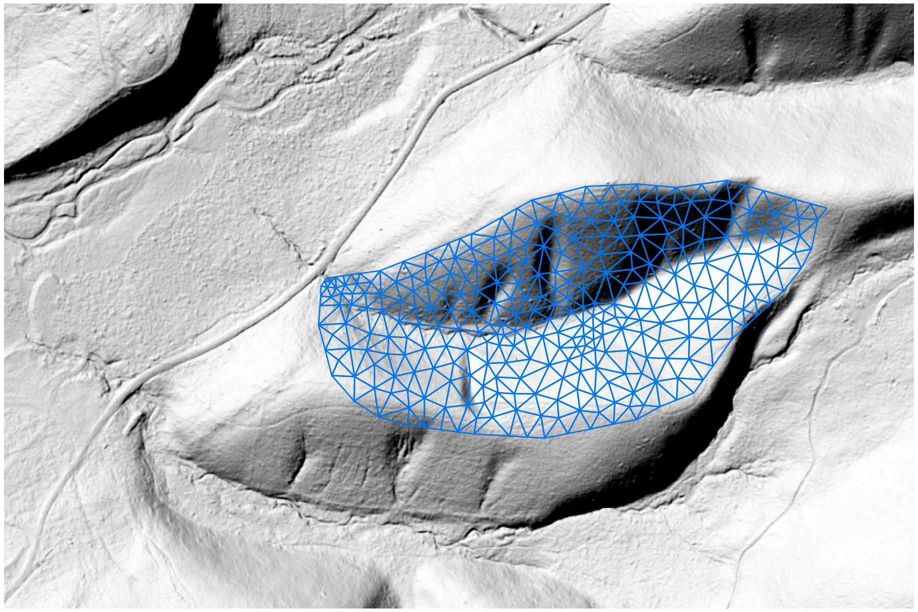
$$\theta A_B \left[C_i \frac{\partial h_i}{\partial t} + h_i \frac{\partial C_i}{\partial t} \right] = -\oint\!\!\oint_{\partial \Omega \mathrm{i}} \mathbf{n} \cdot (\boldsymbol{V} \bar{C})\, dA + \oint\!\!\oint_{\partial \Omega \mathrm{i}} \mathbf{n} \cdot (\mathbf{D} \nabla \bar{C})\, dA + \int_{\Omega \mathrm{i}} q_S C_S \, dV\!\!\!-$$

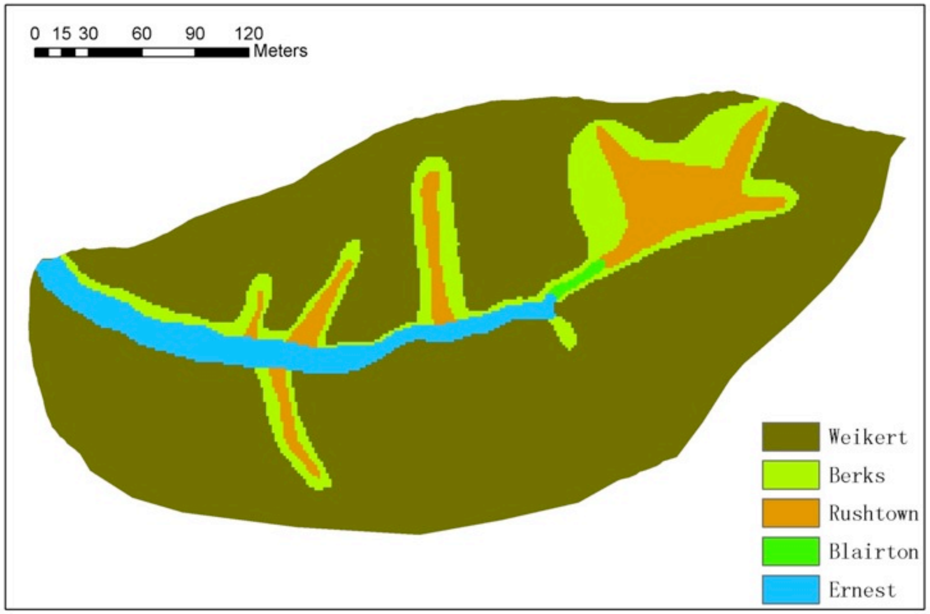
Semi-Discrete Form

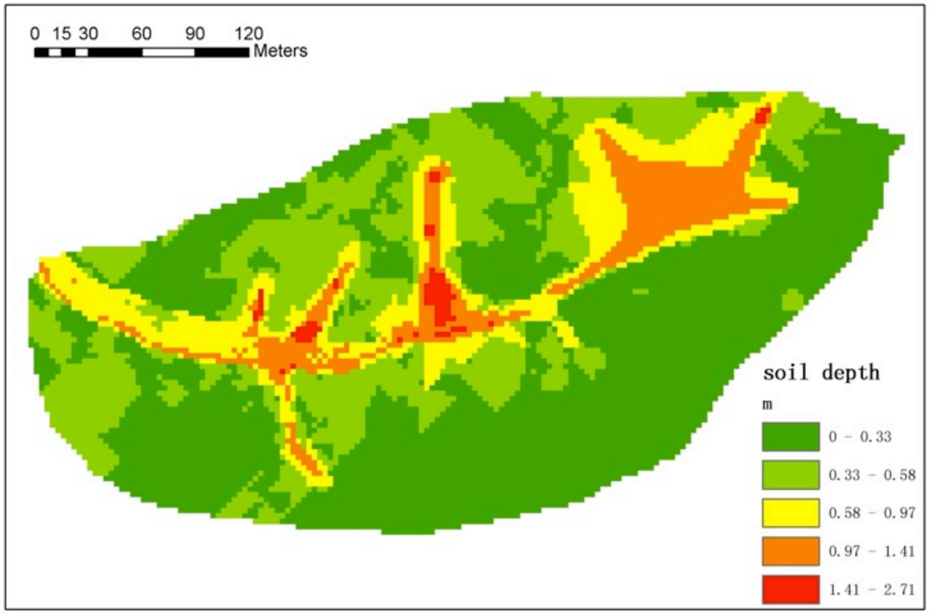
$$\frac{\partial C_i}{\partial t} = \sum_{\partial \Omega \mathrm{i}} \frac{\bar{Q}}{\theta A_B h_i} [C_i - \bar{C}] + \sum_{\Omega \mathrm{i}} \frac{Q_S}{\theta A_B h_i} [C_i - \bar{C_S}] + \sum_{\partial \Omega \mathrm{i}} \frac{\mathbf{n} \cdot (\mathbf{D} \nabla \bar{C}) A}{\theta A_B h_i}$$

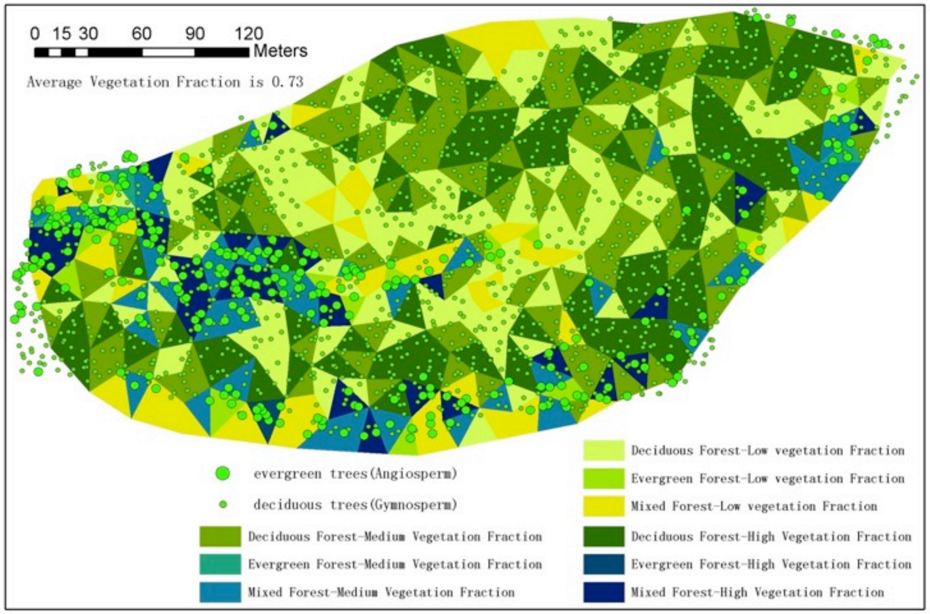
Horizontal Advection | Vertical Flux | Dispersive Flux

CZO Data ->lidar, Soil, Regolith,Veg



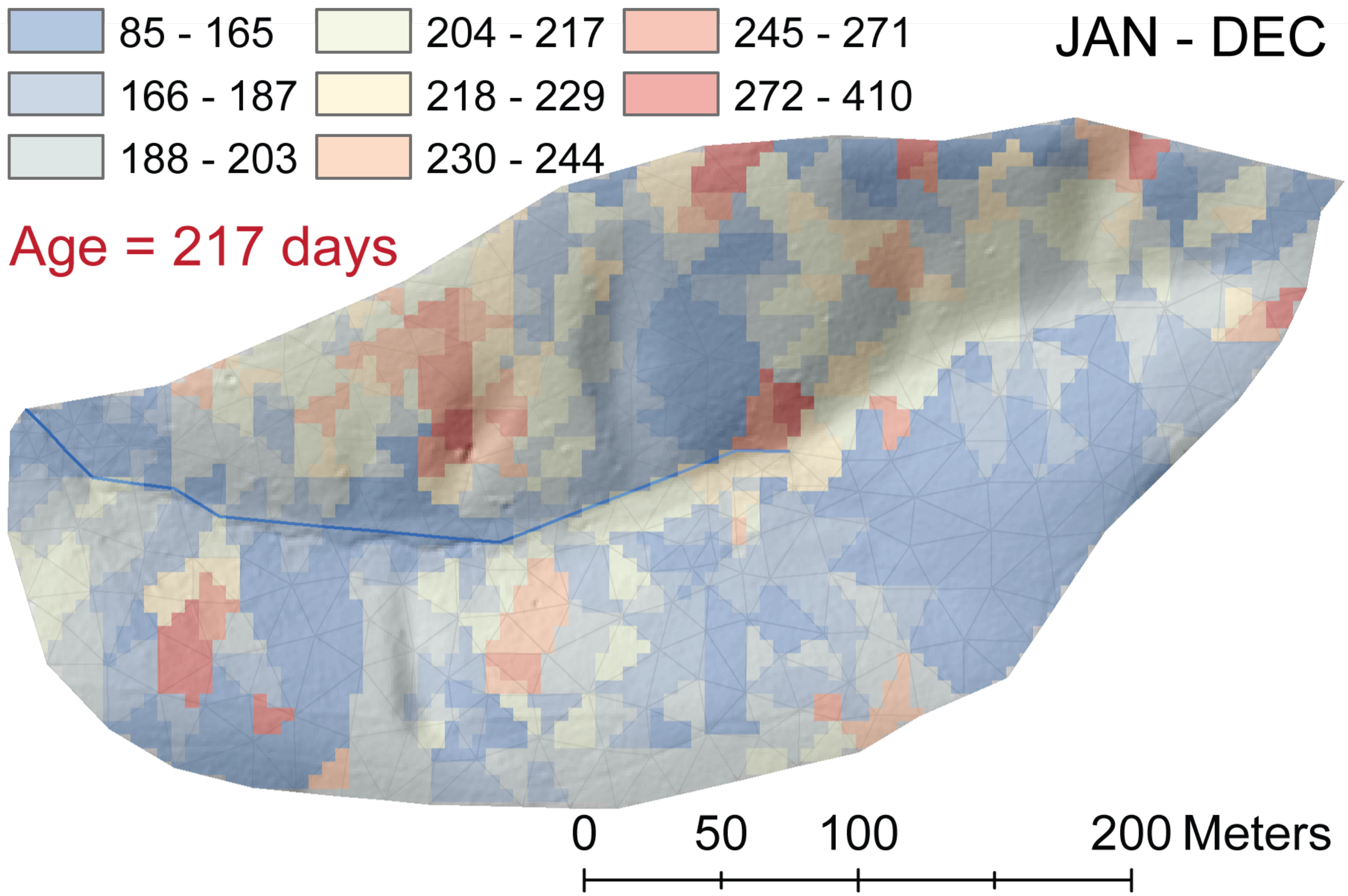




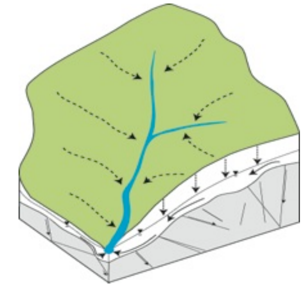


Simulated Average Age of Groundwater + Soil Water At Shale Hills CZO

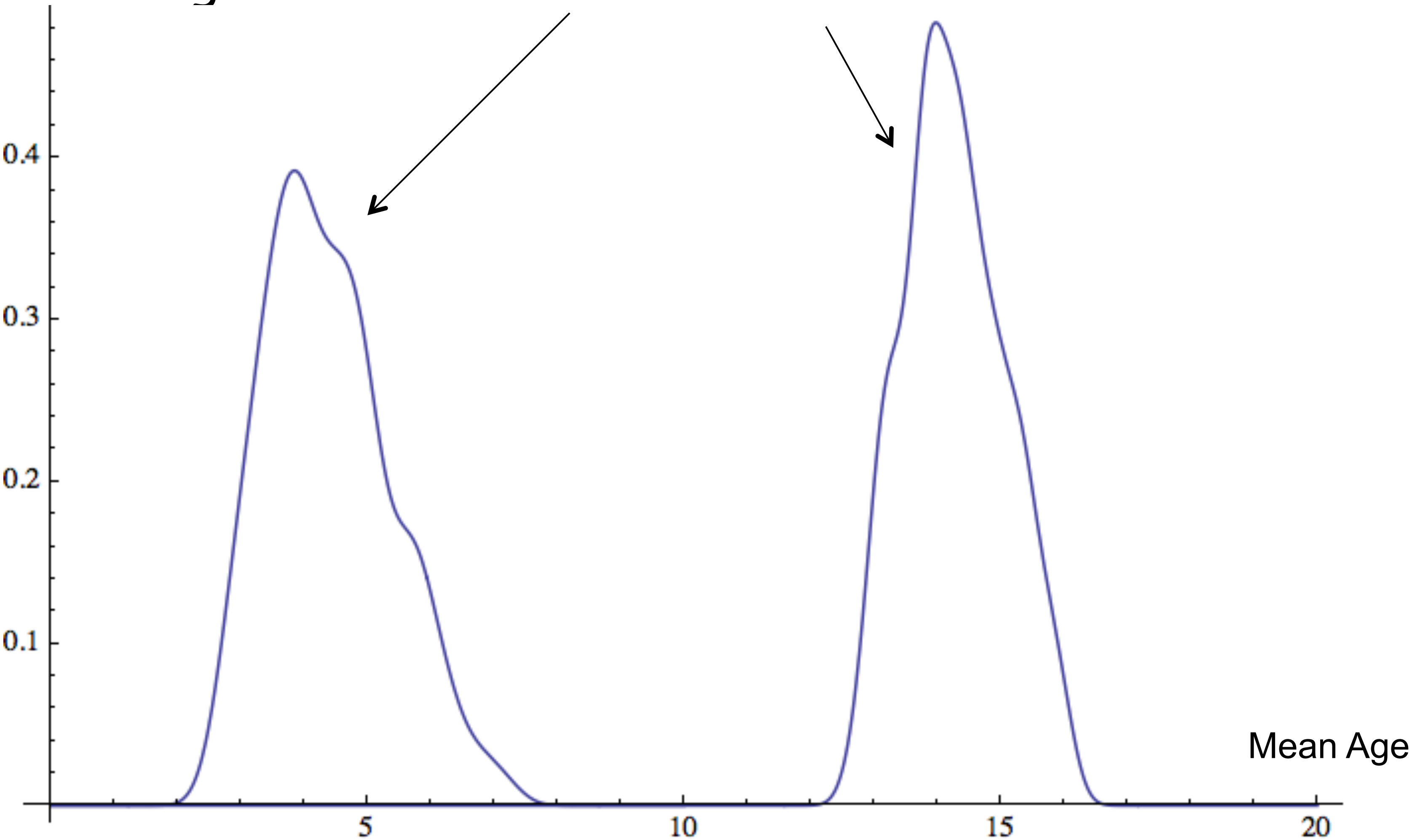
G. Bhatt, PhD 2012



Random Input C_i and Q_i

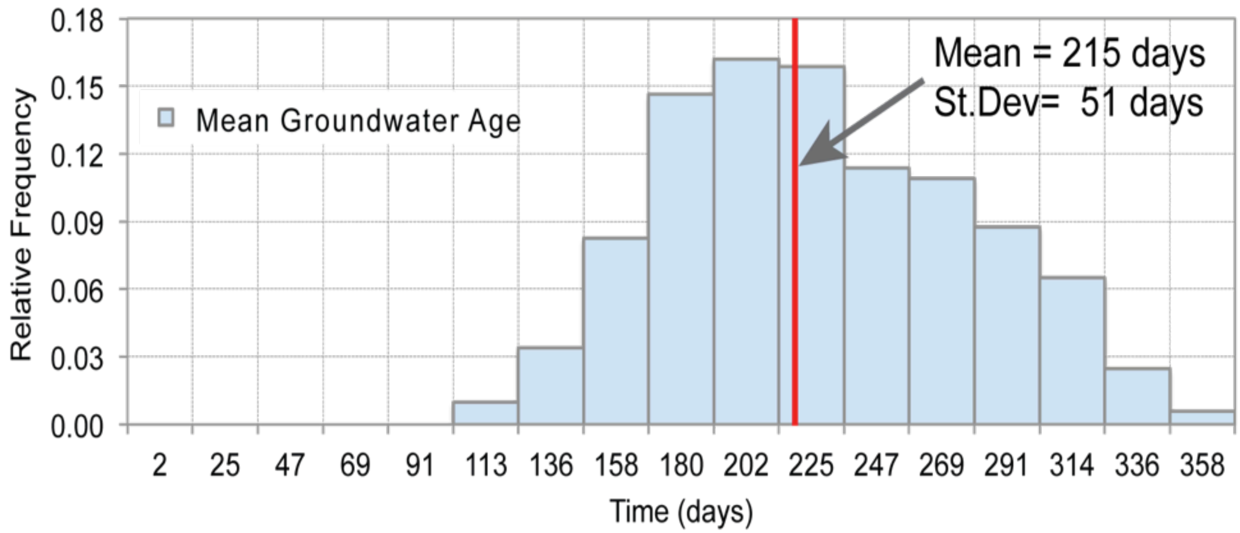


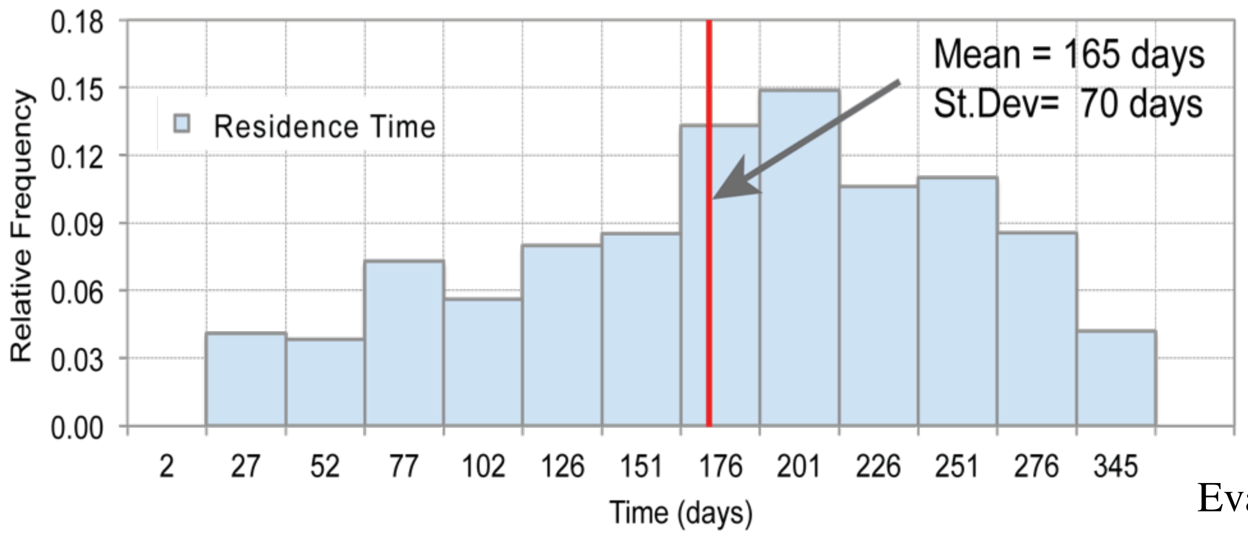
Simulated Age PDF for Mobile and Immobile Water



Relative Frequency Groundwater Age & Runoff Residence Time

G. Bhatt, PhD 2012

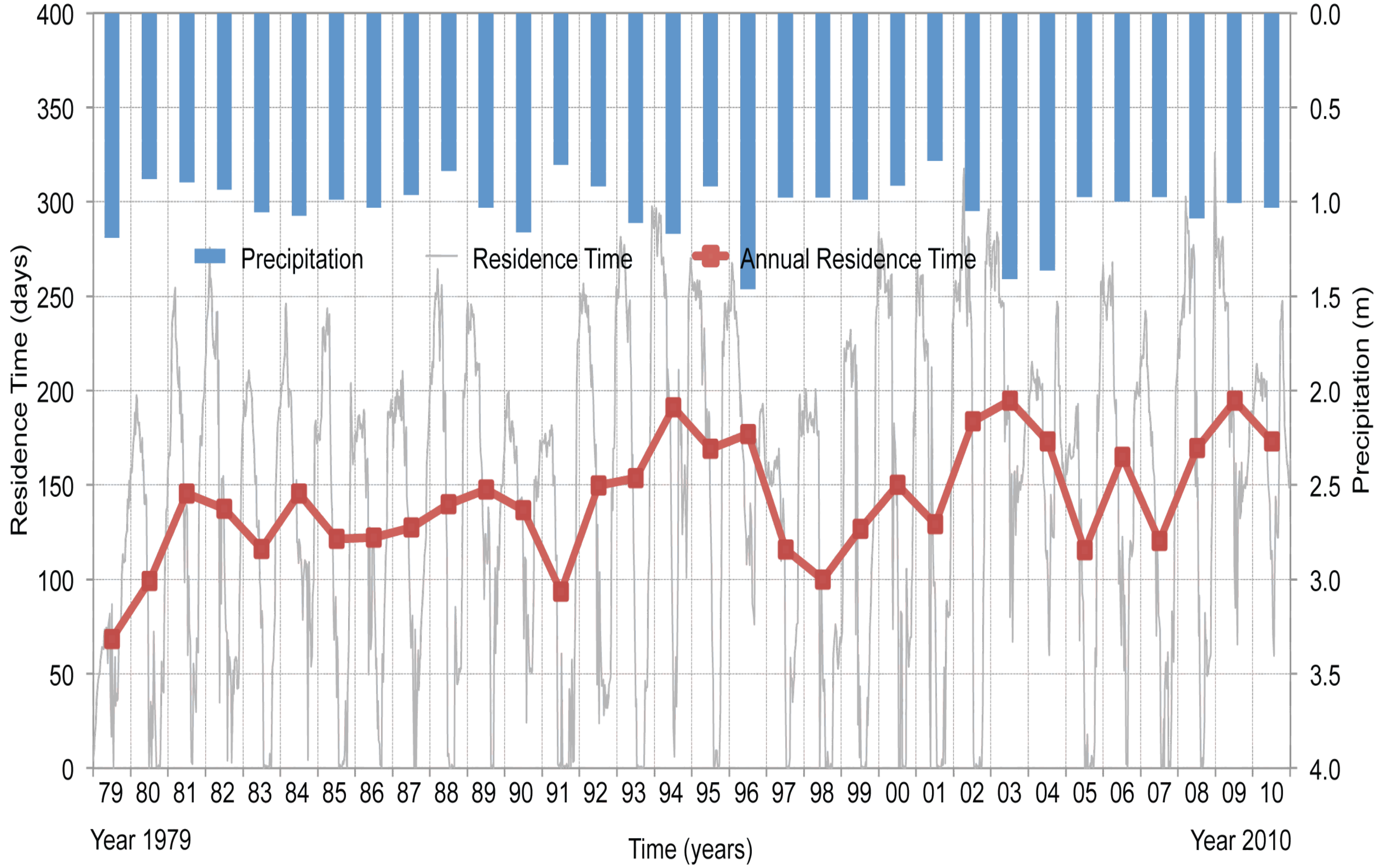




Evan Thomas

1979-2010 Reanalysis Forcing & Dynamic Residence Time of Runoff

G. Bhatt, PhD 2012



Atmospheric Modeling of Stable Isotopes $\delta^{18}O$ in Precipitation A new research product

IsoRSM experiment over northeast US

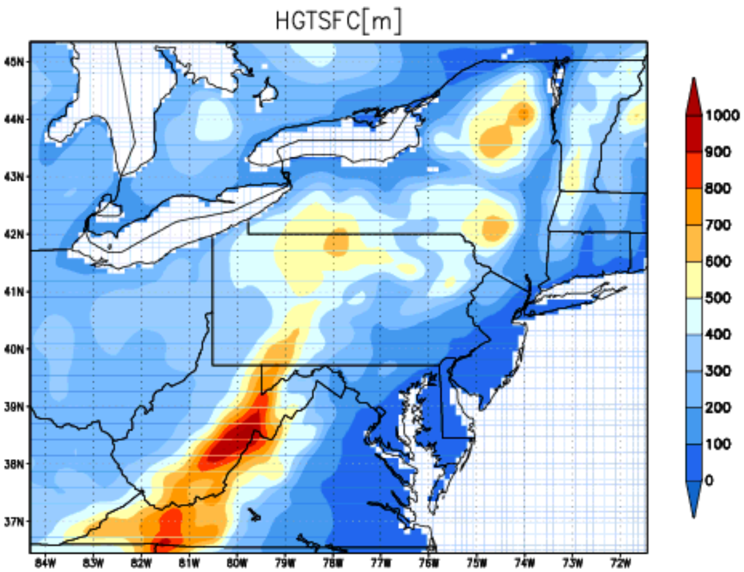
10km Simulation covering 85.5W-71.3W/35.5N-46.2N

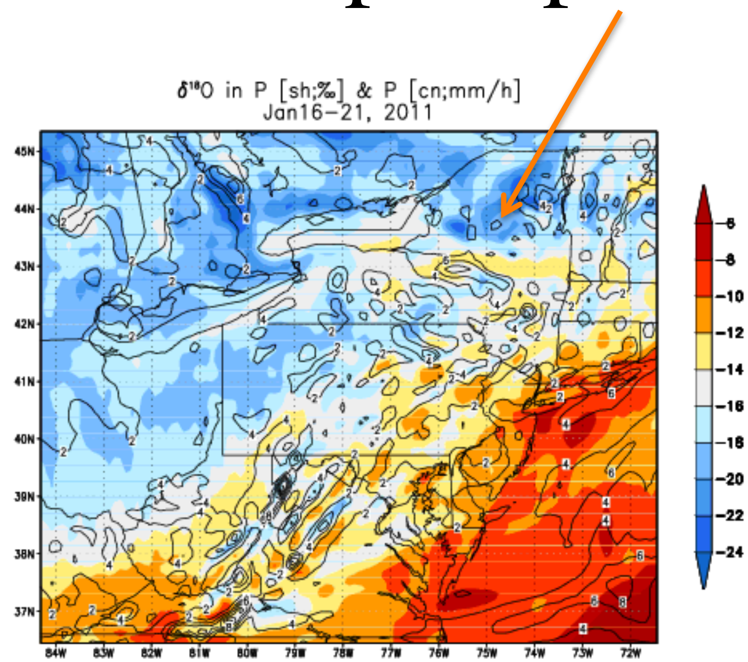
Boundary Conditions: IsoGSM simulation based on NOAA Climate Reanalysis

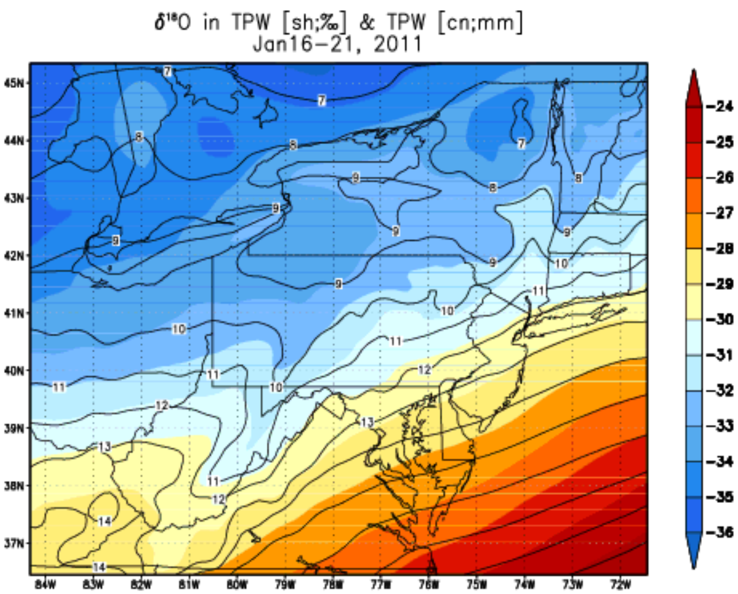
Kei Yoshimura, University of Tokyo, Japan
(Yoshimura et al., 2010)

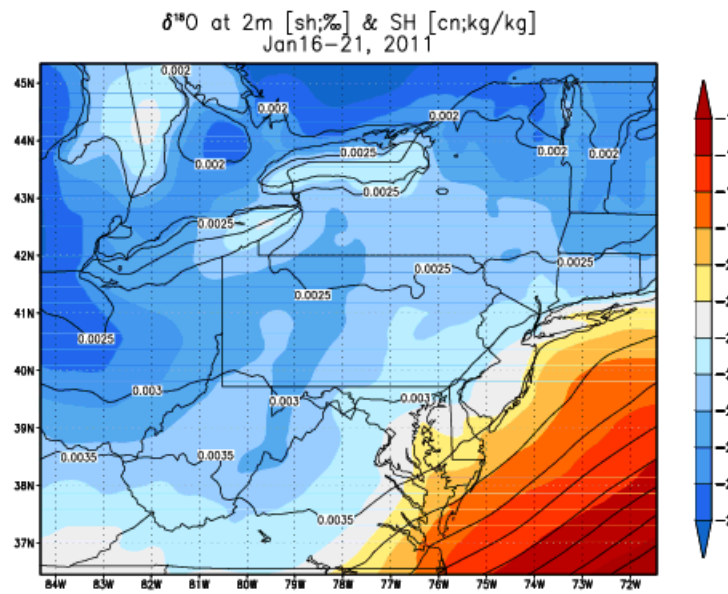
10 km res.

$\delta^{18}O$ in precipitation

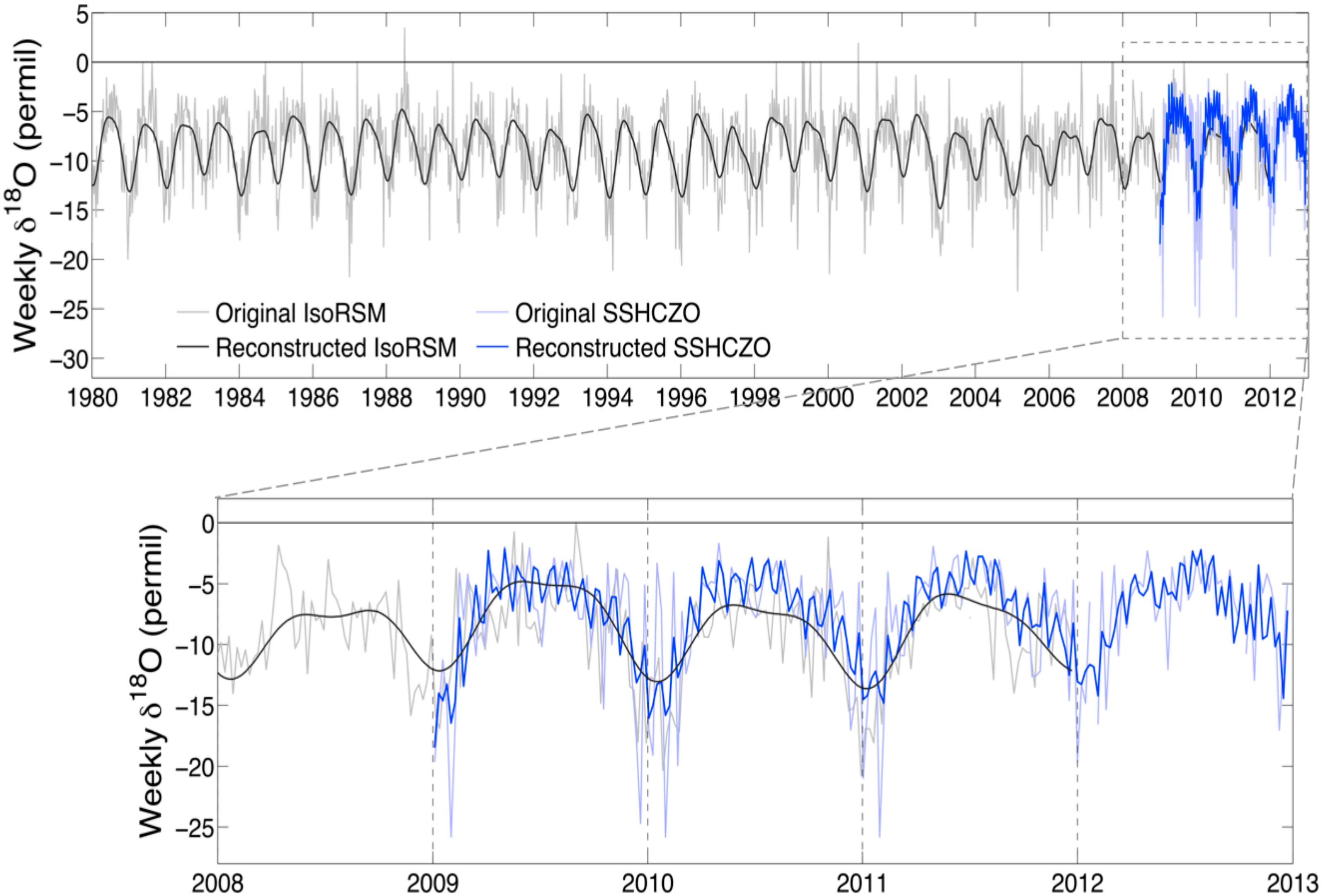






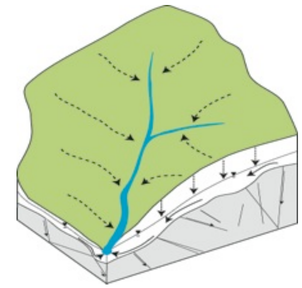


Validation of IsoRSM Stable Isotopes in Precipitation with Shale Hills CZO Data



Evan Thomas, MS Penn State

Conclusions:



The "Mean Age" of waters can be simulated directly using transport theory and stable isotopes

The particular form of the age- or transit-time distribution function is not necessary in this theory.

Mobile-Immobile storage attenuates the seasonal amplitude through lateral diffusive exchange, increasing the relative age of infiltrating waters

Vegetation using immobile water is not detached from the mobile phase but rather exchange occurs by capillary diffusion

The isoscape is a powerful concept for assessing space-time patterns of age and residence time at the catchment scale

Thank You