From Pattern to Prediction:

Combining chemical, isotopic, and discharge data to understand karst aquifers

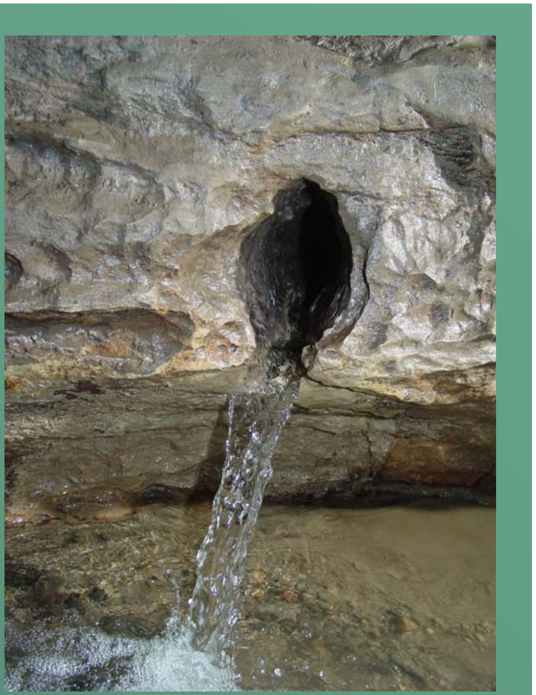


Photo: Allen Lewerer

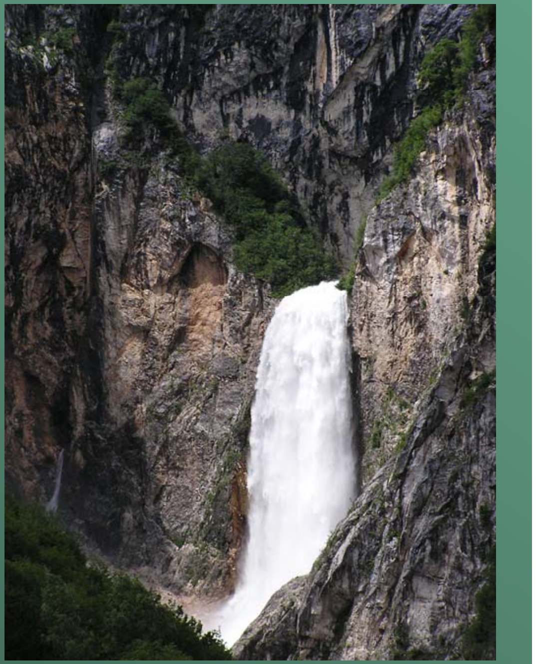


Photo: Dan Doctor

Daniel H. Doctor

Eastern Earth Surface Processes Science Center

Reston, VA

U.S. Department of the Interior
U.S. Geological Survey

Outline of this talk

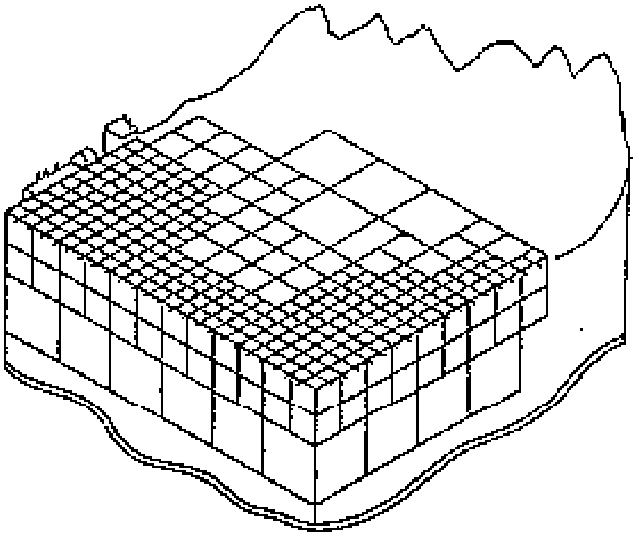
- Ground water vs. surface water modeling approaches
- Conceptual models
- Linking hydrologic and chemical patterns
- Future directions

Groundwater studies

- Little hydrologic data to work with (wells)
- Physics is known→governing equations
- Problem: discretization, model geometry

GROUNDWATER MODELS

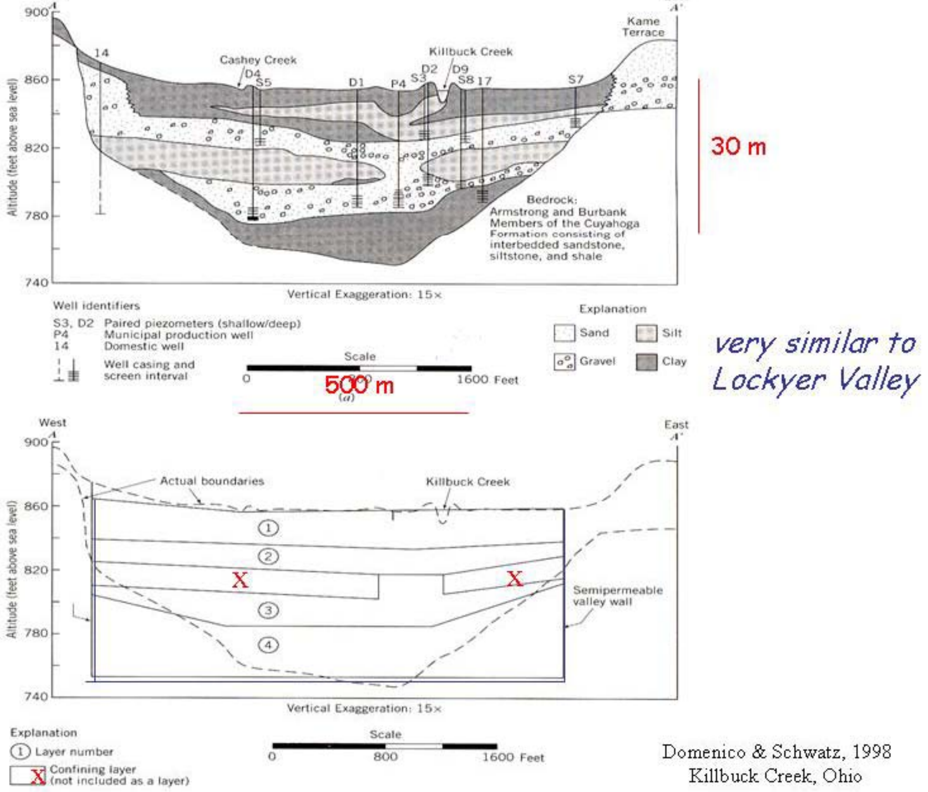
- **Model geometry—natural patterns?**



Develop hydrogeological units for model

geological cross section

conceptualised units for FDM

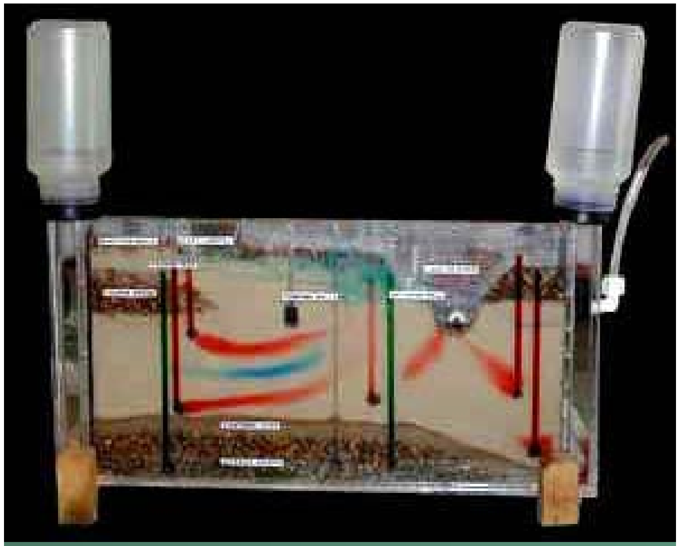


30 m

500 m

very similar to Lockyer Valley

Domenico & Schwatz, 1998
Killbuck Creek, Ohio

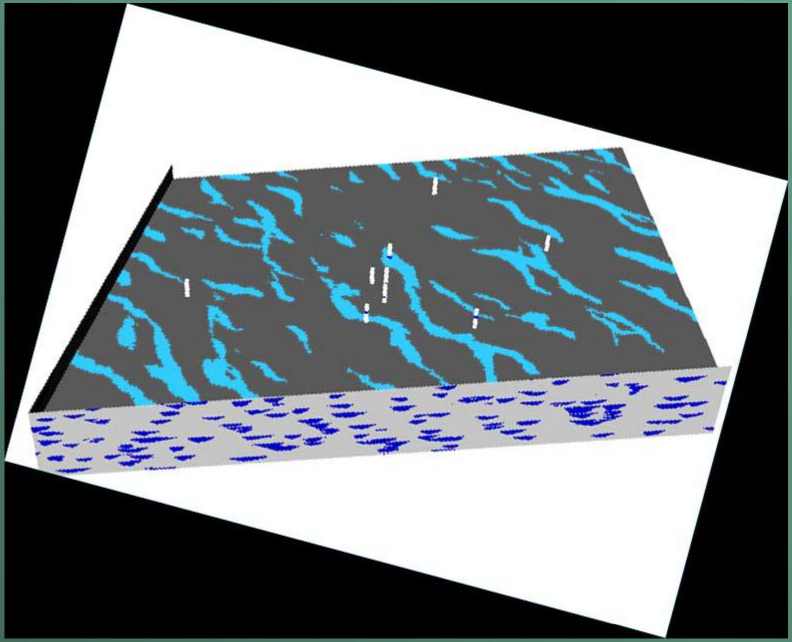


Complete the sequence…

- We are trained from an early age to recognize patterns
- Why has the science of hydrogeology focused on mimicking "*equivalent homogeneous porous media*"?
- The "silicon siren"

MADE Site-Lessons learned

"Recent studies at the Macrodispersion Experiment (MADE) site in Columbus, Mississippi have indicated that the preferential flow paths resulting from aquifer heterogeneities at **decimeter (dm) and smaller scales** appear to have a dominant effect on plume-scale solute transport."



http://pangea.stanford.edu/research/groups/hydrogeology/research.php?rg_id=15&rgpr_id=26

Catchment Studies

- Lots of data
  - weirs, piezometers, lysimeters, rain gages, evaporation pans, etc.

- Geometry is relatively well-constrained
  - topography, surface network, subsurface characteristics

- Governing equations?
  - Simplified systems approach works best (‘lumped’ parameter models)

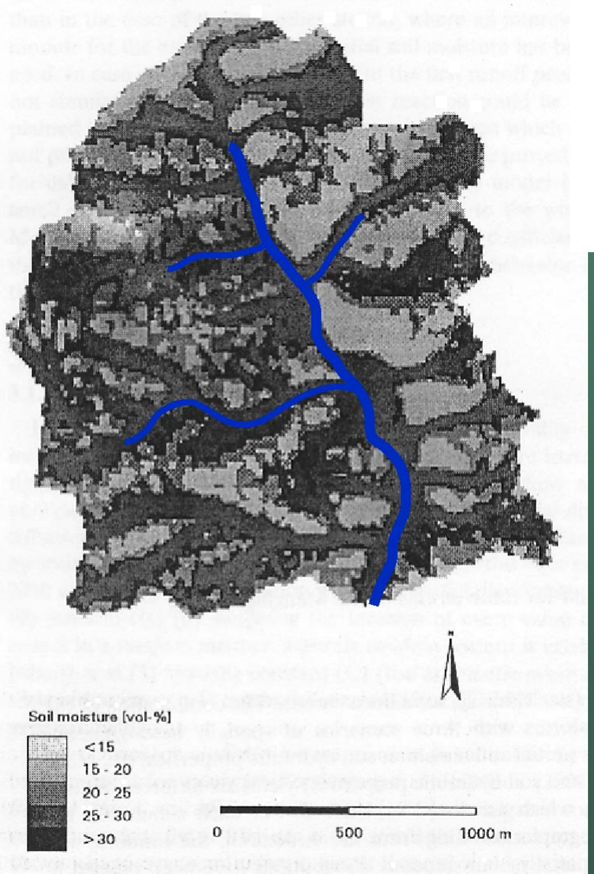
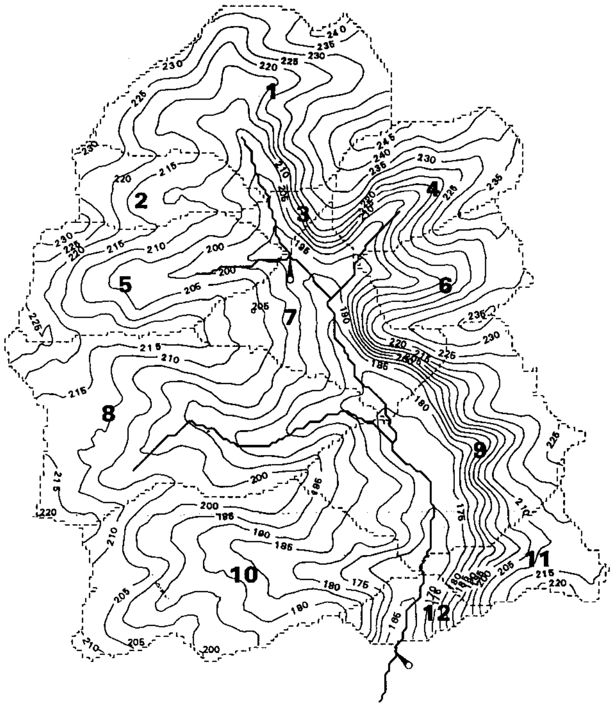


Figure 4. The measured/interpolated soil moisture of the 0- to 60-cm layer on June 20, 1994, in Menzingen.



Merz and Plate, 1997

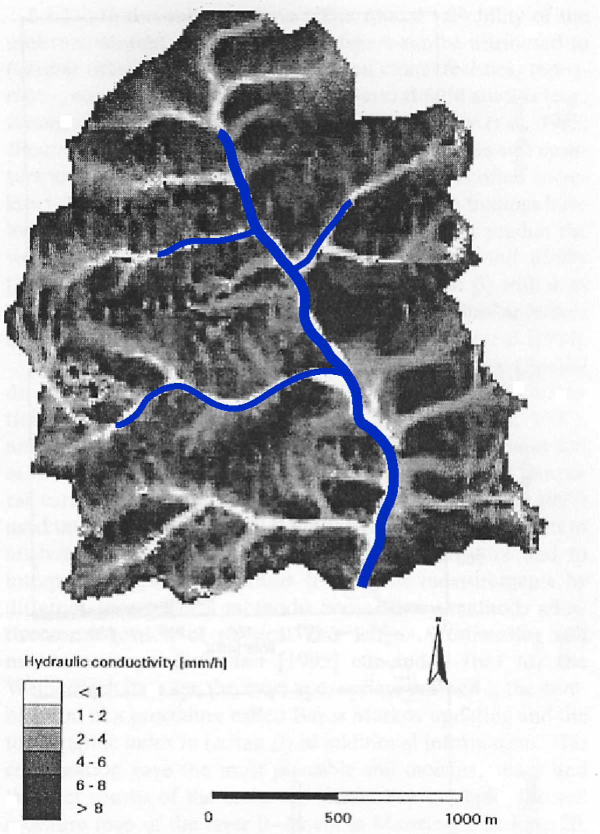


Figure 5. Assumed spatial distribution of saturated hydraulic conductivity.

Conclusions from graphical method:

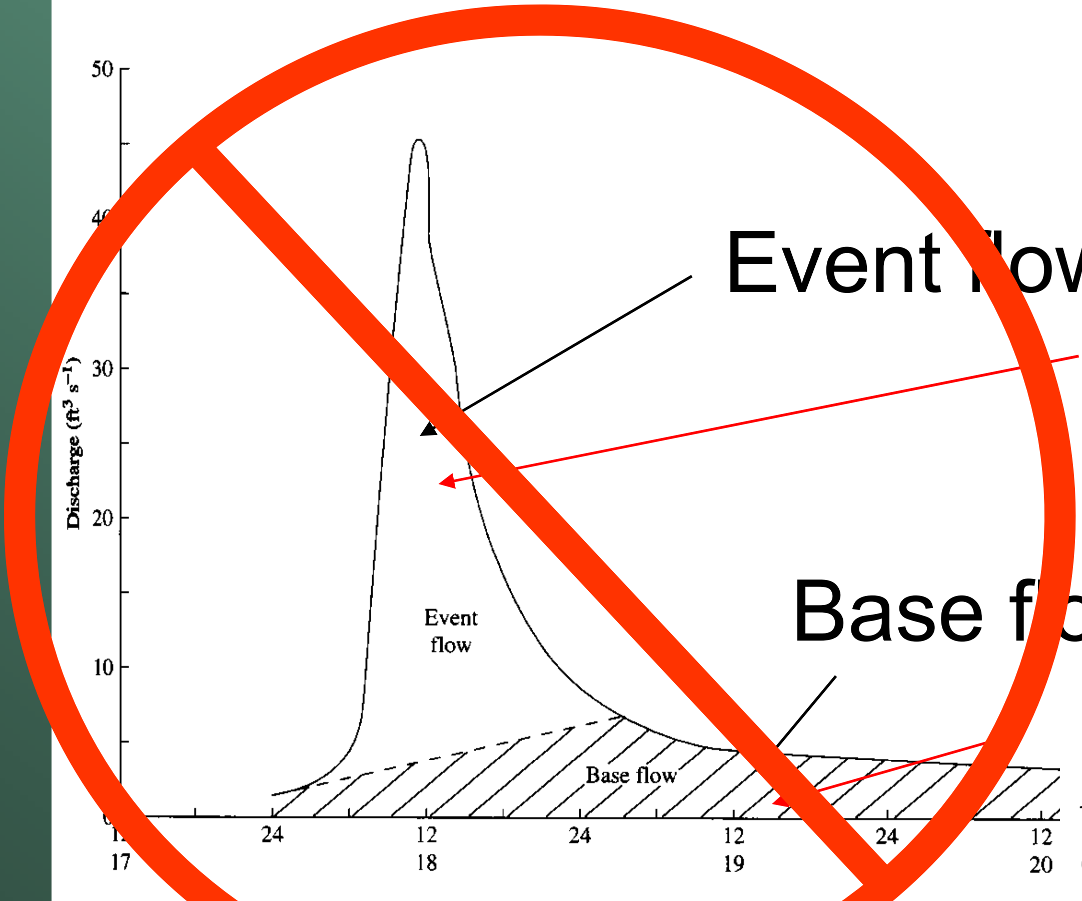


FIGURE 9-5

Hydrograph separatio lied to the hydrograph of Watershed W-3, S pers River Research Watershed, Danville, VT, to rain of 18 September 1973. See Ex 1.

Event flow=60%

Quick Flow,
Assumed to be
precipitation

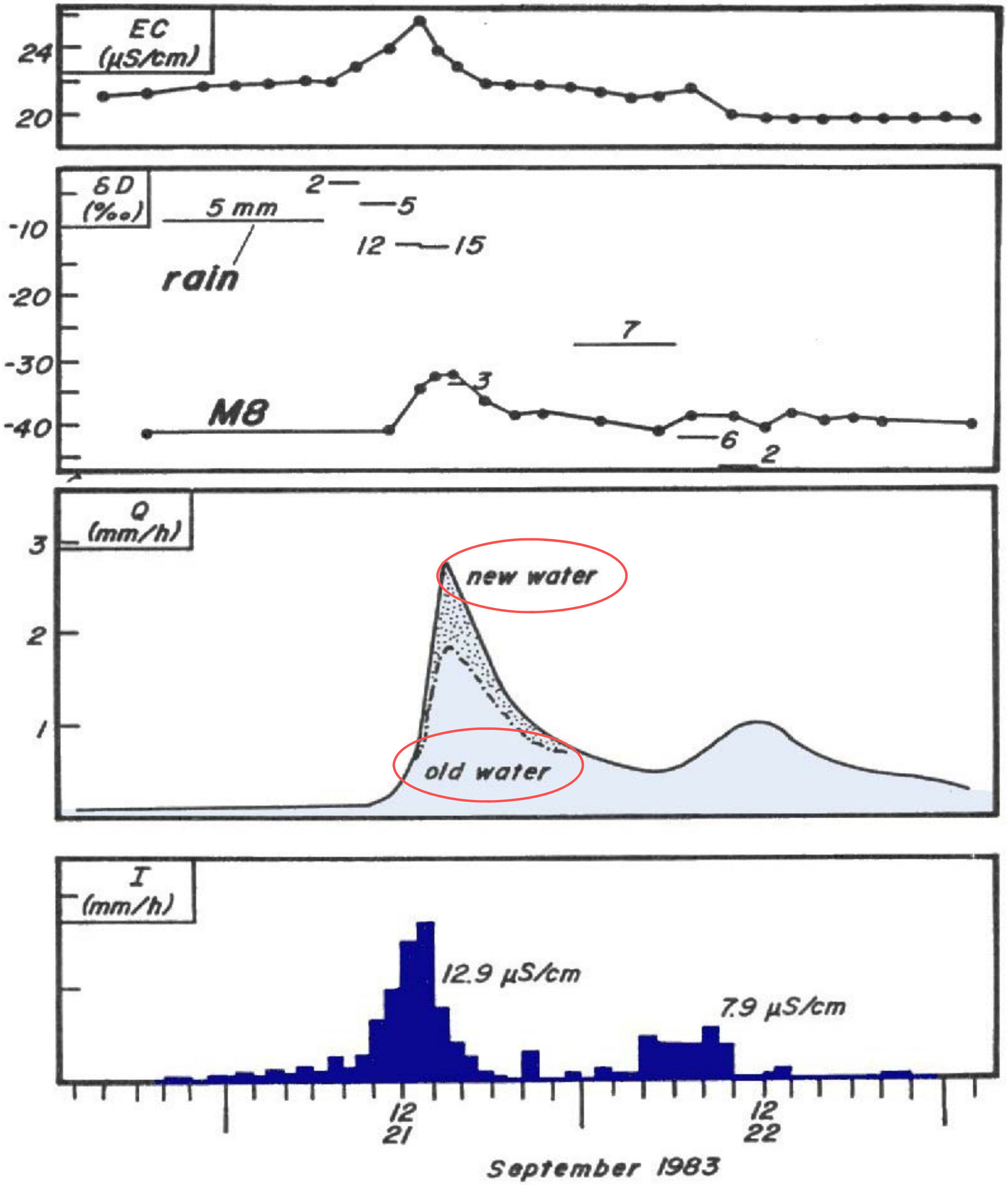
Base flow=40%

Slow Flow—
Assumed to be
Groundwater/interflow

Dingman, 1997

Conclusion from isotopic hydrograph separation:

Groundwater is the main component of storm flow in many streams

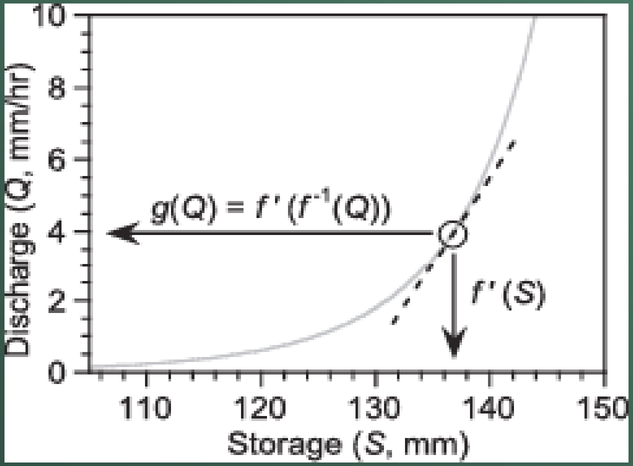


Anderson and Burt, 1990

Main problem:
Storage-discharge relationship

- "The challenge is to find appropriate functional forms for representing the **hysteretic storage-discharge relationship**." (Beven, 2006)

- **Kirchner, WRR, 2009**



$$dS/dt = P - E - Q$$

"Sensitivity function":

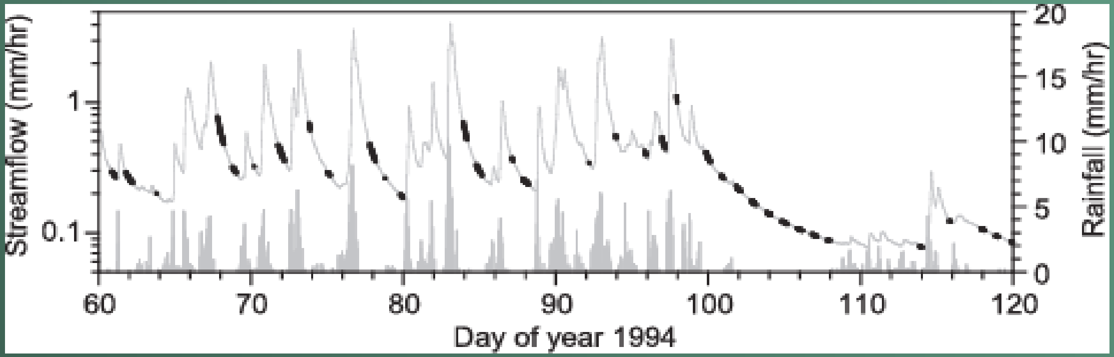
$$g(Q) = dQ/dS$$

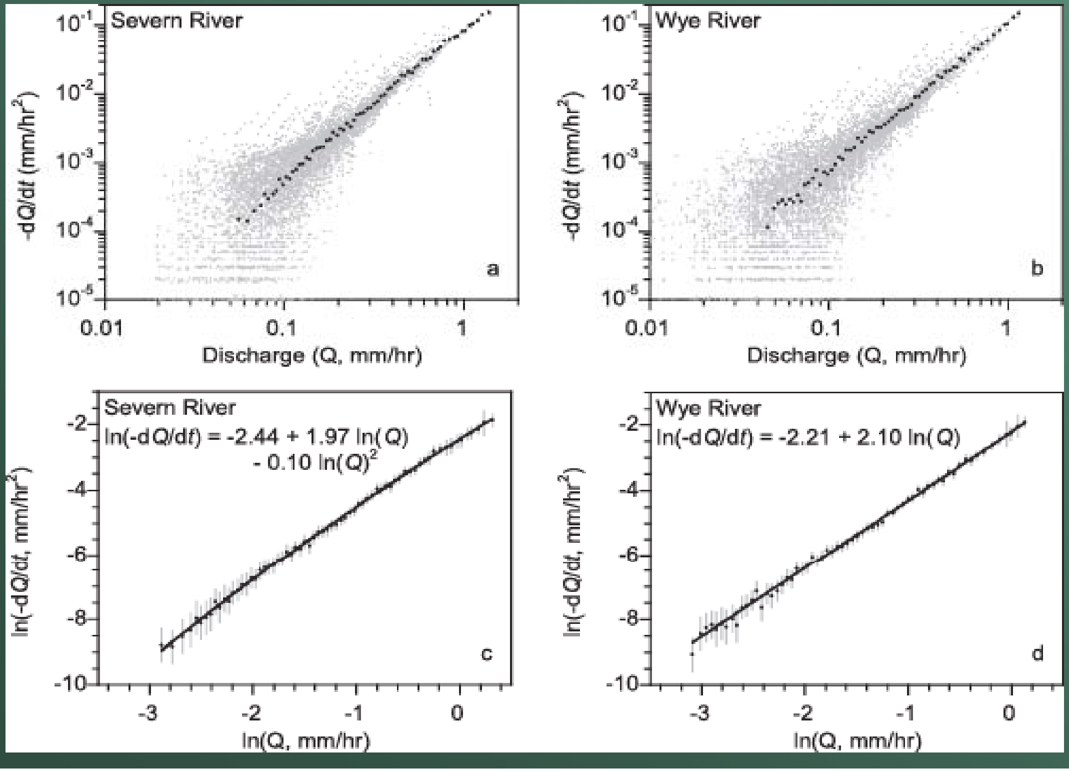
when P<<Q, E<<Q :

$$g(Q) = \frac{-dQ/dt}{Q}$$

How to estimate the change in discharge per change in storage, g(Q)?

- Hydrograph recession analysis





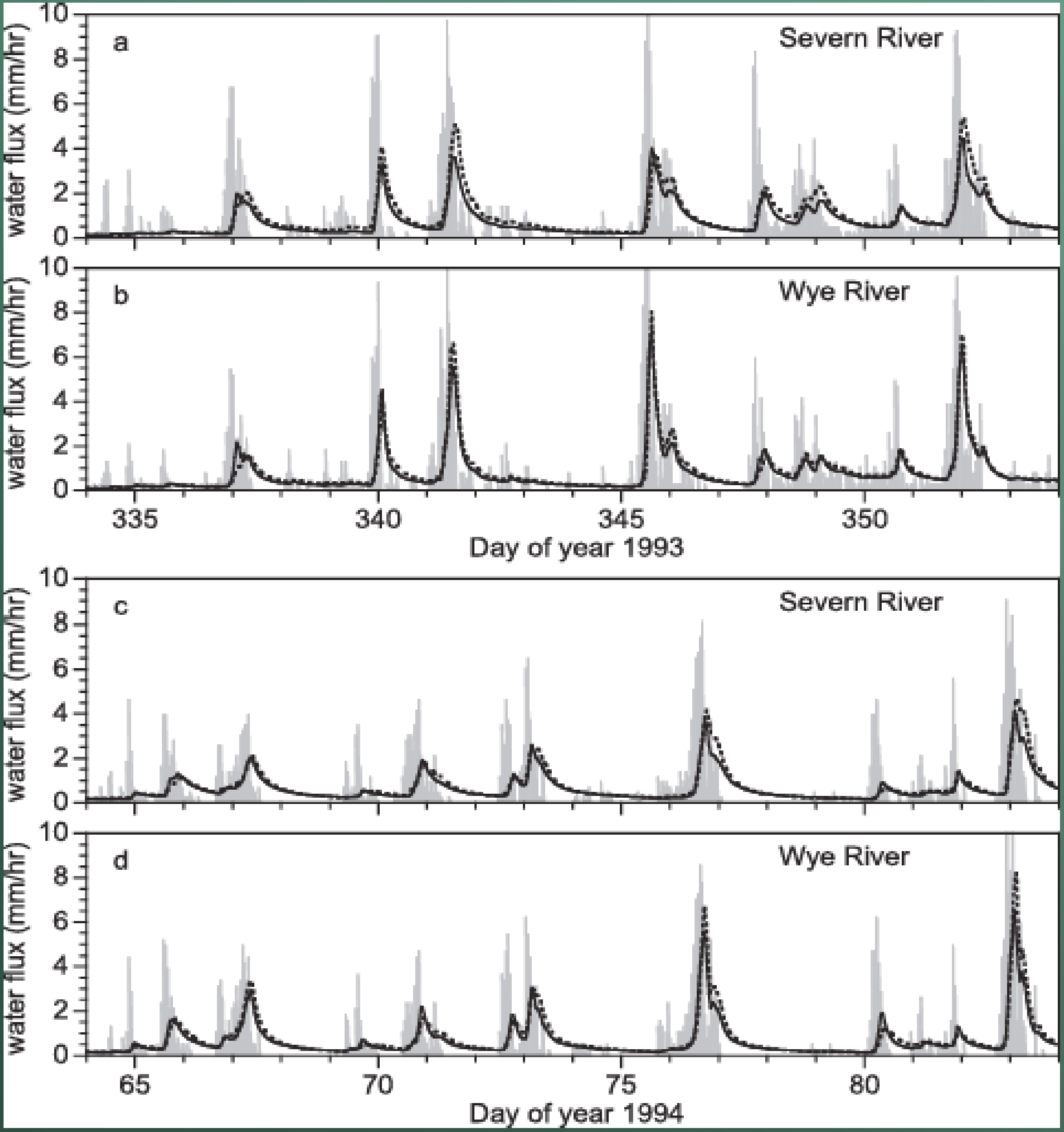
when P<<Q, E<<Q :

$$g(Q) = \frac{-dQ/dt}{Q}$$

Rainless nighttime intervals

Form is quadratic here, though need not be specified

MODEL PREDICTION:



Model parameters determined from recessions alone; no parameters were calibrated to the time series

Brutsaert-Nieber Method

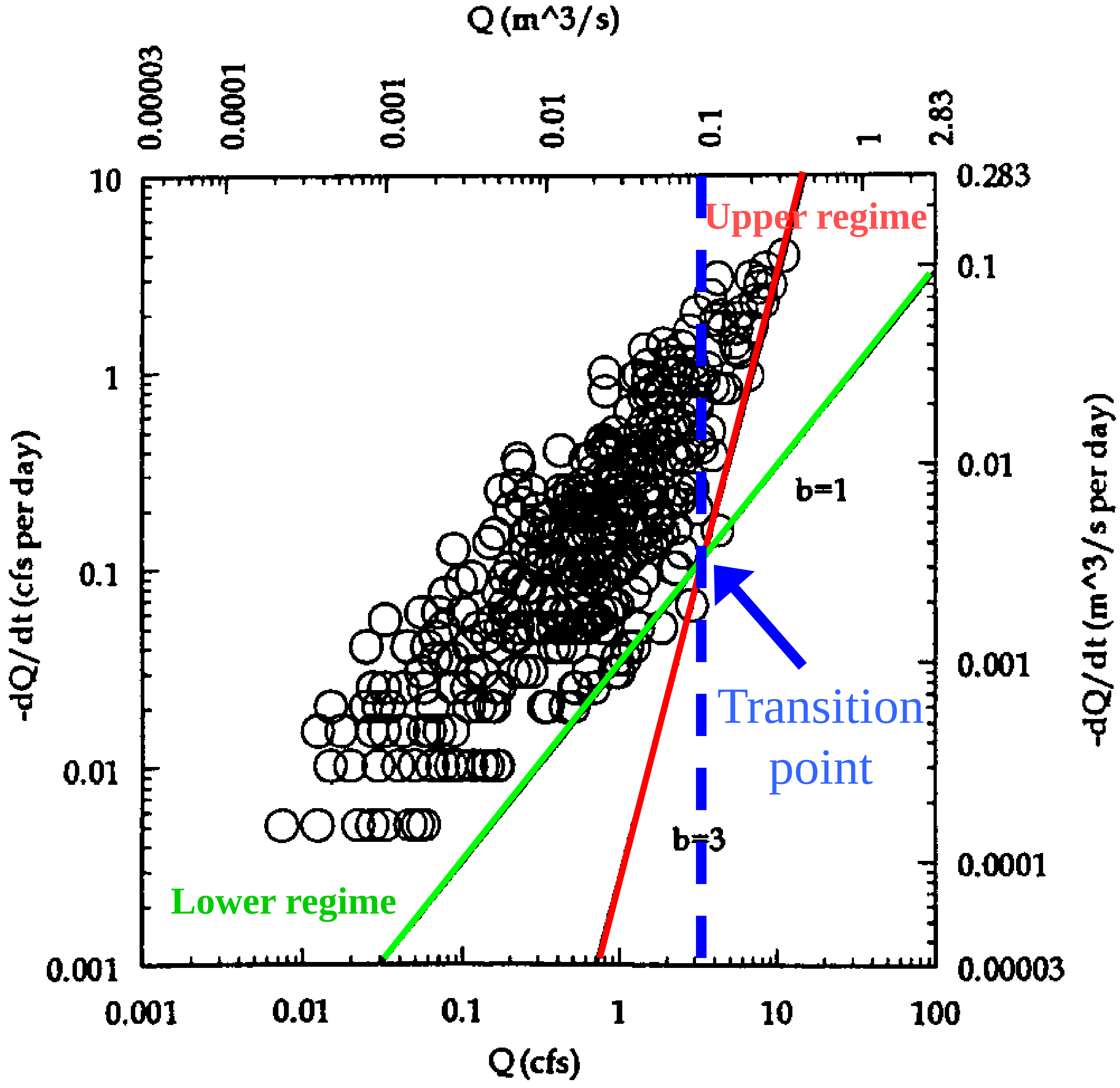
(Brutsaert & Nieber, WRR, 1977)

Based on a solution to the Boussinesq equation (for an idealized, unconfined, horizontal 1-D aquifer) of the form:

$$\mathbf{dQ/dt = -}\boldsymbol{a}\mathbf{Q}^{\boldsymbol{b}}$$

- *a* and *b* are constants

- The equation above defines a linear lower envelope on a log-log plot of the slope of the hydrograph (dQ/dt) vs. Q


Q (m^3/s)
0.00003
0.0001
0.001
0.01
0.1
1
2.83
10
1
0.1
0.01
0.001
0.283
0.1
0.01
0.001
0.0001
0.00003
0.001
0.01
0.1
1
10
100
Q (cfs)
-dQ/dt (cfs per day)
-dQ/dt (m^3/s per day)
Upper regime
Lower regime
b=1
b=3
Transition point

Conceptual model of a 1-D aquifer:

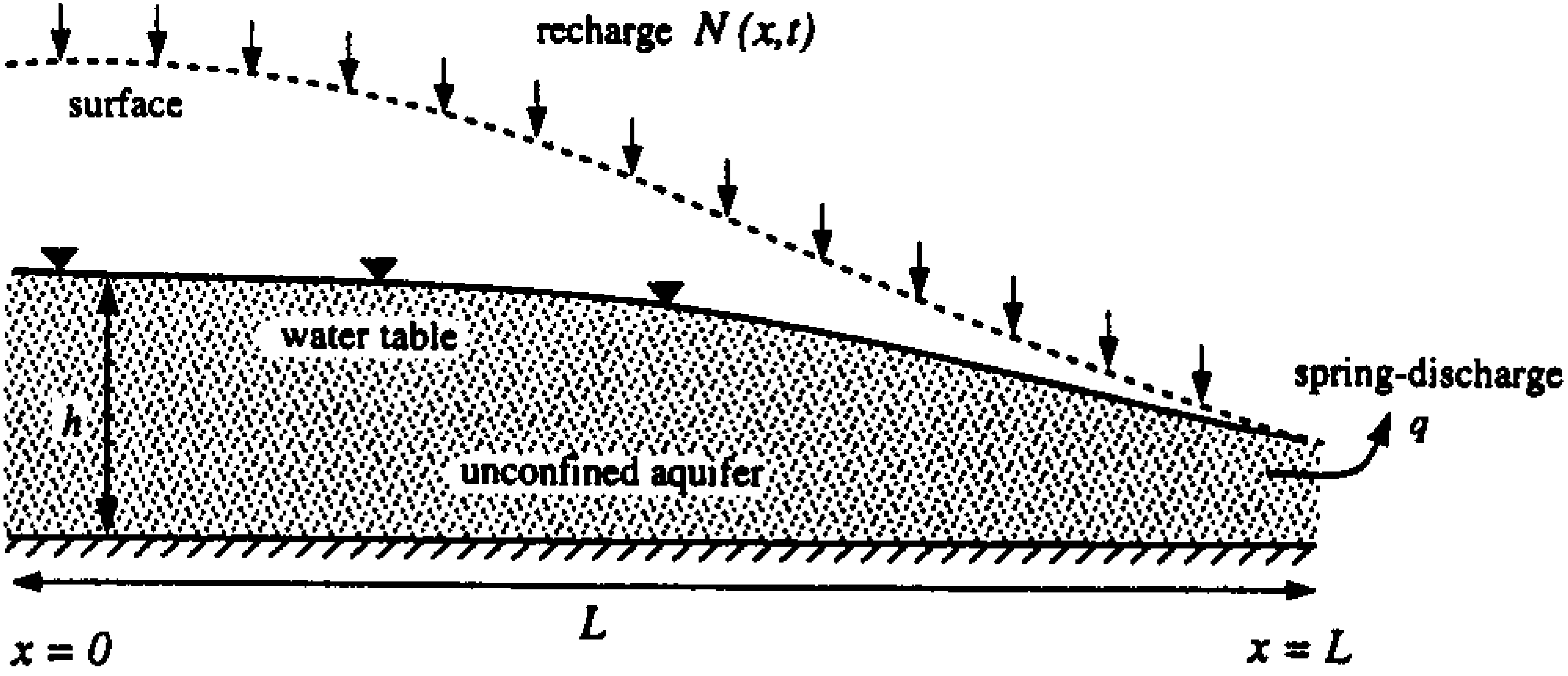
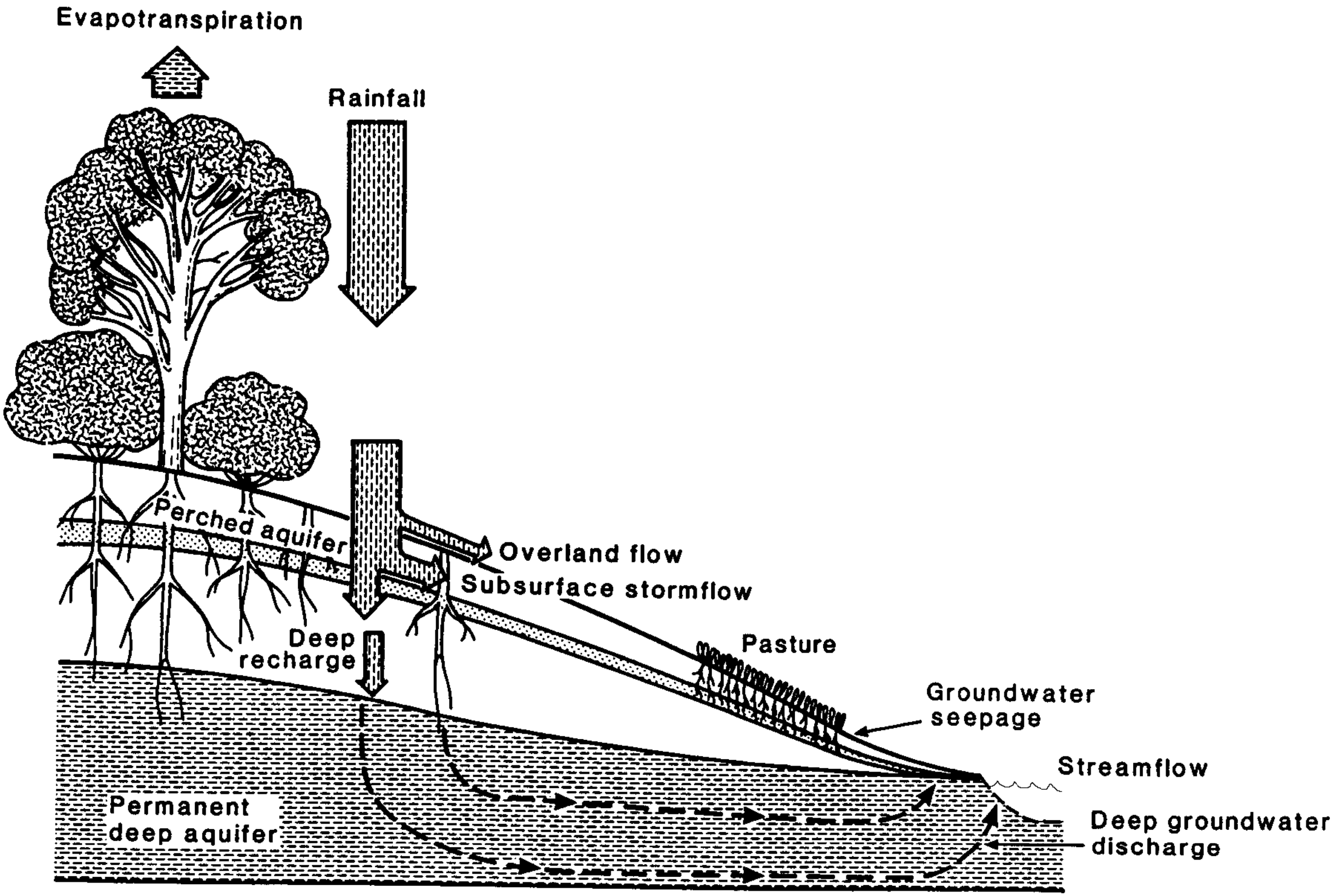


Figure X. Geometry of the one-dimensional model.

Conceptual model of a catchment



Turner and Macpherson, 1990

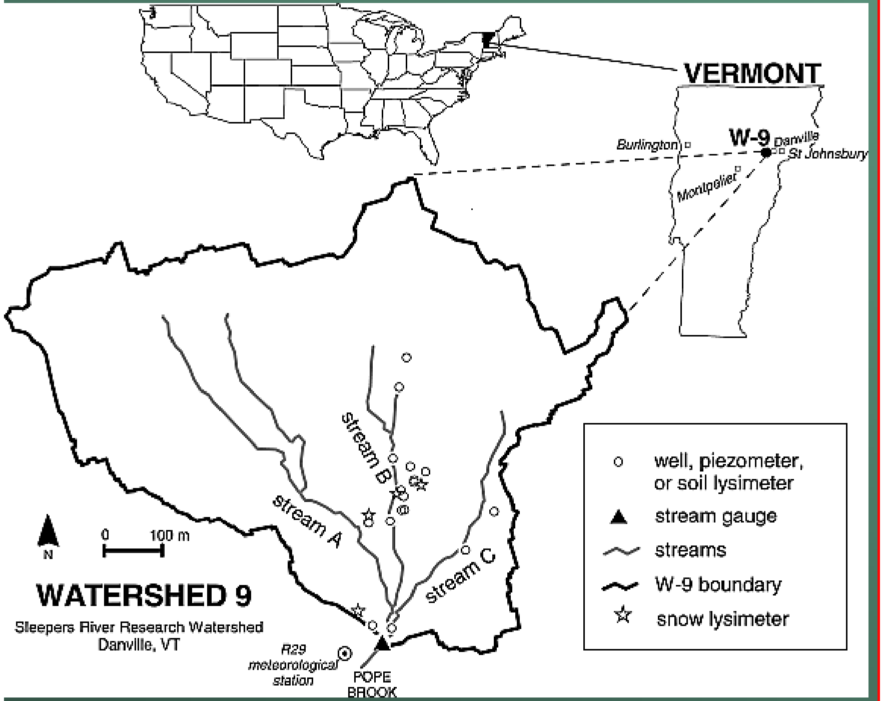
How do recessions reveal contributions from storage?

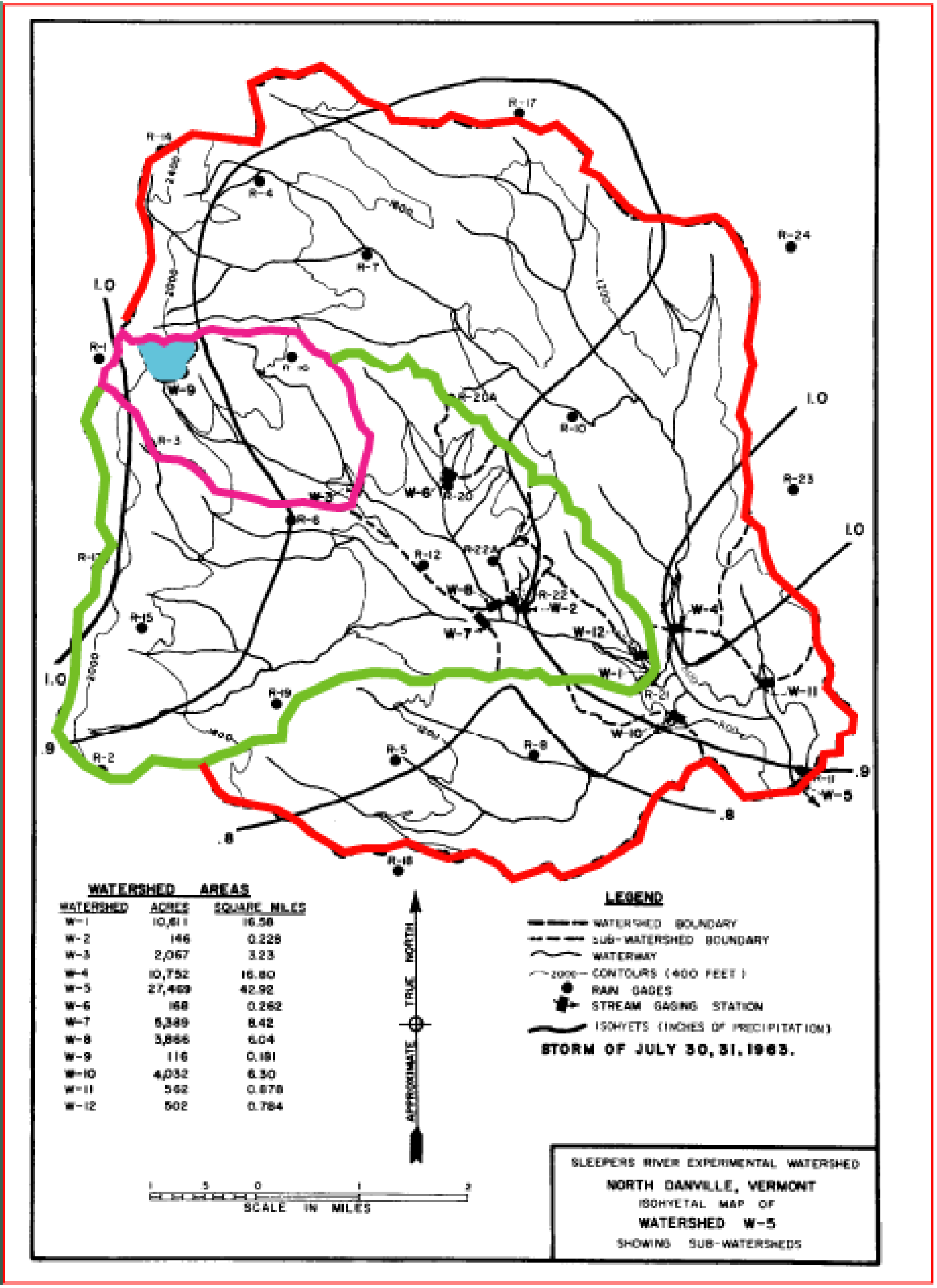
- Use ambient tracers (chemistry and isotopes)

- CATCHMENT EXAMPLE
  - Sleepers River Research Watershed, Vermont

- KARST EXAMPLE
  - Classical karst, Slovenia/Italy

Sleepers River Research Watershed

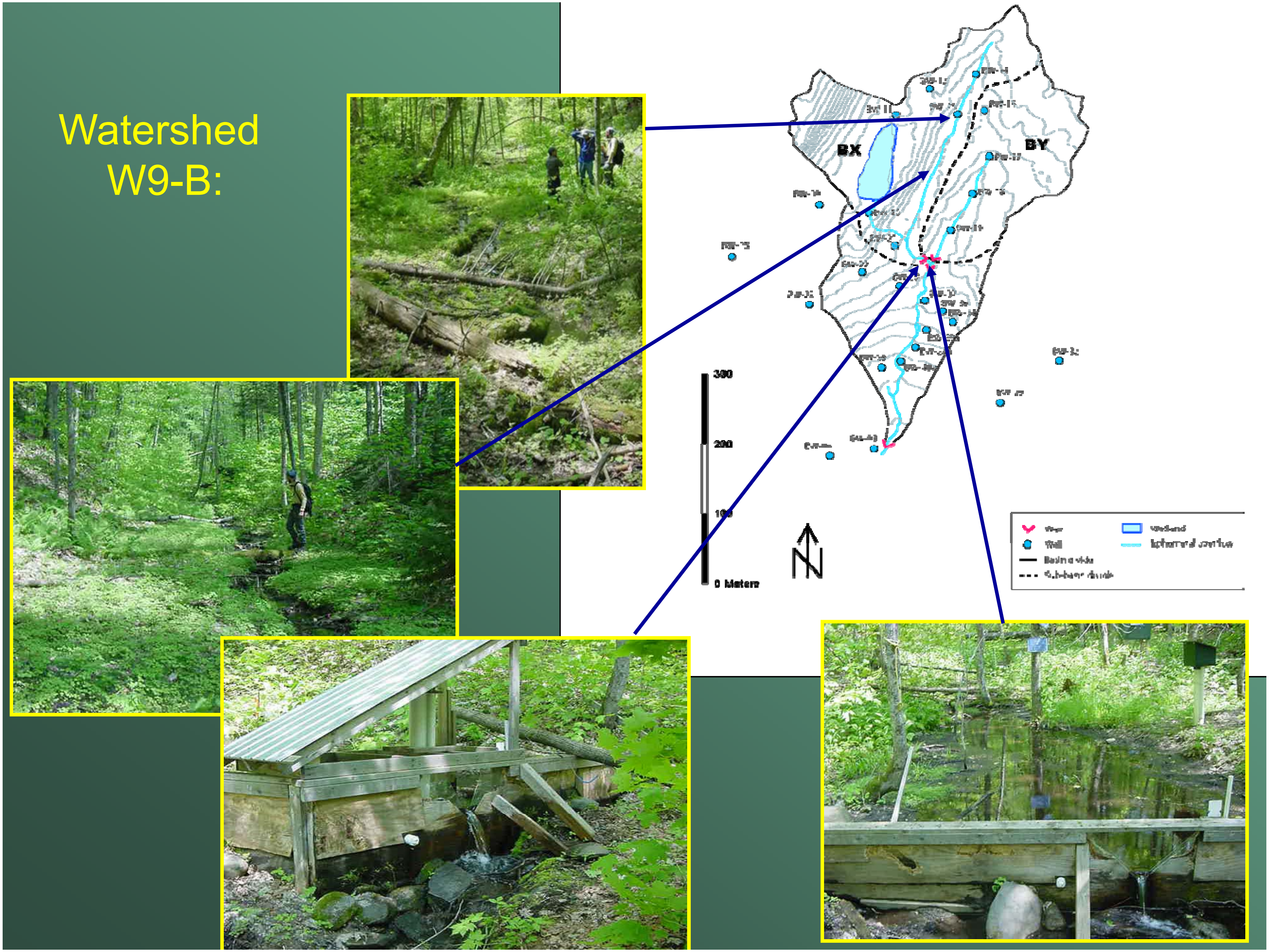




WATERSHED AREAS

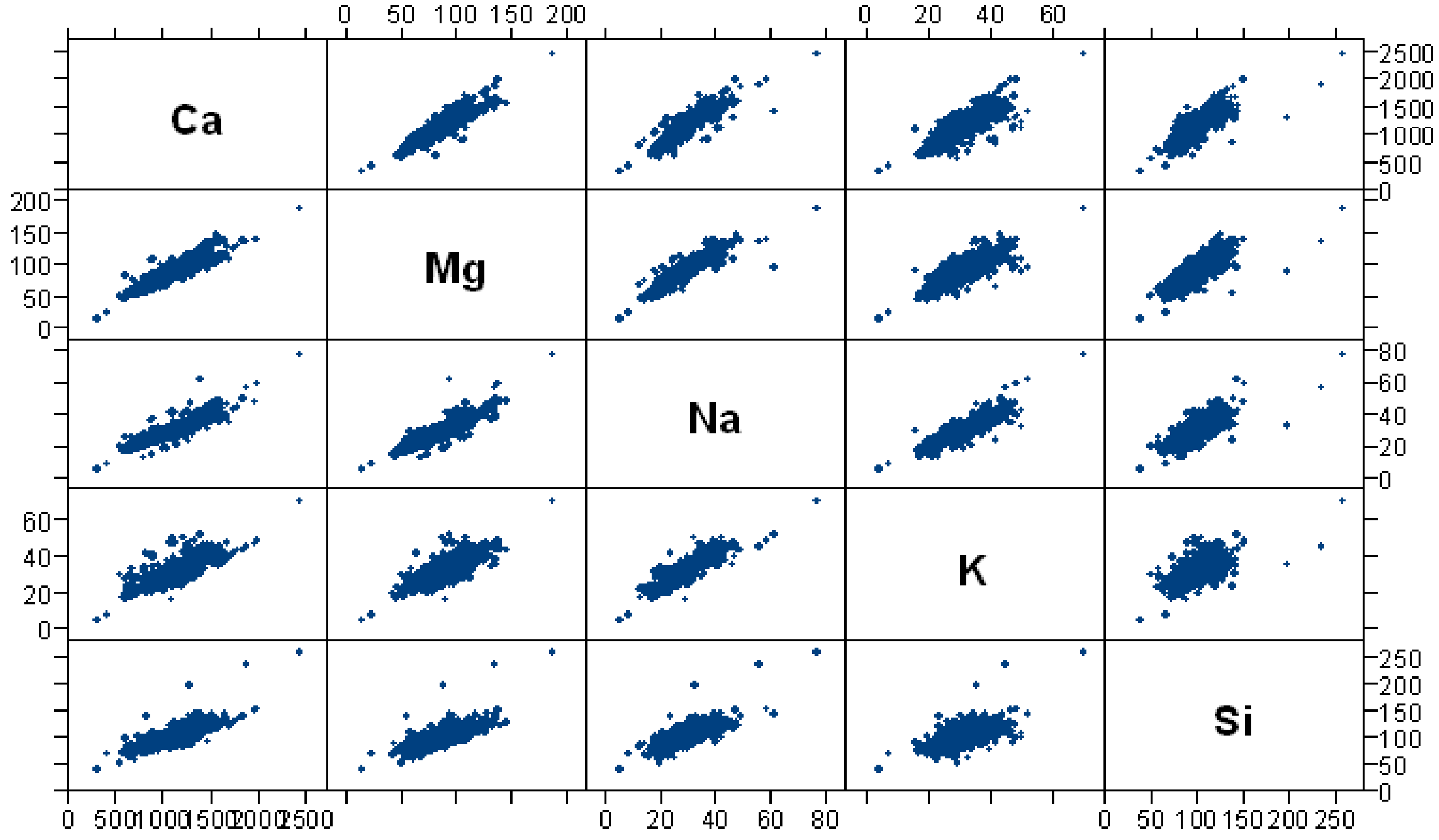
WATERSHED	ACRES	SQUARE MILES
W-1	10,611	16.58
W-2	146	0.228
W-3	2,067	3.23
W-4	10,752	16.80
W-5	27,469	42.92
W-6	168	0.262
W-7	5,389	8.42
W-8	3,866	6.04
W-9	116	0.181
W-10	4,032	6.30
W-11	562	0.878
W-12	502	0.784

Watershed W9-B:

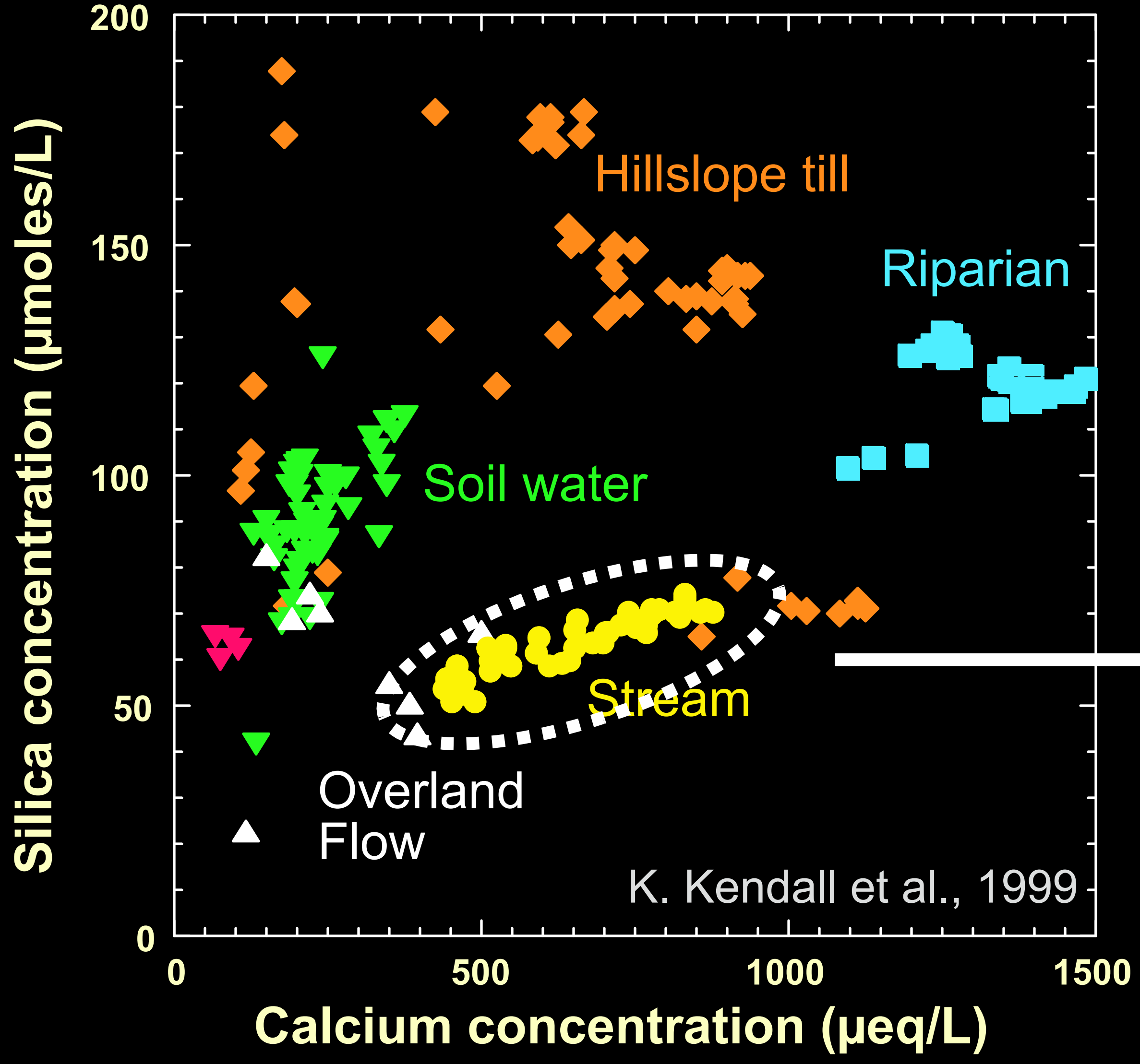


Sleepers River, W-9

Cations (µeq/L)

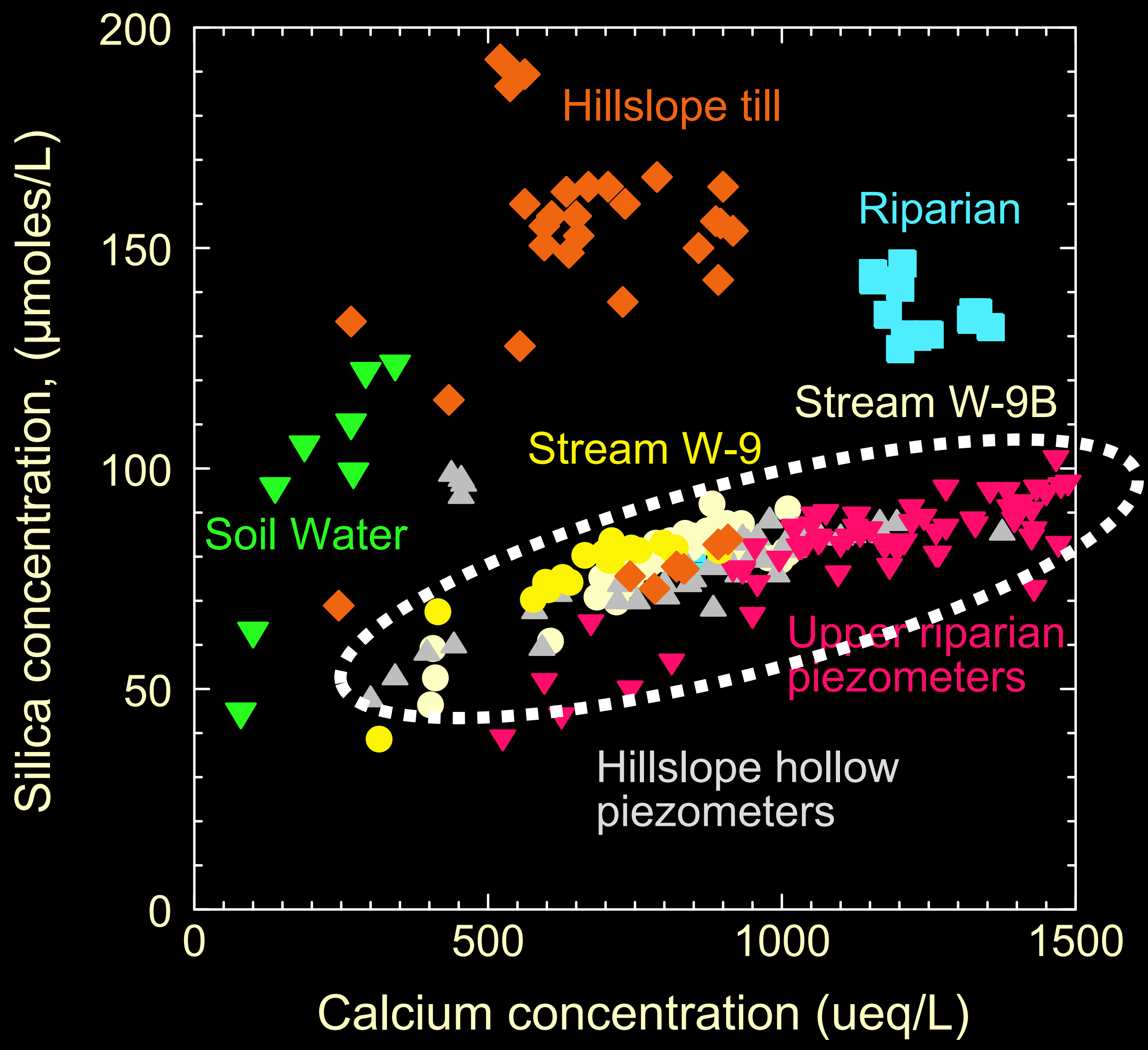


1996 snowmelt

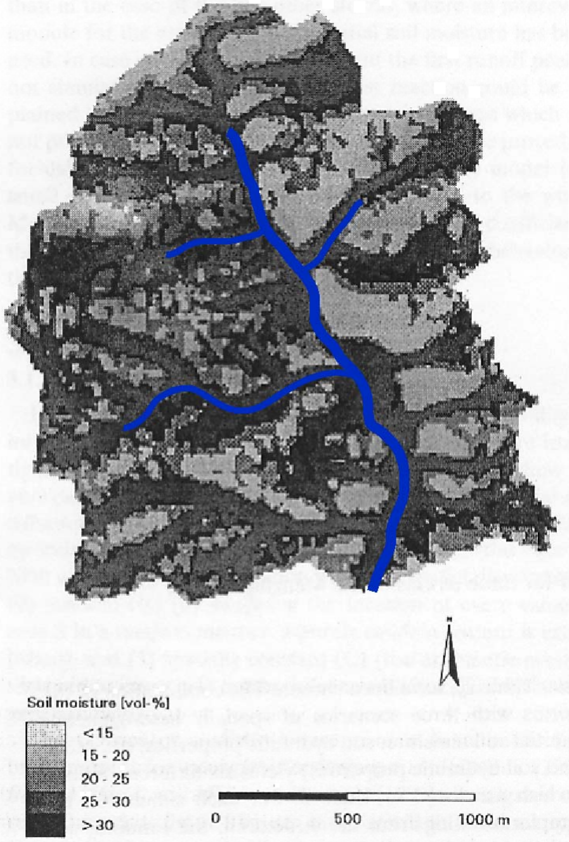


WTF?

1999 snowmelt



Piezometers in upstream hollows



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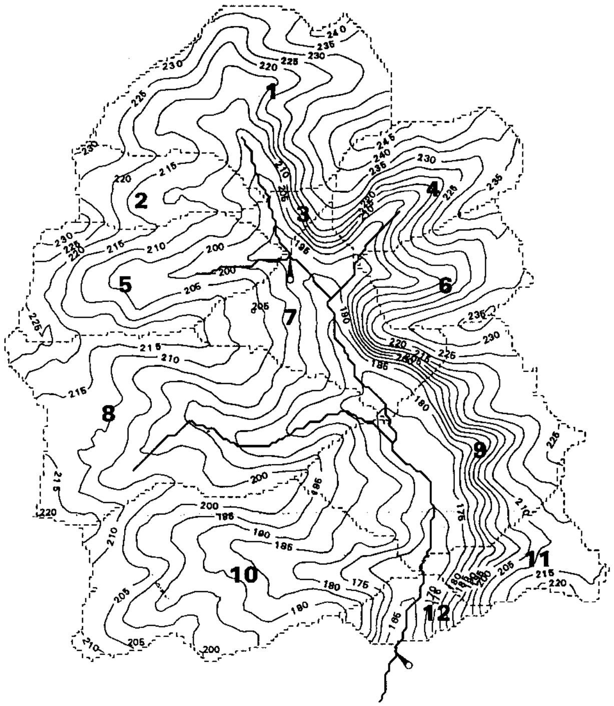


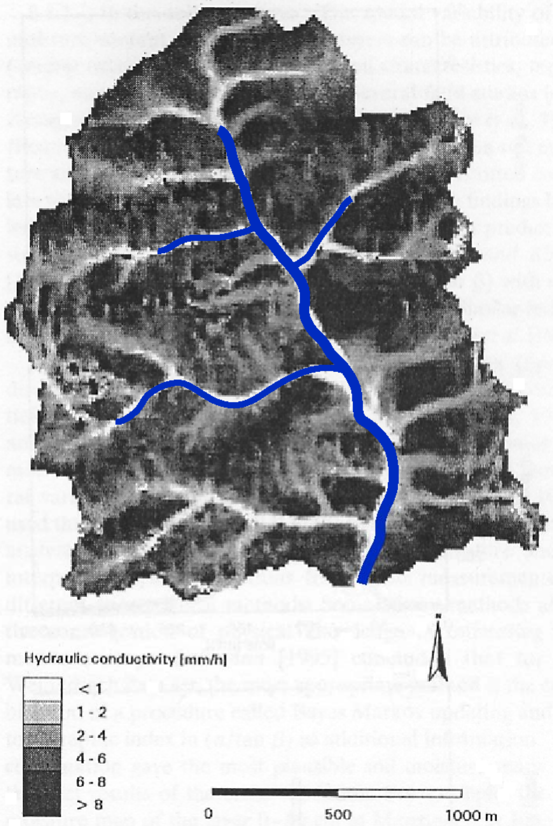
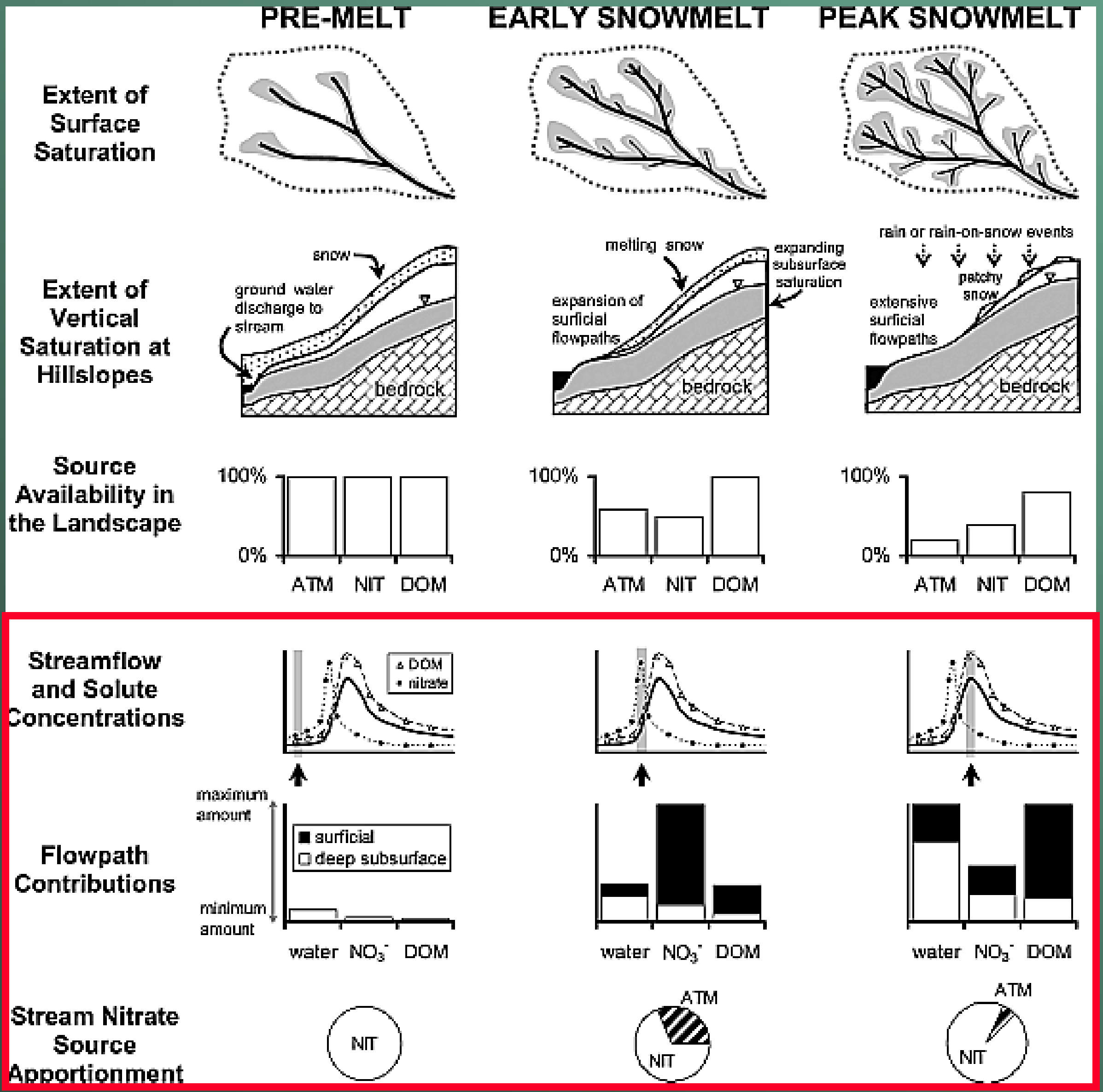


Figure 5. Assumed spatial distribution of saturated hydraulic conductivity.

Merz and Plate, 1997

Expansion of riparian source areas:



Flowpath contributions vary according to flow regime

Sebestyen et al., 2008

Subsurface flow

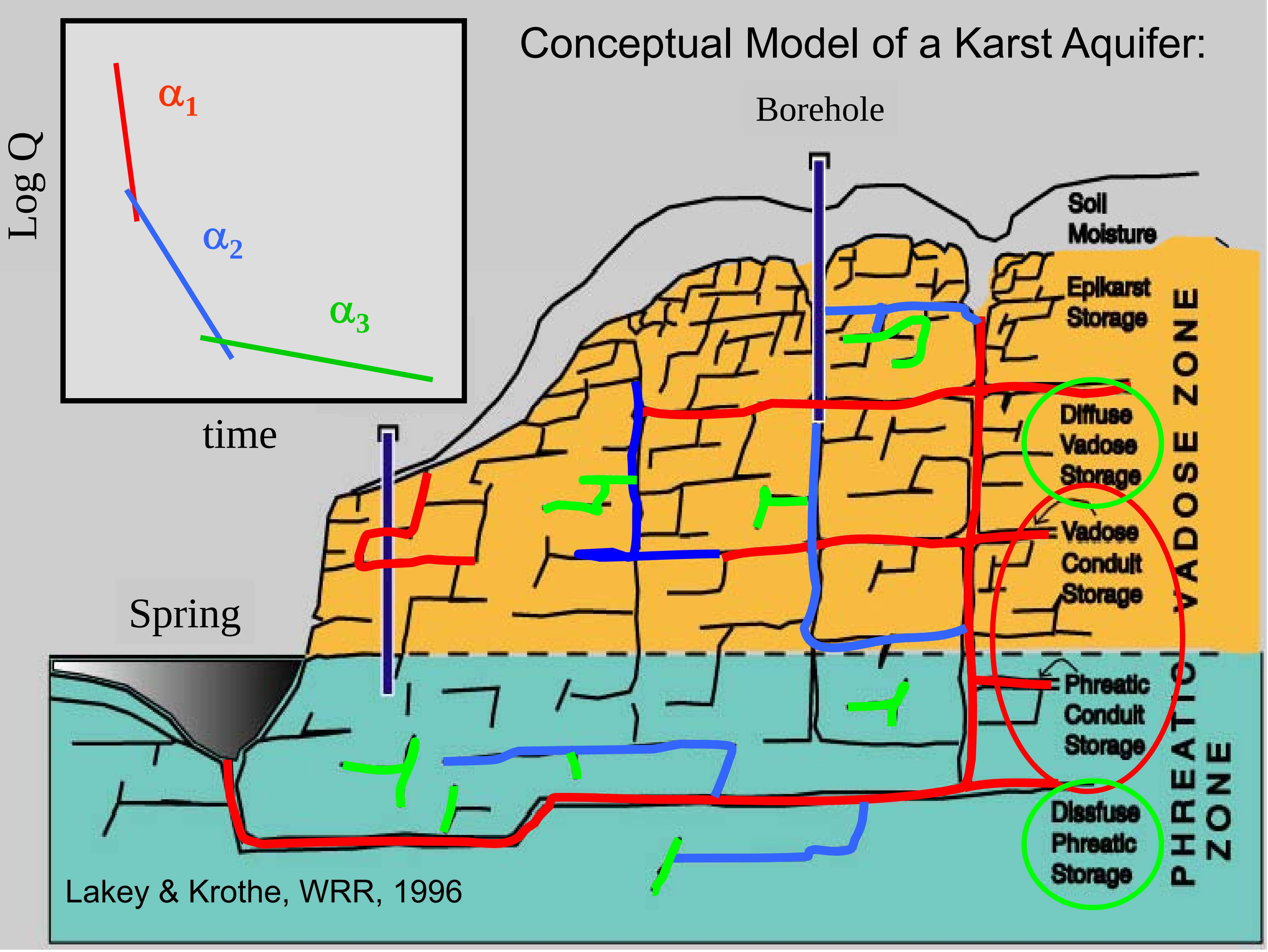
Macropores in till

PREFERENTIAL FLOW IN KARST

Karst studies

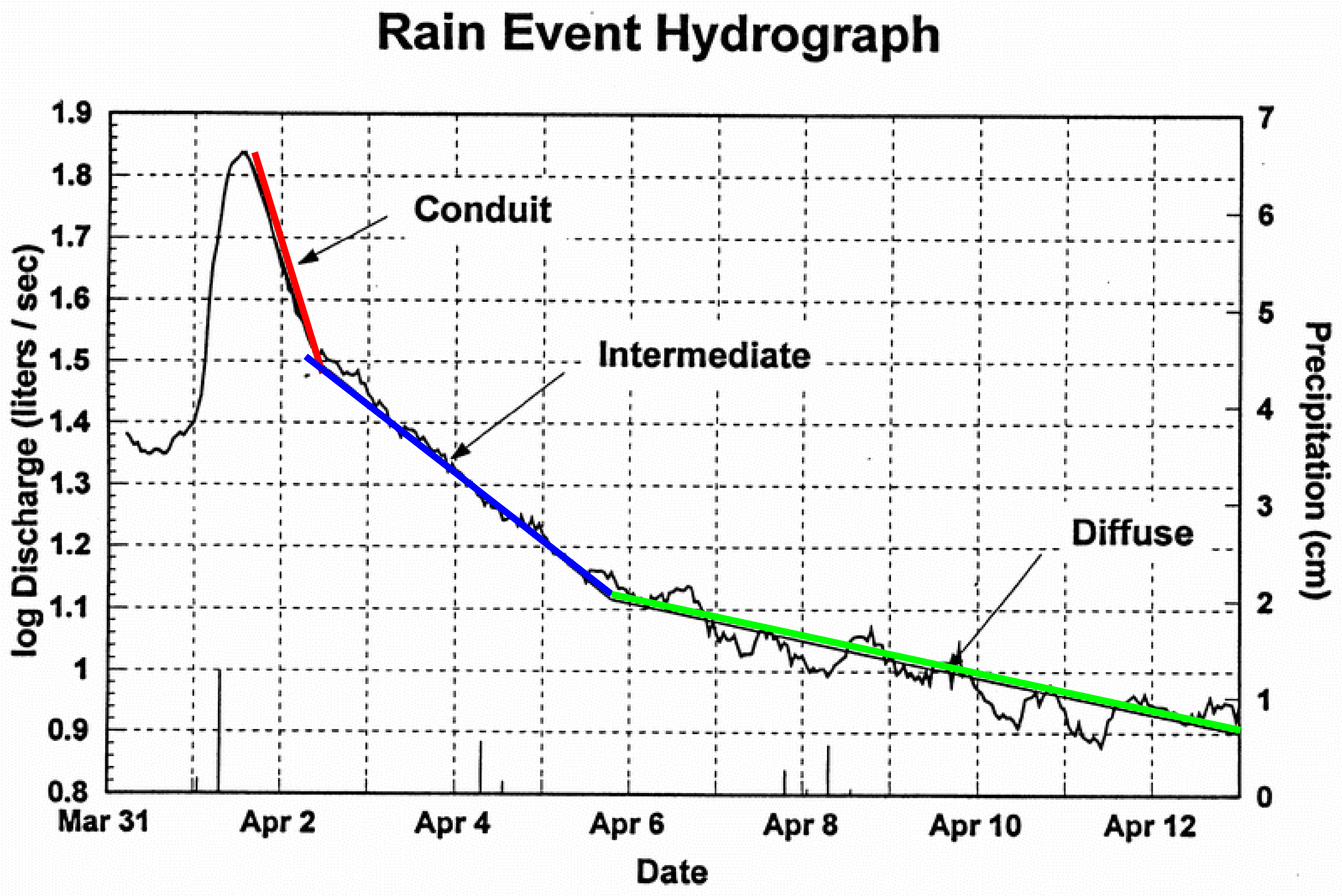
- Good discharge data
- Poorly constrained geometry
- Governing equations? Pick your favorite

Conceptual Model of a Karst Aquifer:

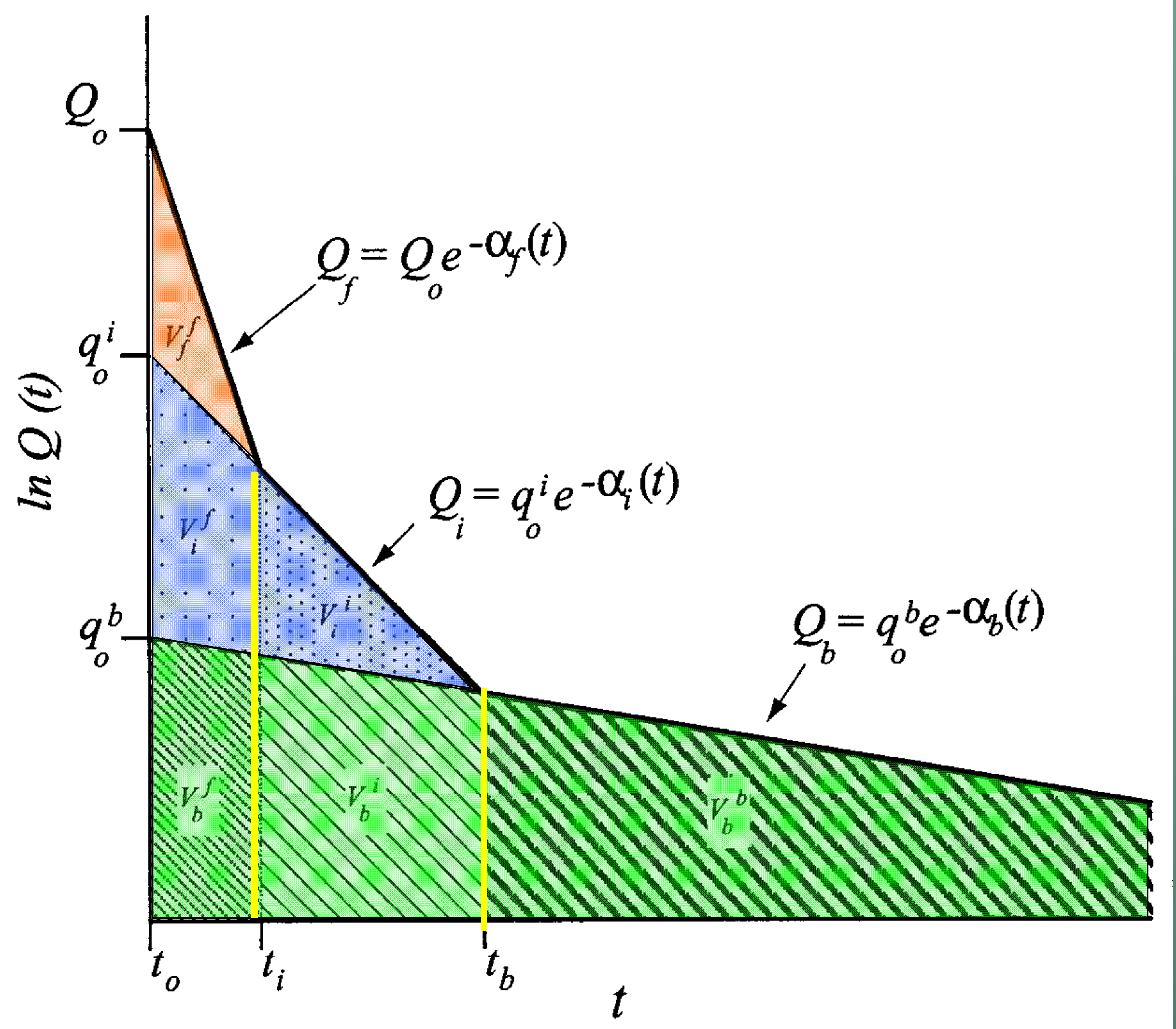


Lakey & Krothe, WRR, 1996

Karst spring recession behavior

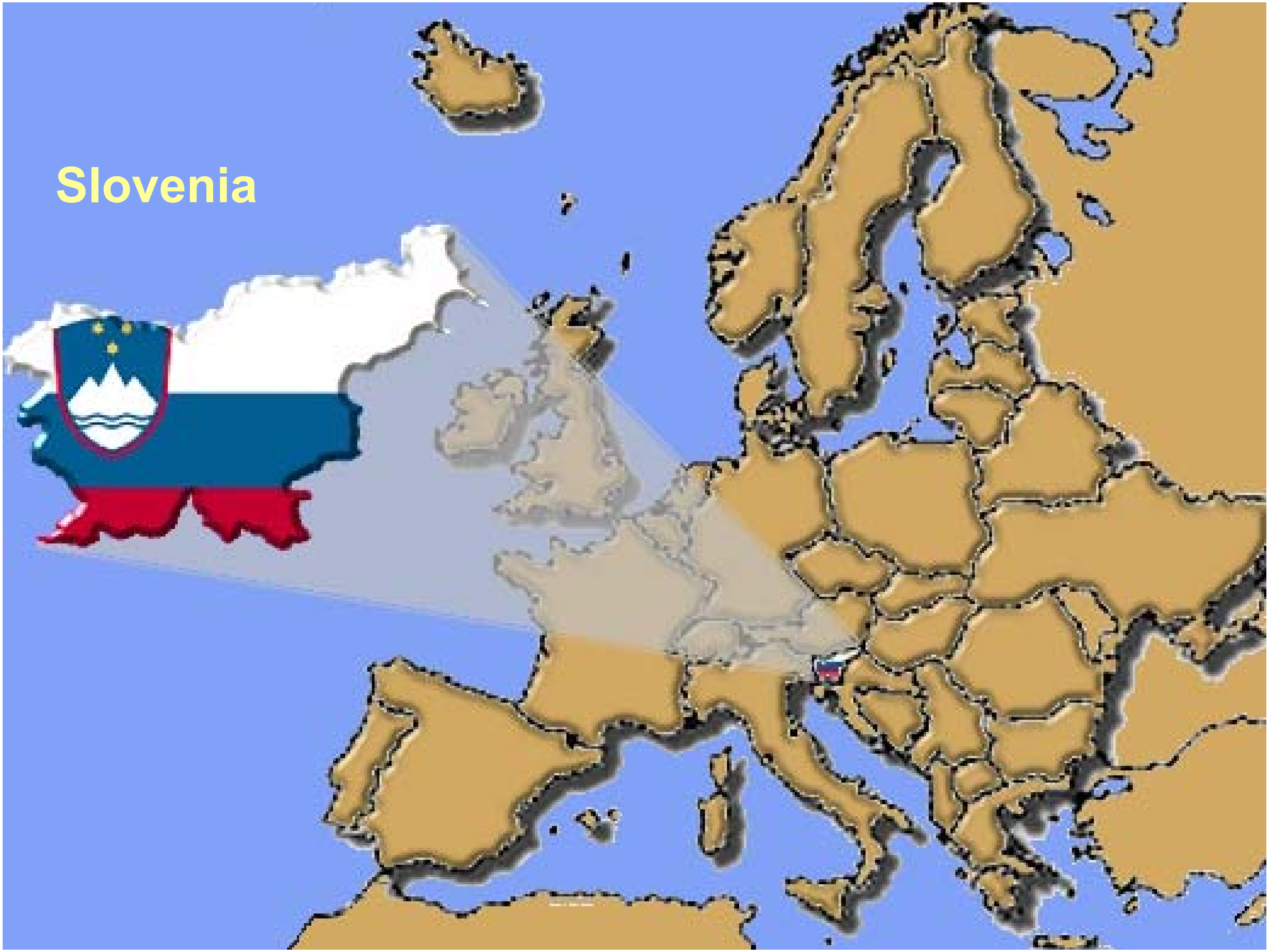


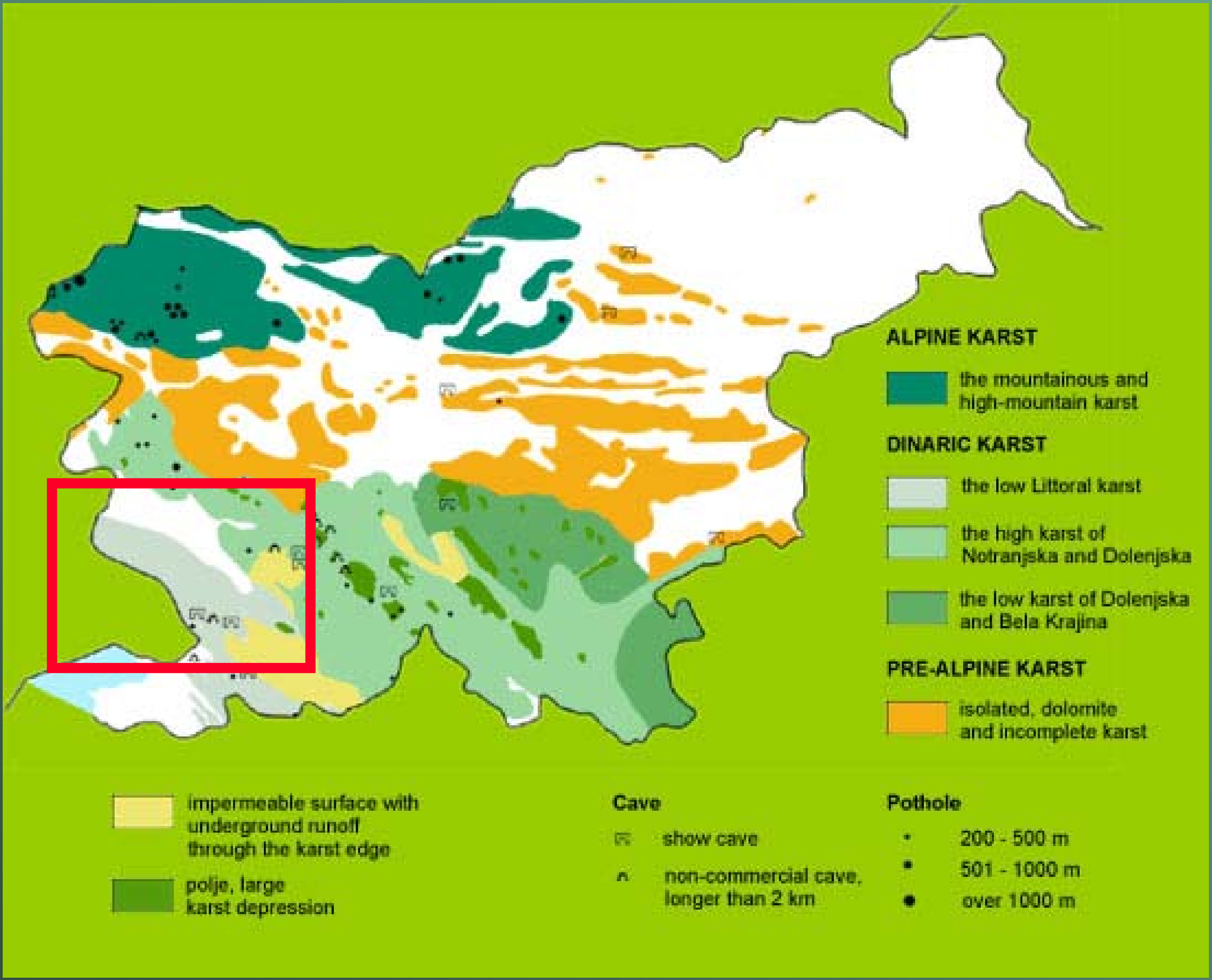
Baedke & Krothe, WRR, 2001



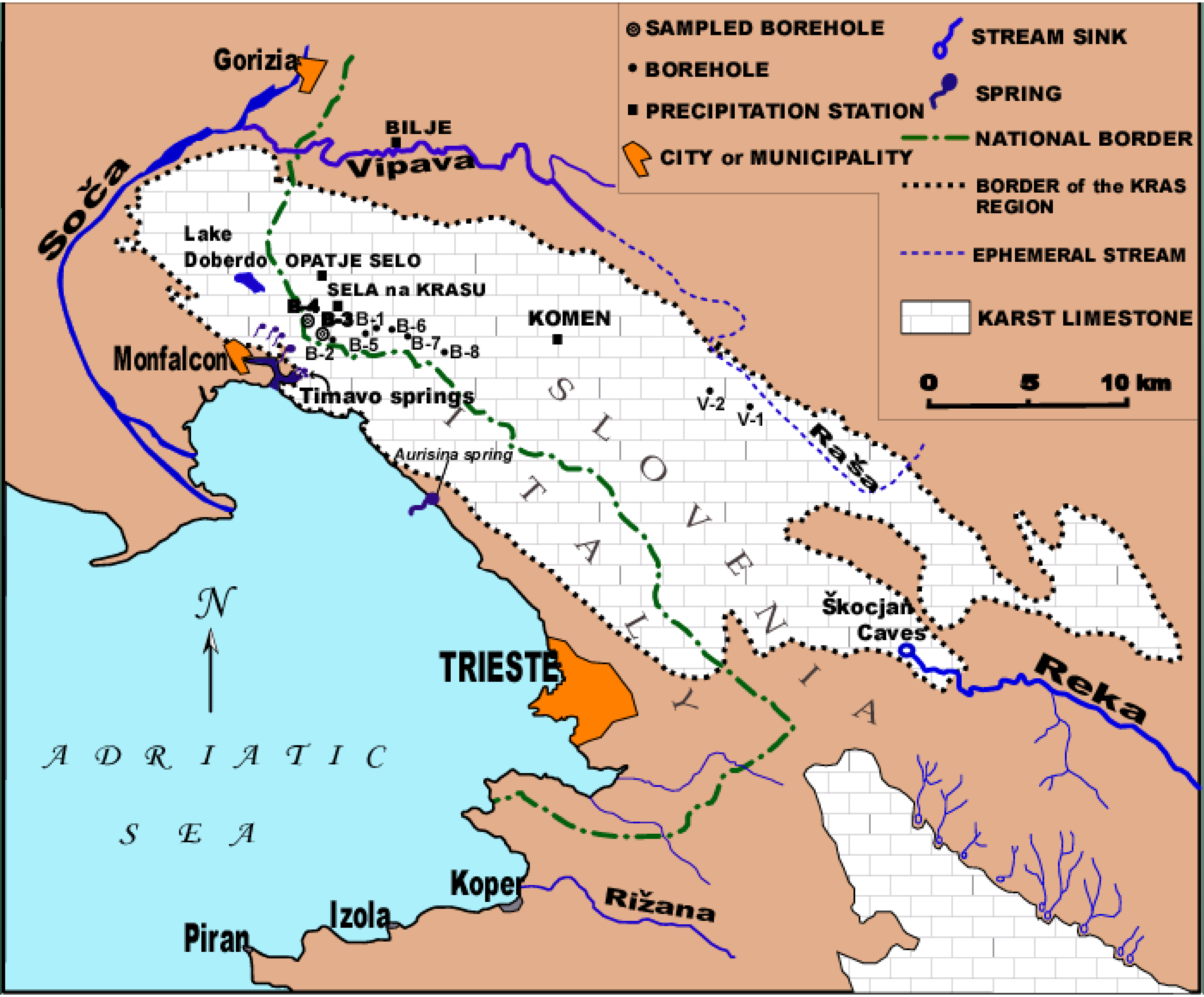
Doctor & Alexander, 2005

Slovenia

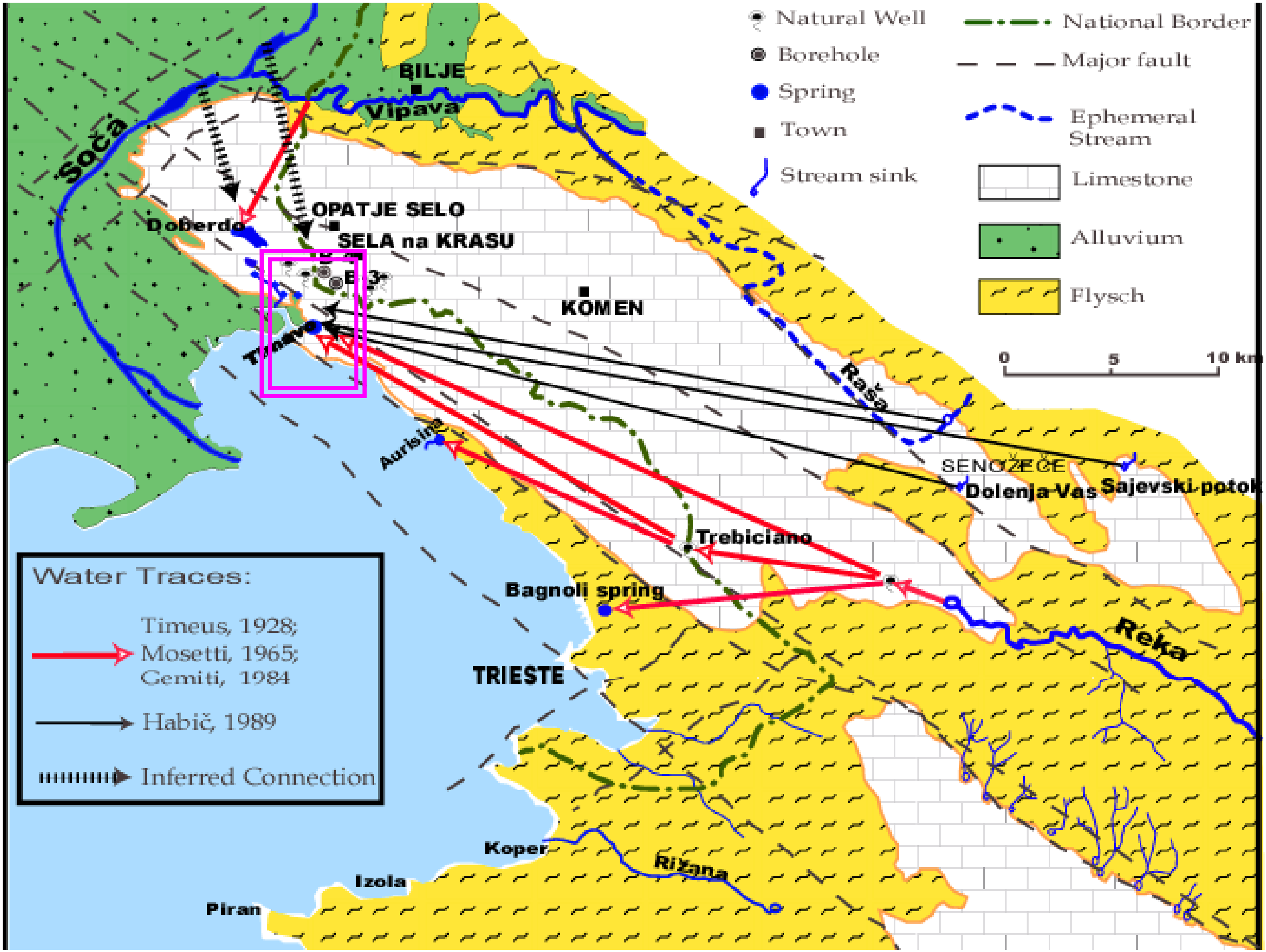


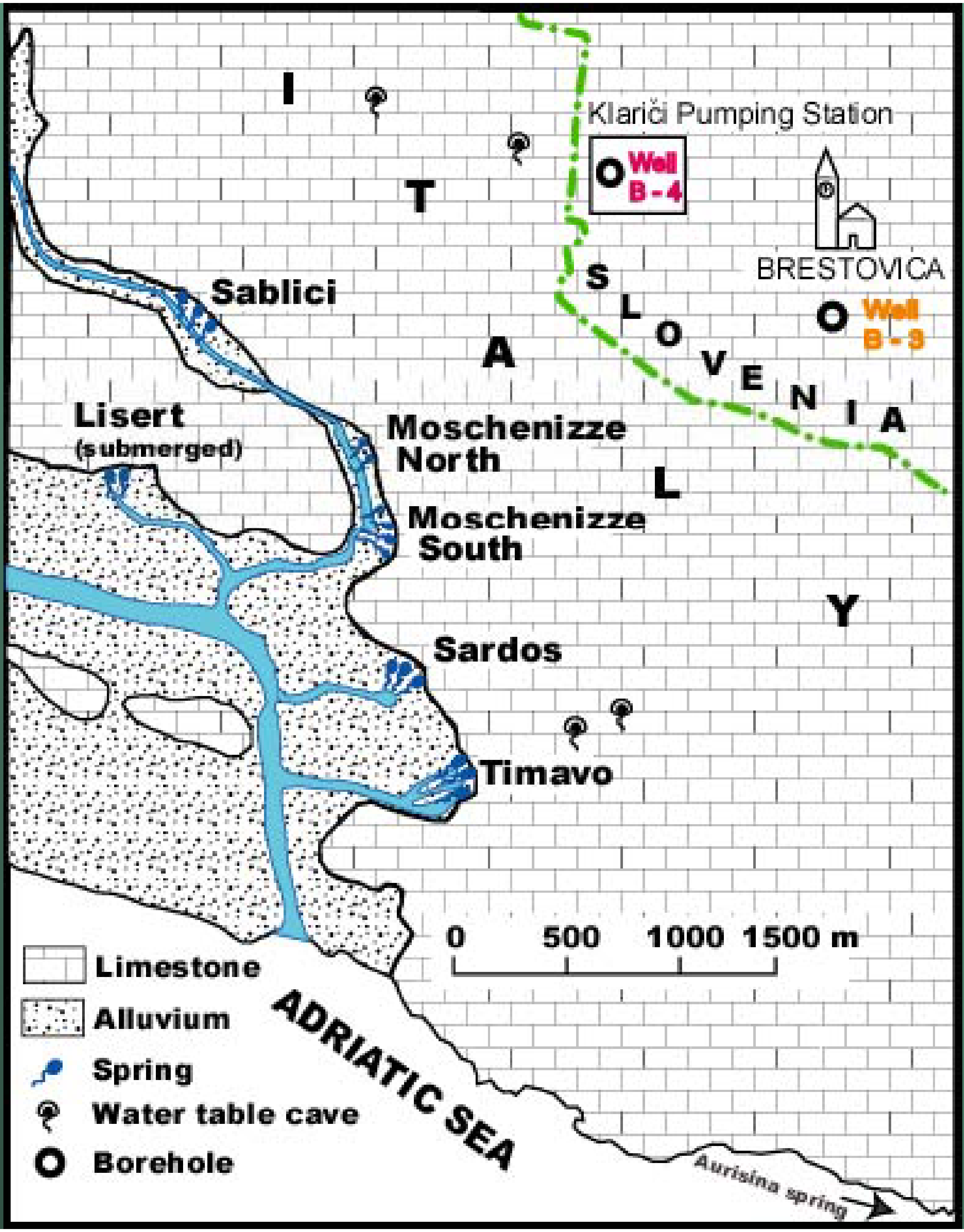

ALPINE KARST
the mountainous and high-mountain karst
DINARIC KARST
the low Littoral karst
the high karst of Notranjska and Dolenjska
the low karst of Dolenjska and Bela Krajina
PRE-ALPINE KARST
isolated, dolomite and incomplete karst
impermeable surface with underground runoff through the karst edge
polje, large karst depression
Cave
show cave
non-commercial cave, longer than 2 km
Pothole
200 - 500 m
501 - 1000 m
over 1000 m

Habic, 1998



⊚ SAMPLED BOREHOLE
• BOREHOLE
■ PRECIPITATION STATION
CITY or MUNICIPALITY
STREAM SINK
SPRING
NATIONAL BORDER
BORDER of the KRAS REGION
EPHEMERAL STREAM
KARST LIMESTONE
0
5
10 km
Gorizia
BILJE
Vipava
Soča
Lake Doberdo
OPATJE SELO
SELA na KRASU
B-4
B-3
B-1
B-6
B-2
B-5
B-7
B-8
KOMEN
Monfalcone
Timavo springs
Aurisina spring
V-2
V-1
Raša
SLOVENIA
ITALY
Škocjan Caves
Reka
TRIESTE
N
ADRIATIC SEA
Koper
Rižana
Izola
Piran

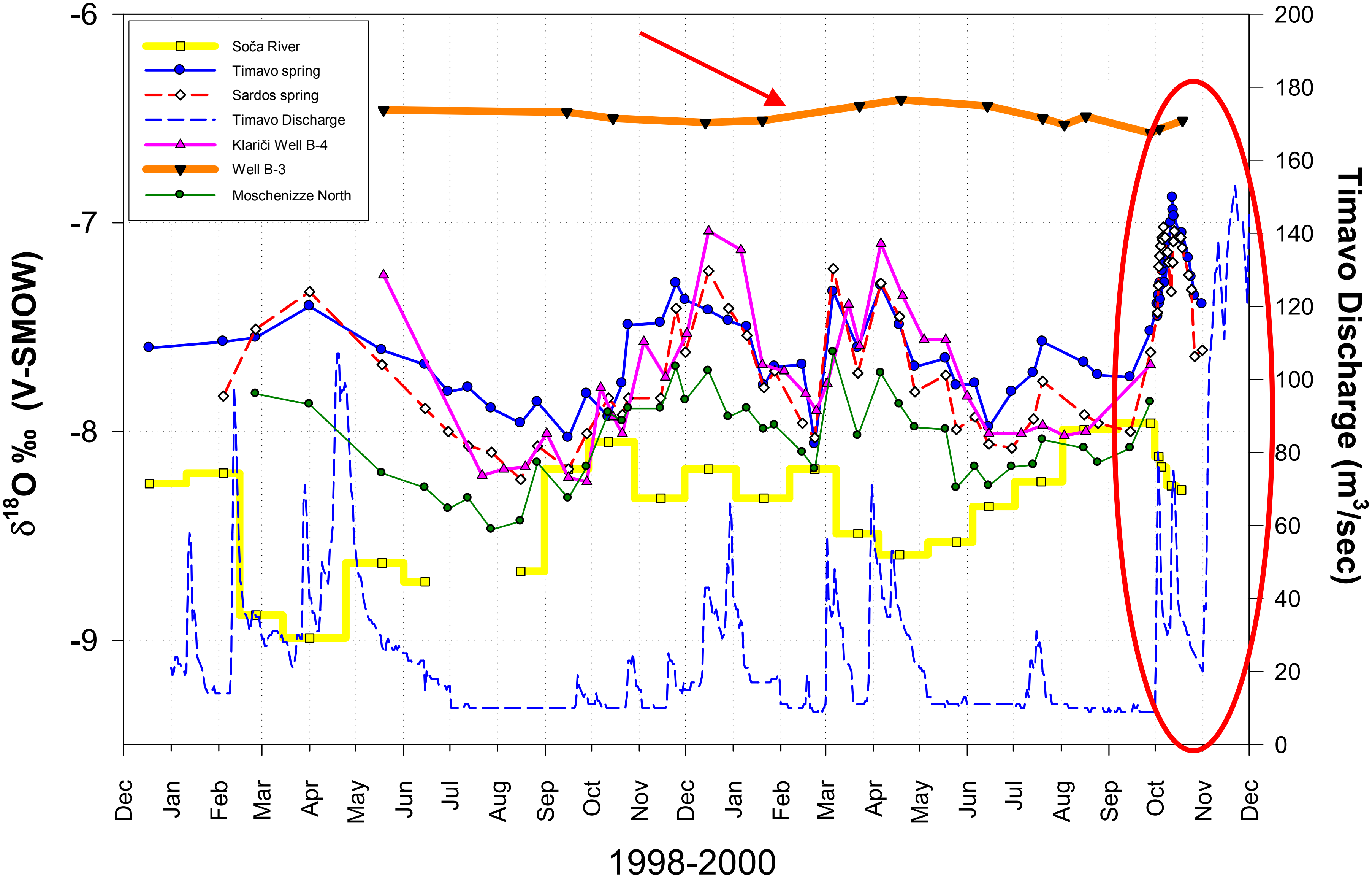

Natural Well
Borehole
Spring
Town
Stream sink
National Border
Major fault
Ephemeral Stream
Limestone
Alluvium
Flysch
0
5
10 km
BILJE
Vipava
Soča
Doberdo
OPATJE SELO
SELA na KRASU
B-3
KOMEN
Timavo
Raša
Aurisina
SENOŽEČE
Dolenja Vas
Sajevski potok
Trebiciano
Bagnoli spring
Reka
TRIESTE
Koper
Izola
Piran
Rižana
Water Traces:
Timeus, 1928;
Mosetti, 1965;
Gemiti, 1984
Habič, 1989
Inferred Connection

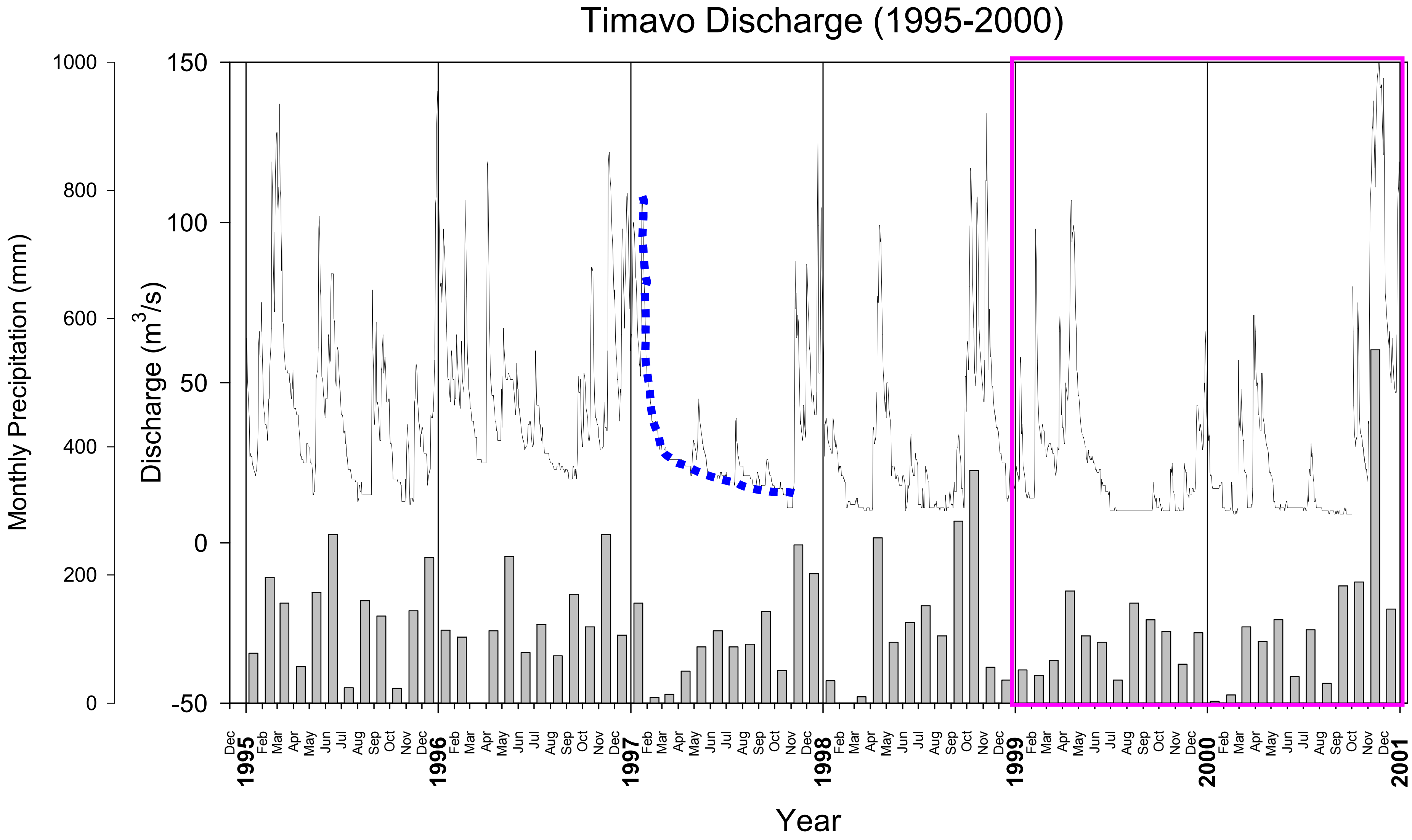

I T A L Y
S L O V E N I A
Klariči Pumping Station
Well B - 4
BRESTOVICA
Well B - 3
Sablici
Lisert (submerged)
Moschenizze North
Moschenizze South
Sardos
Timavo
0 500 1000 1500 m
ADRIATIC SEA
Aurisina spring
Limestone
Alluvium
Spring
Water table cave
Borehole

The Timavo Springs: Low flow

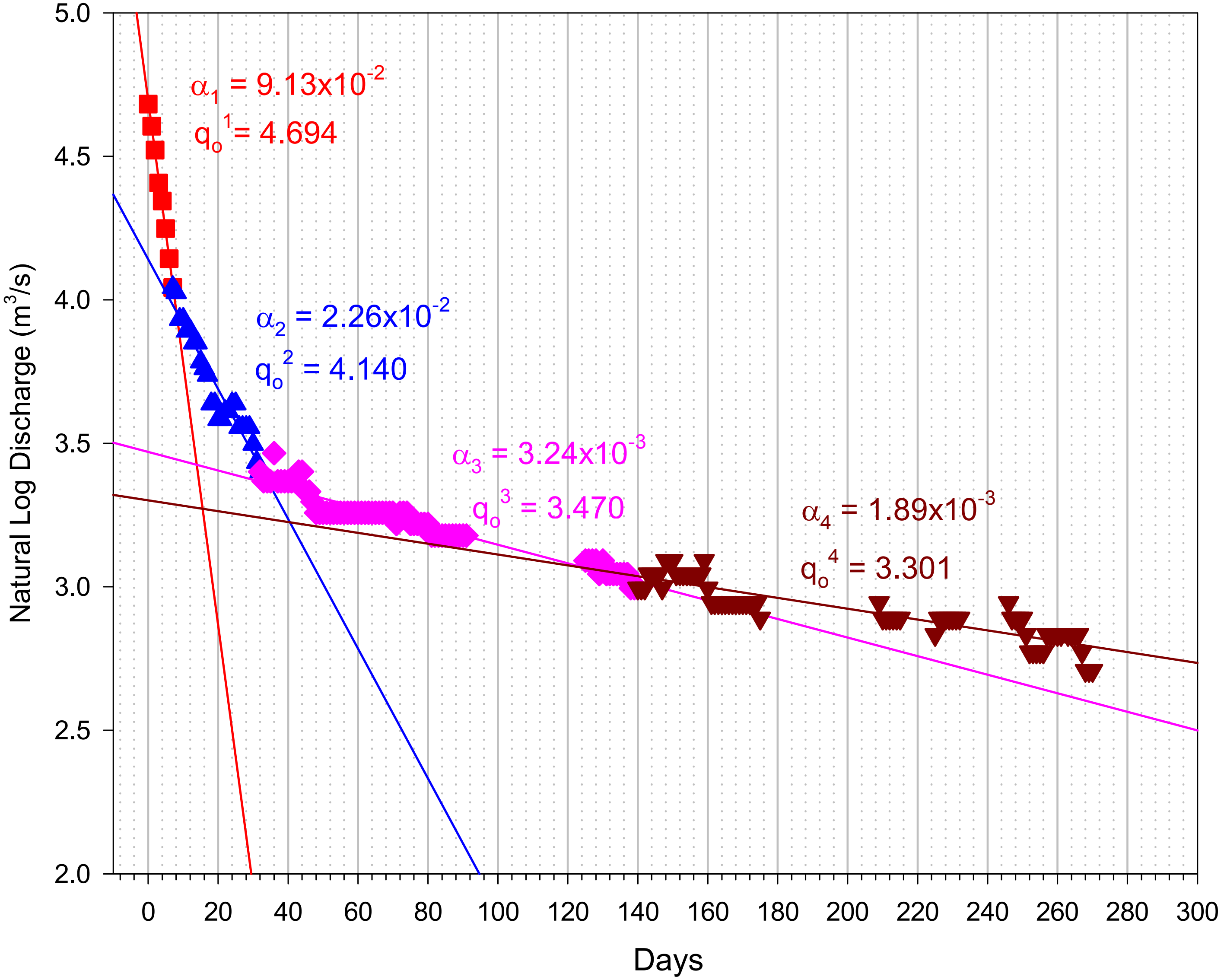
The Timavo Springs: Flood flow

Oxygen isotopic compositions of Kras waters 1998-2000

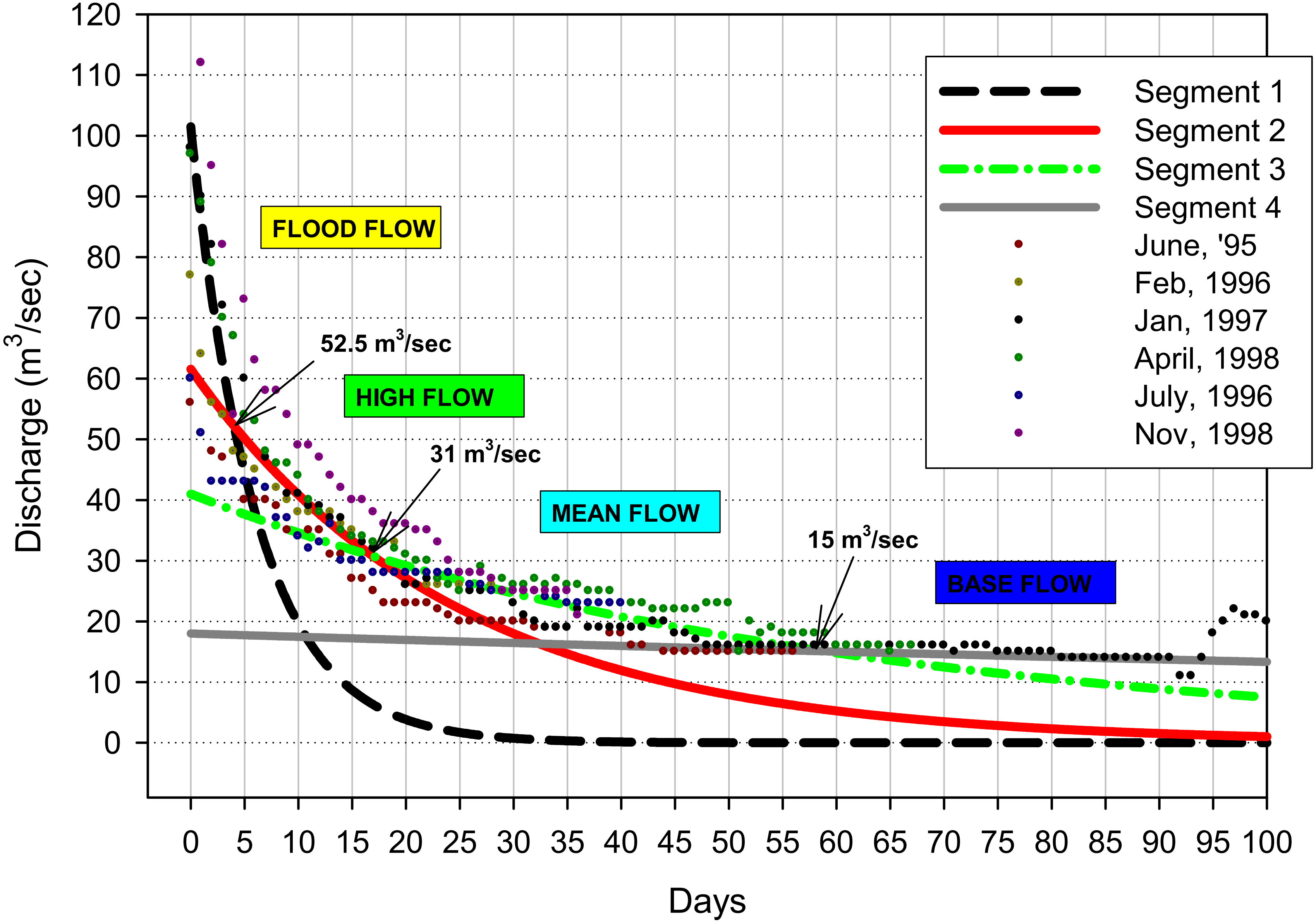



Timavo Discharge (1995-2000)
Monthly Precipitation (mm)
1000
800
600
400
200
0
Discharge (m³/s)
150
100
50
0
-50
Dec
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
1995
1996
1997
1998
1999
2000
2001
Year

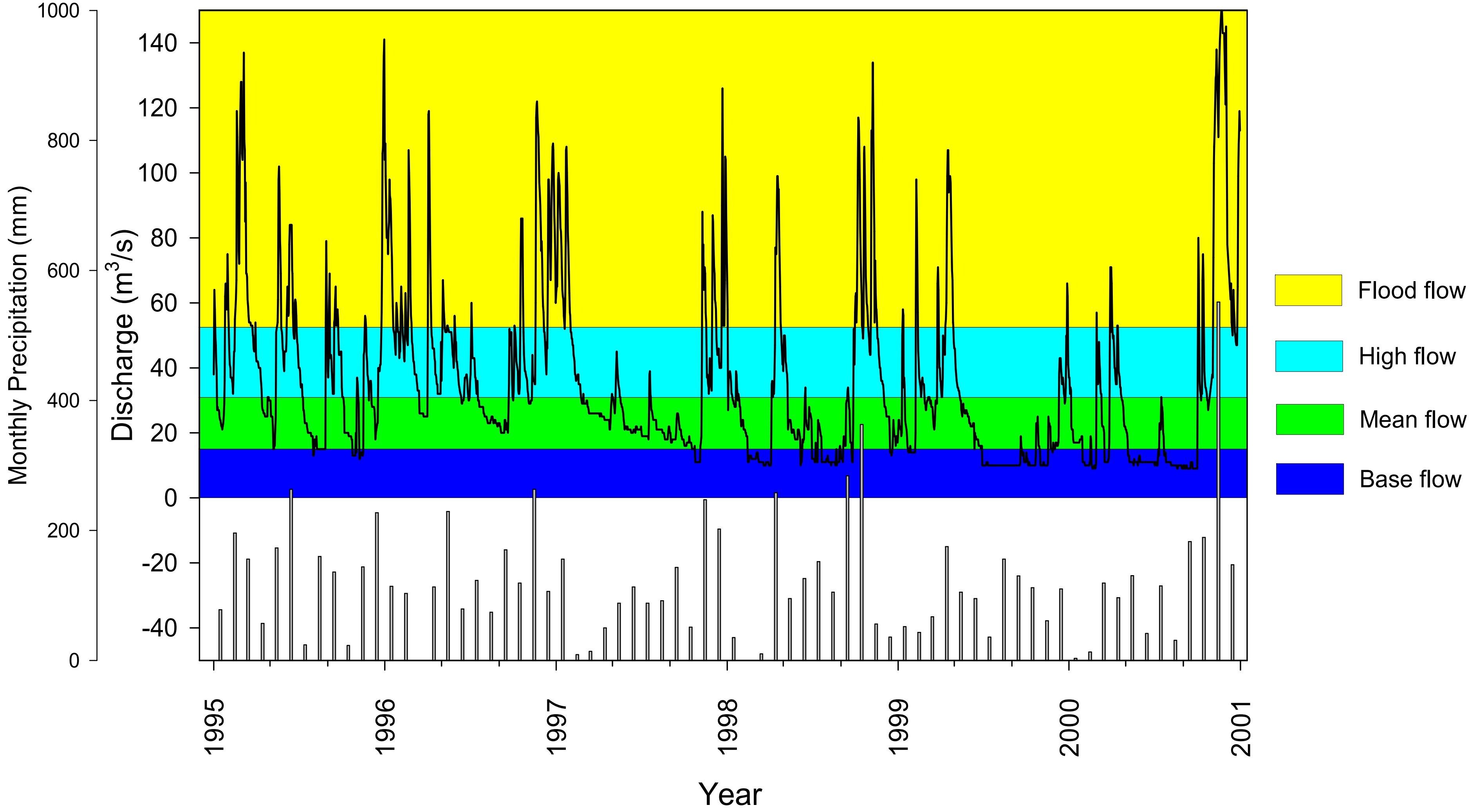
Representative hydrograph recession of the Timavo springs
(Jan. 23 - Oct. 20,1997)



Master Recession Curve of the Timavo springs

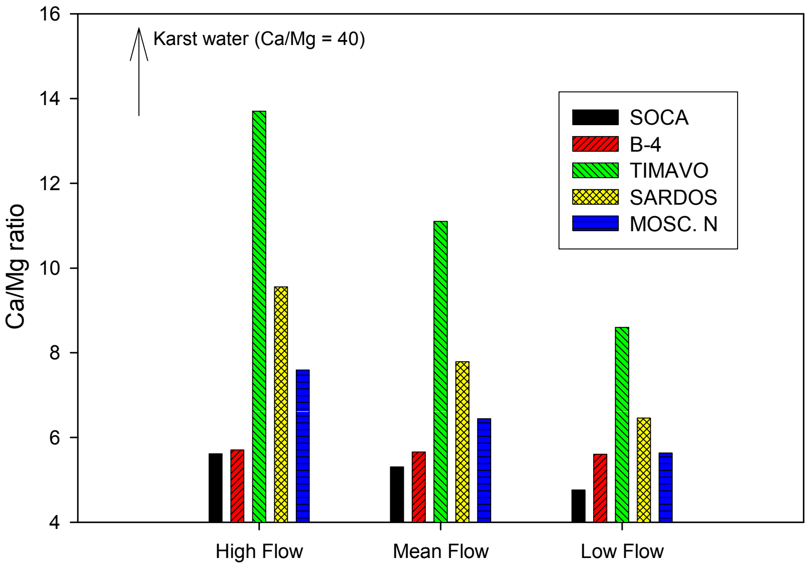


Discharge of the Timavo springs (1995-2000)

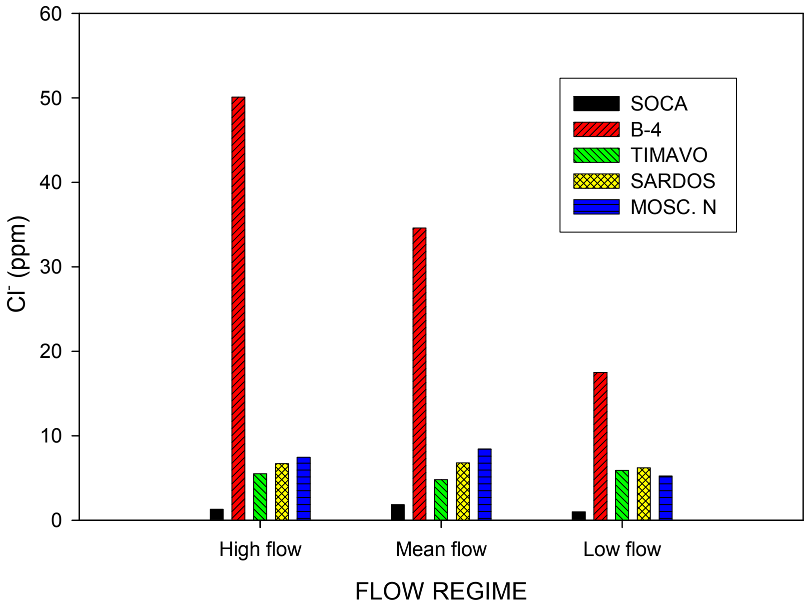


Chemical change with flow regime

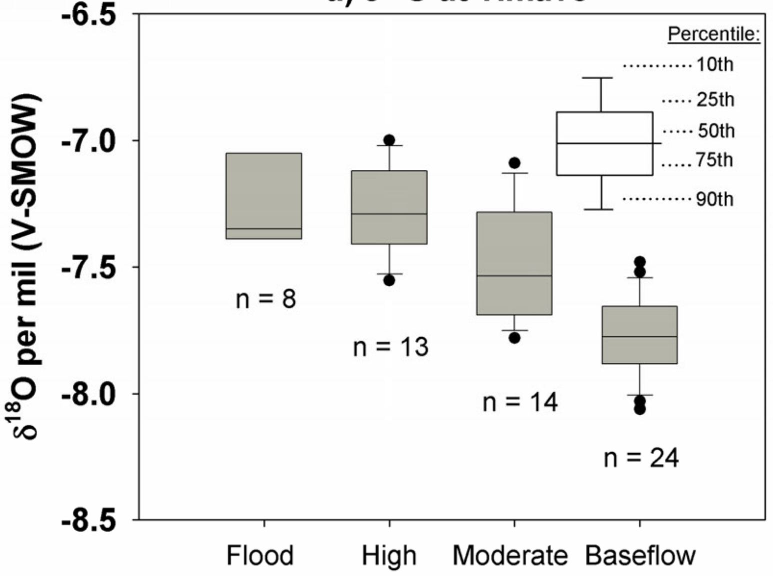
Average Ca/Mg ratio according to flow regime



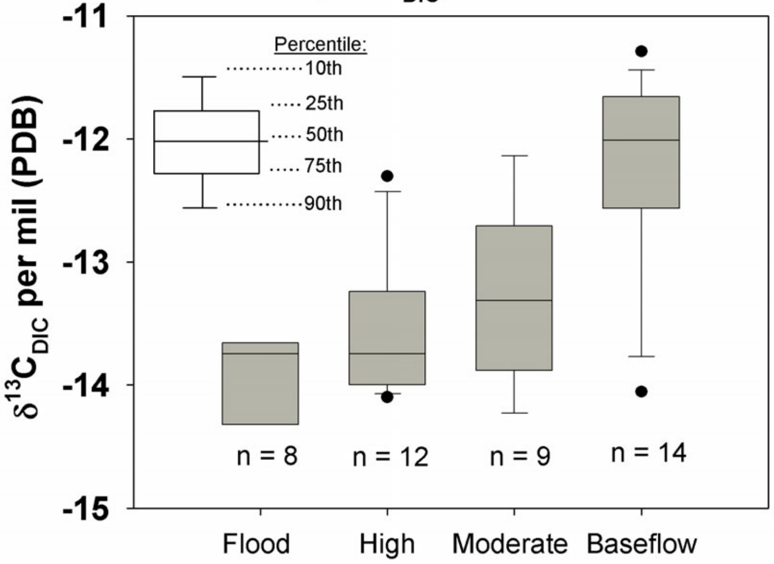
Average Cl^- concentrations according to flow regime



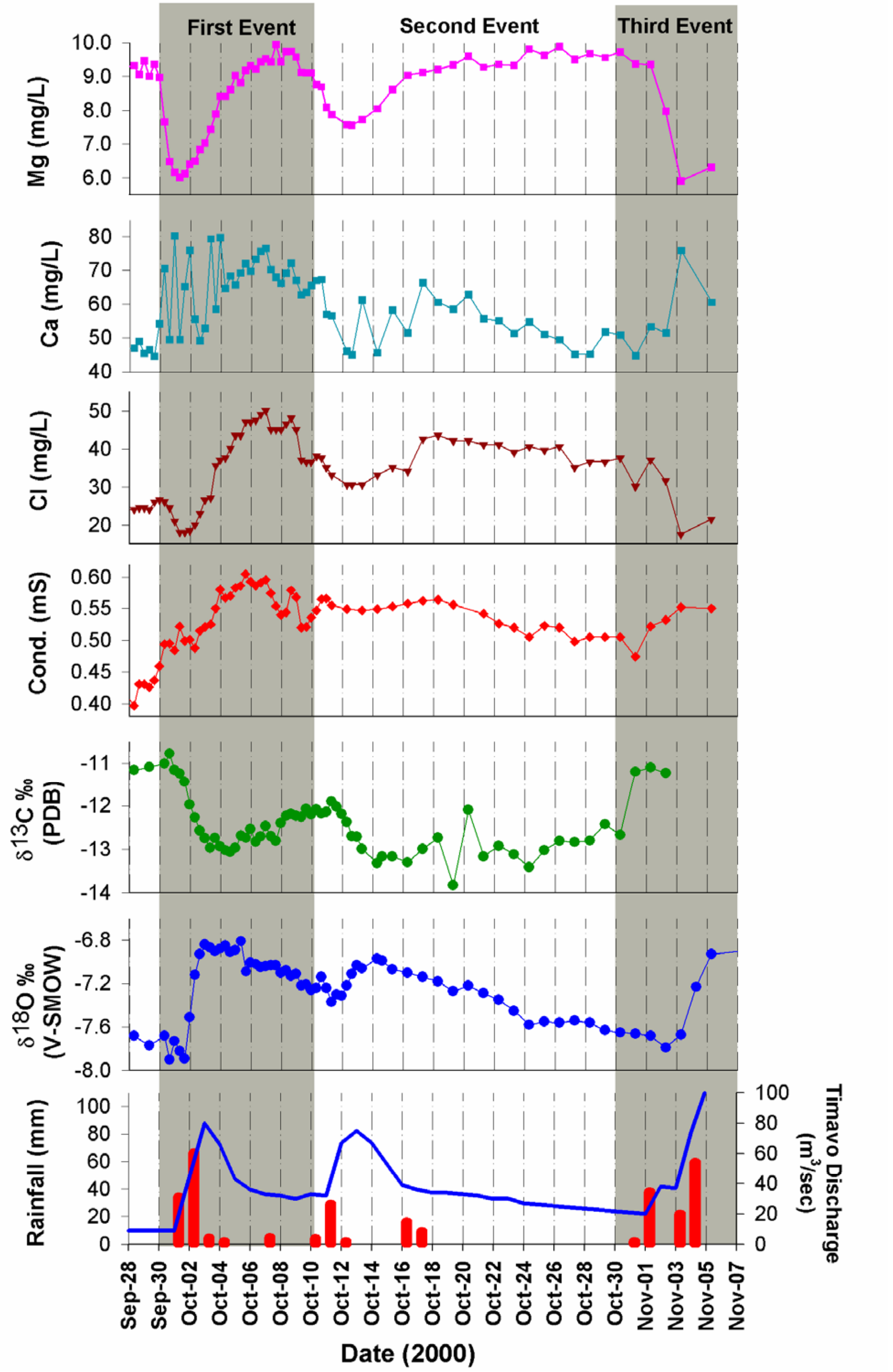
a) $\delta^{18}O$ at Timavo



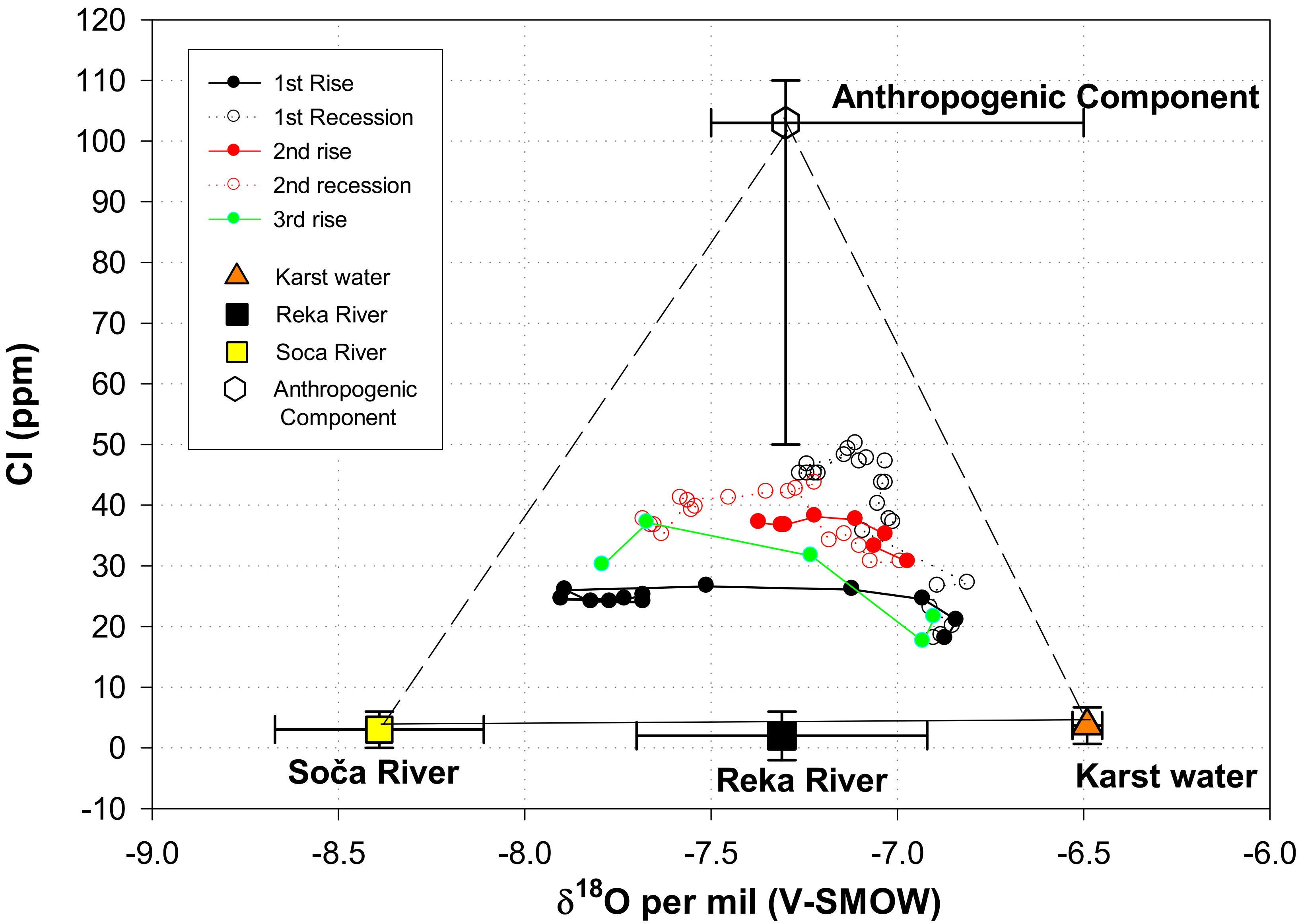
b) $\delta^{13}C_{DIC}$ at Timavo



Chemical and isotopic parameters measured in a well during storm events



(Doctor et al., Hydrogeology Journal, 2006)



Anthropogenic Component
Soča River
Reka River
Karst water
1st Rise
1st Recession
2nd rise
2nd recession
3rd rise
Karst water
Reka River
Soca River
Anthropogenic Component
Cl (ppm)
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-9.0
-8.5
-8.0
-7.5
-7.0
-6.5
-6.0
δ18O per mil (V-SMOW)

Principle Components Analysis (PCA) and End Member Mixing Analysis (EMMA)

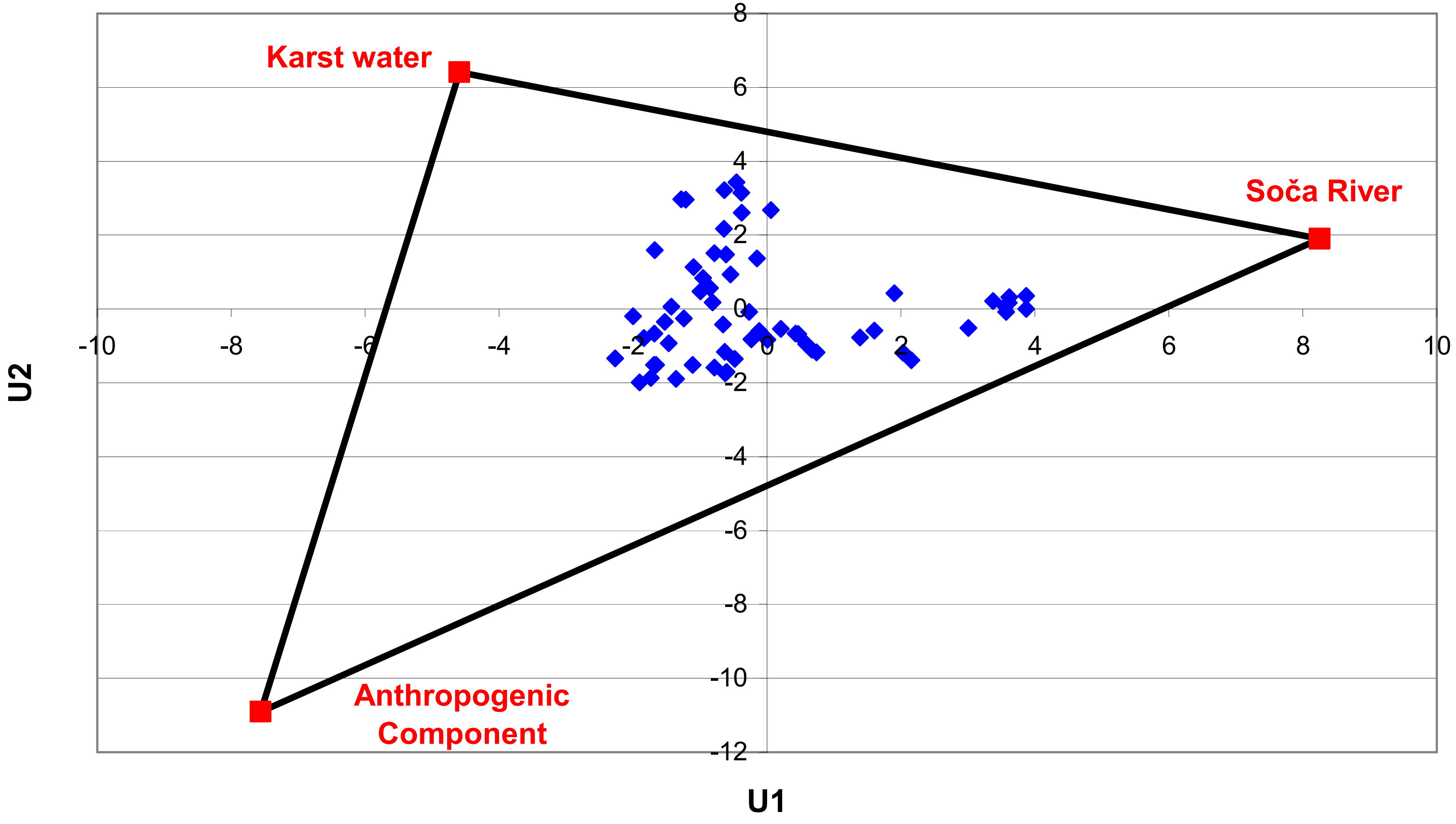
PCA → Factor analysis

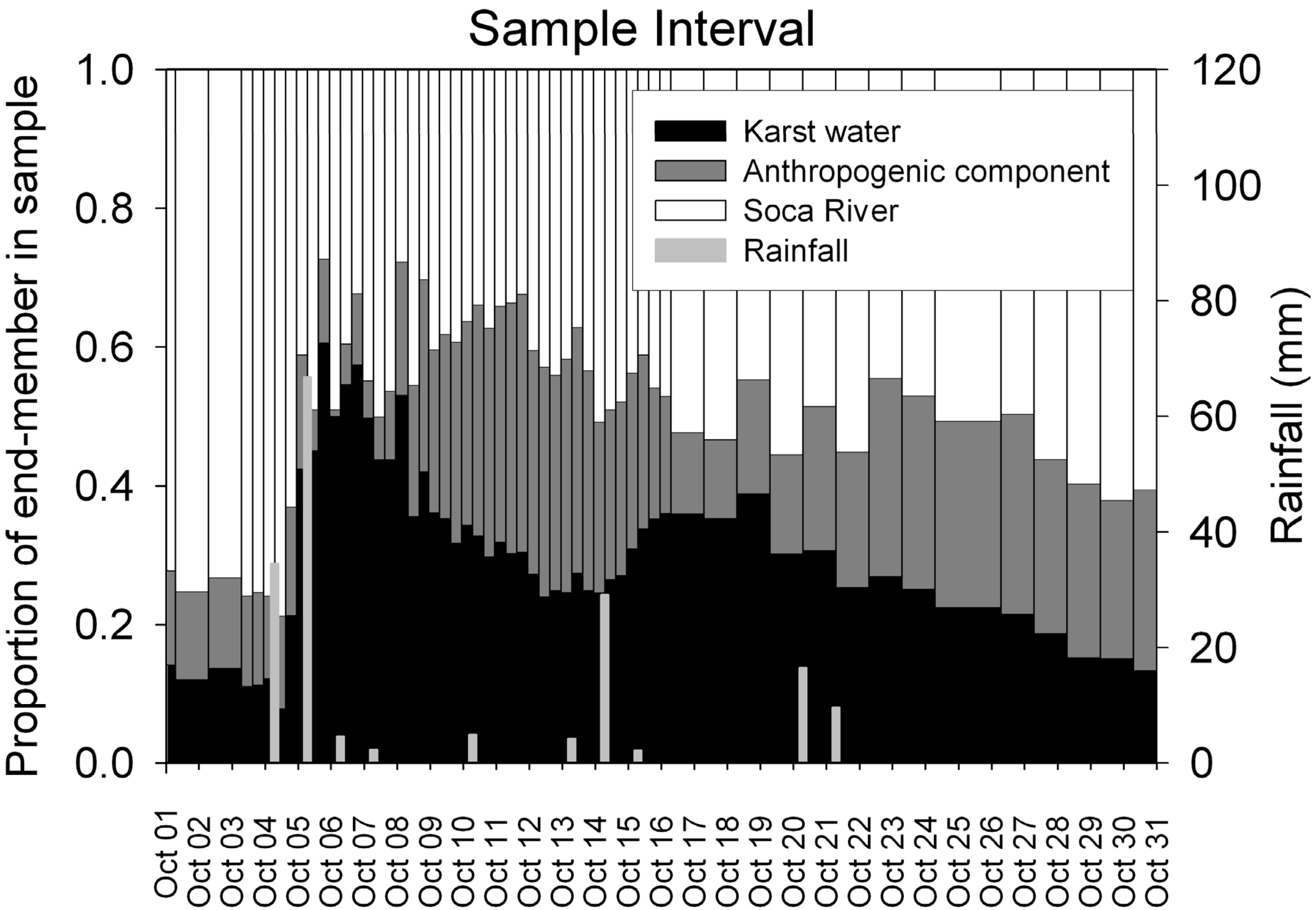
Reduces numerous parameters into a smaller set of new variables ("components") which account for the majority of the data variance.

EMMA → Mixing analysis

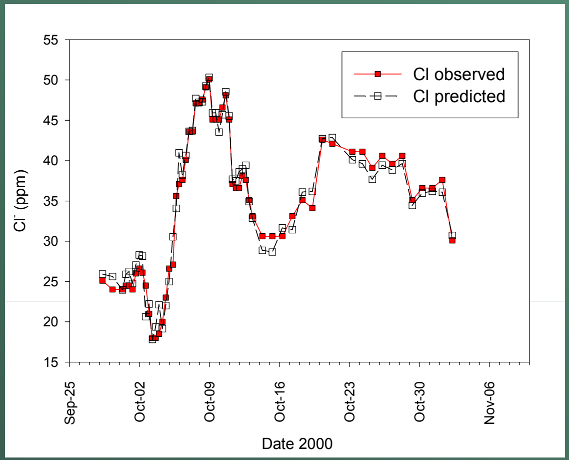
Project observed samples and estimated end-members into 2D mixing space, and calculate proportions of each end-member contained within each observed sample.

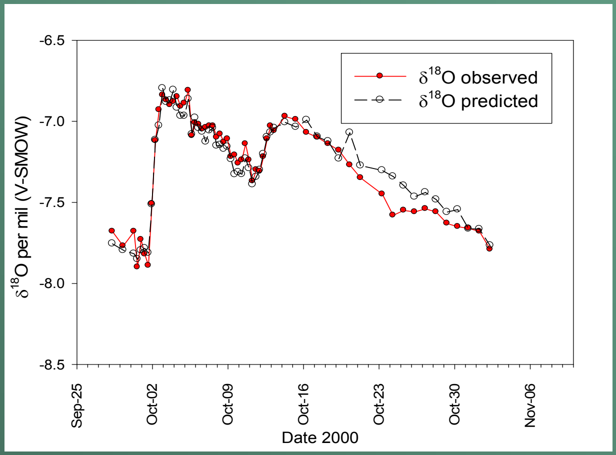
PC-space Mixing Diagram
Well B-4 Storm Events, 2000 (6-parameter PCA/EMMA)

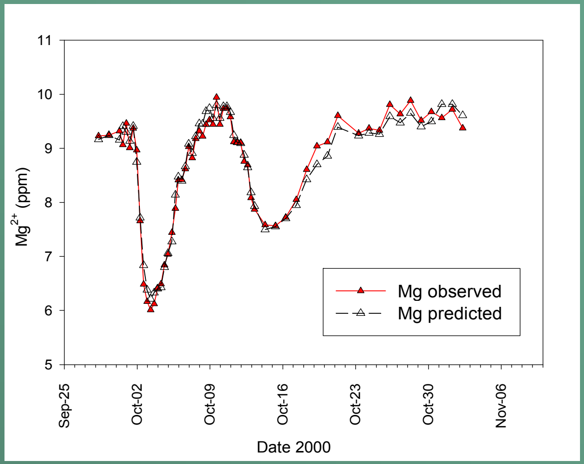


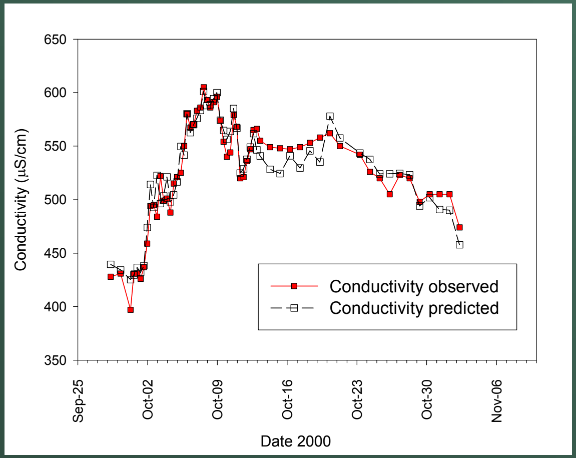

Sample Interval
Proportion of end-member in sample
1.0
0.8
0.6
0.4
0.2
0.0
Rainfall (mm)
120
100
80
60
40
20
0
Karst water
Anthropogenic component
Soca River
Rainfall
Oct 01
Oct 02
Oct 03
Oct 04
Oct 05
Oct 06
Oct 07
Oct 08
Oct 09
Oct 10
Oct 11
Oct 12
Oct 13
Oct 14
Oct 15
Oct 16
Oct 17
Oct 18
Oct 19
Oct 20
Oct 21
Oct 22
Oct 23
Oct 24
Oct 25
Oct 26
Oct 27
Oct 28
Oct 29
Oct 30
Oct 31

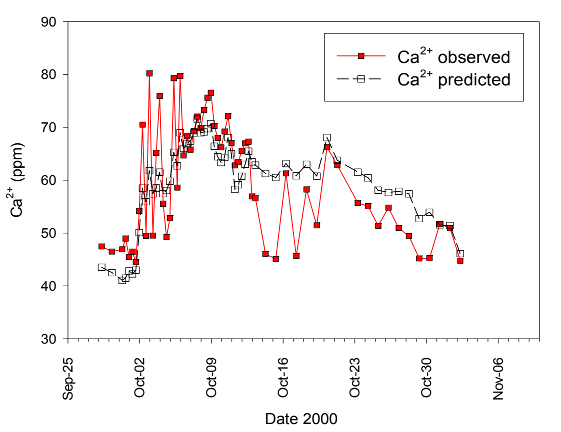
Measured vs. predicted chemistry and isotopic composition at well B-4 during storm events of 2000

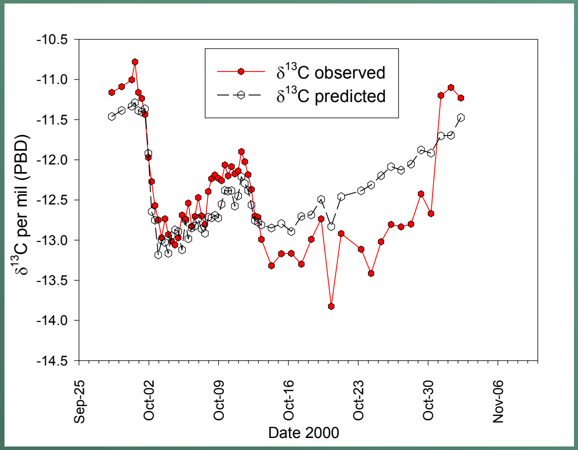




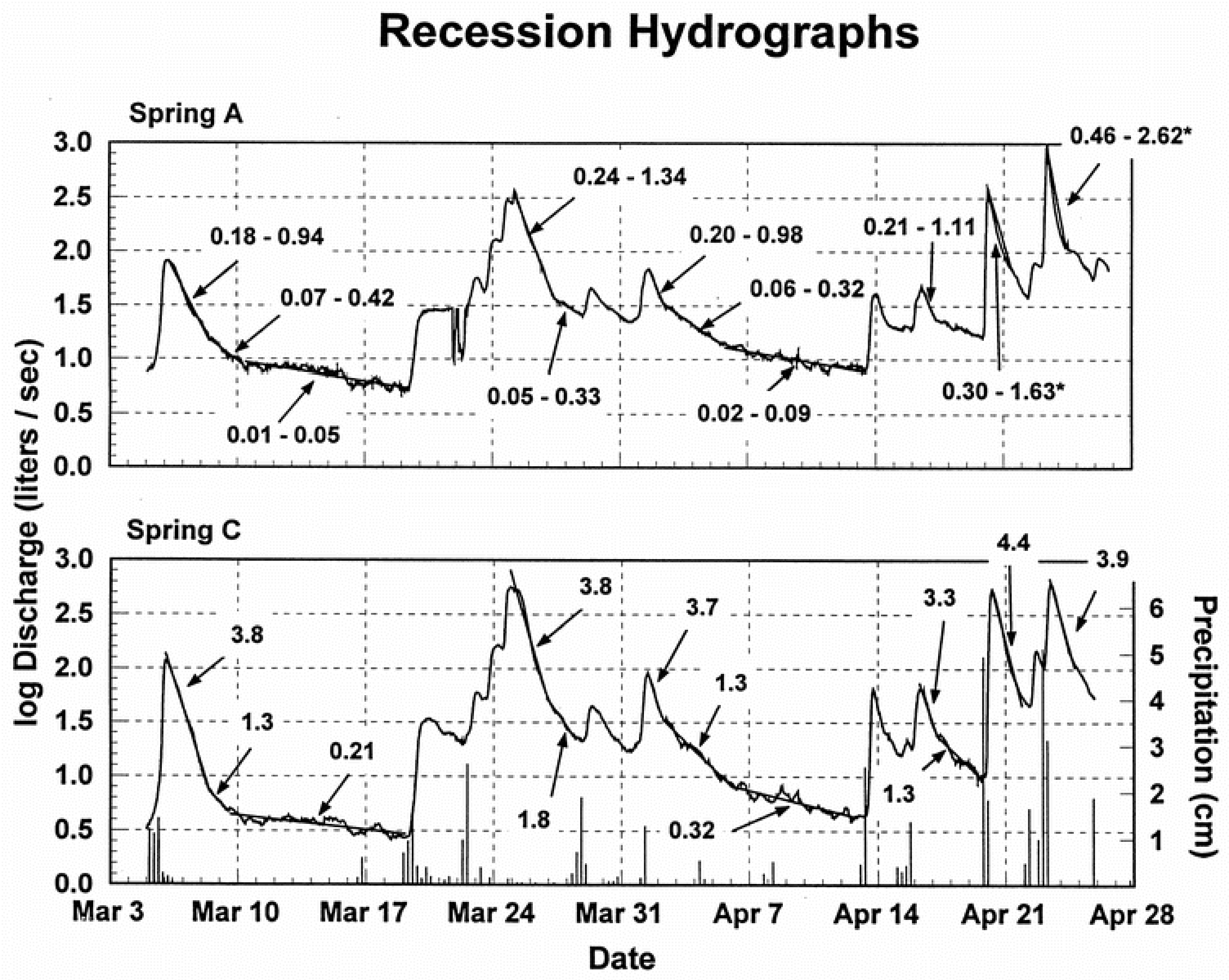






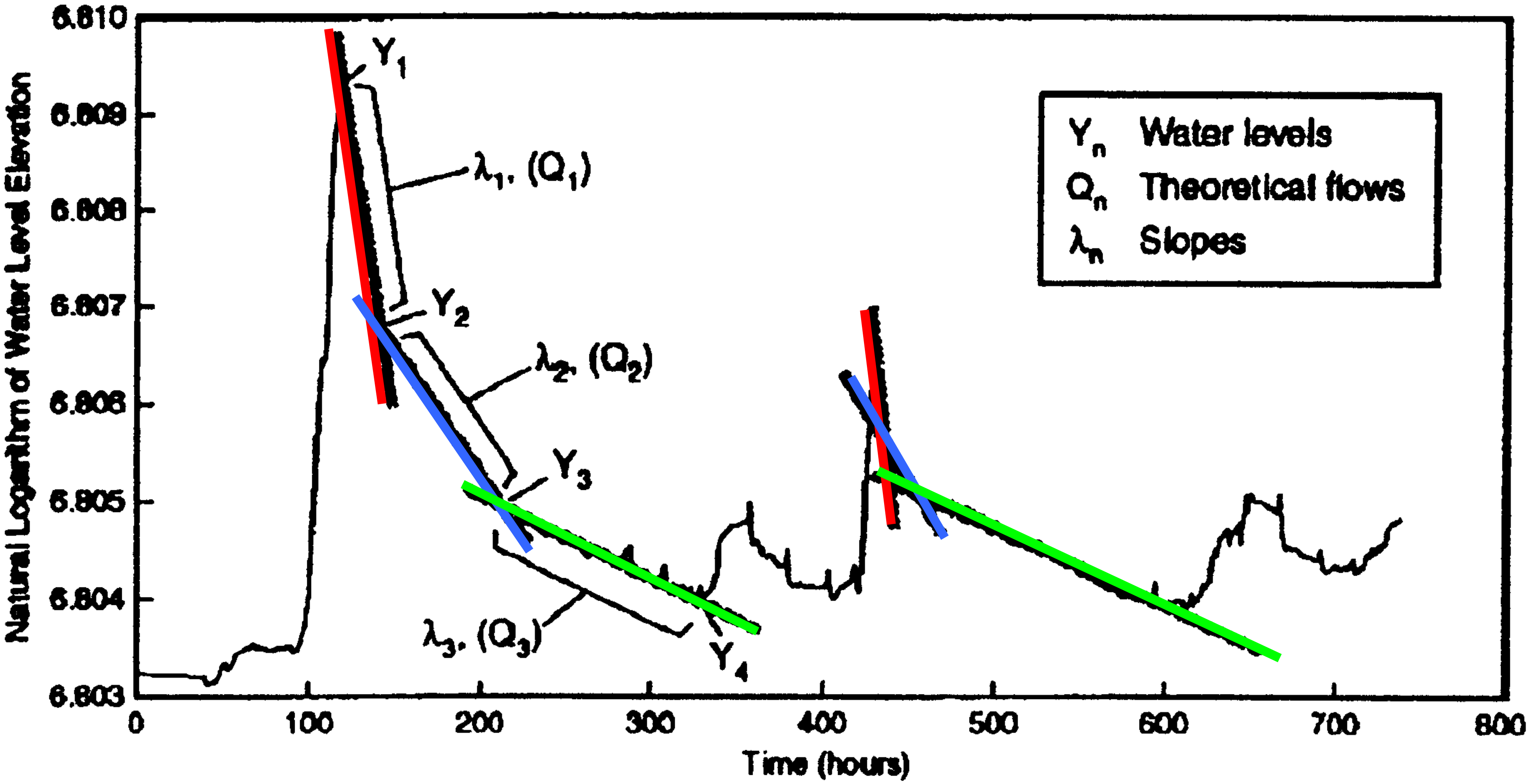


Can this approach work across different scales?



Baedke & Krothe, WRR, 2001

WELL HYDROGRAPHS IN KARST

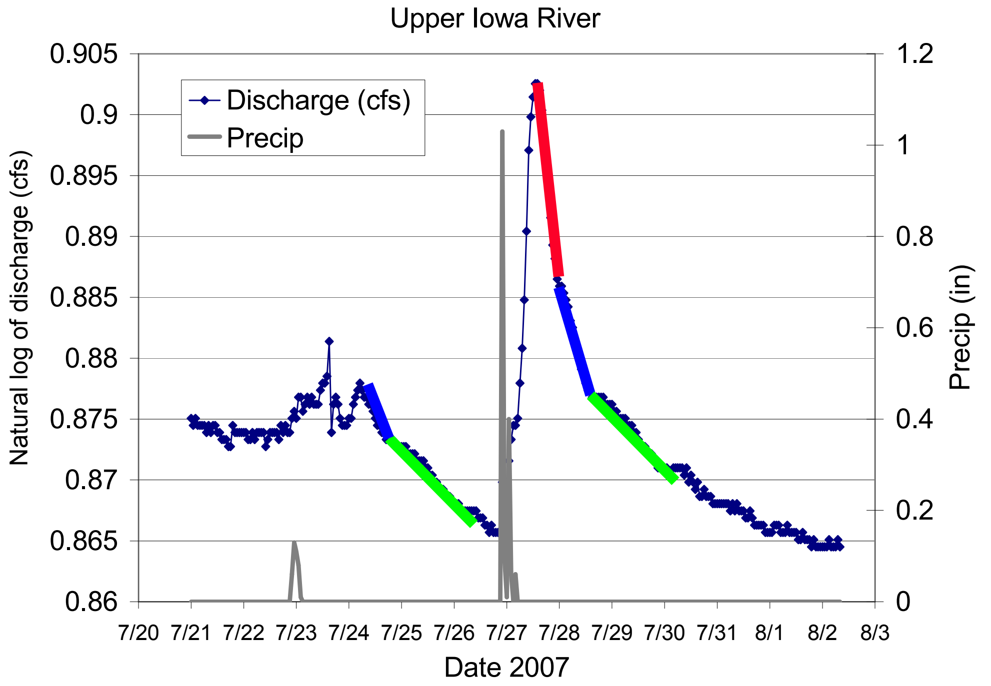


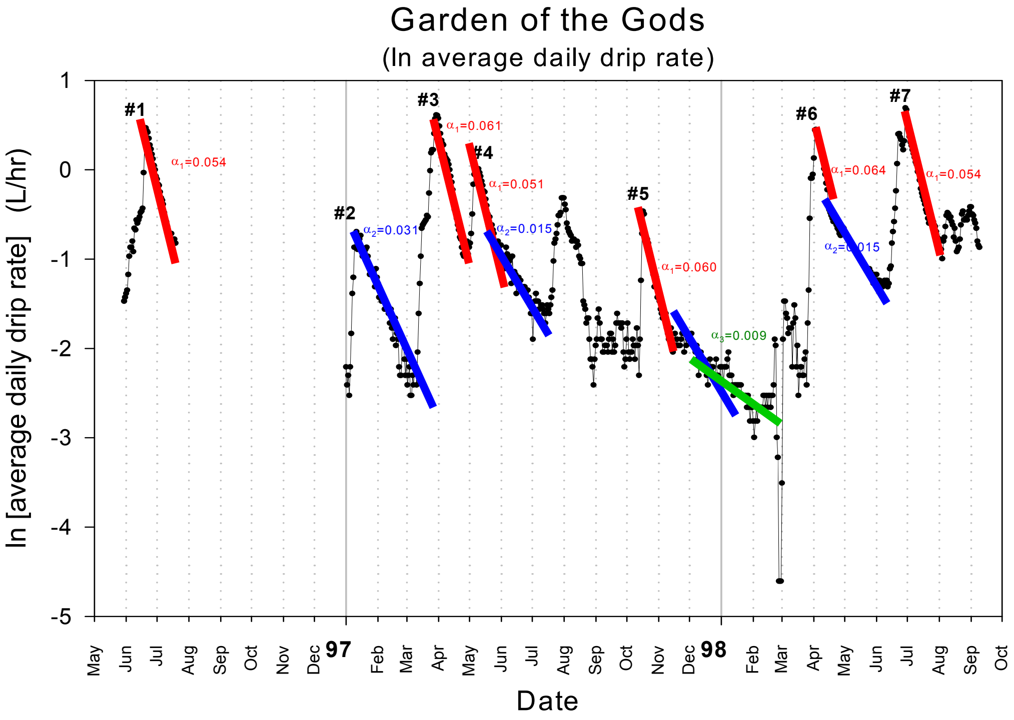
Powers and Shevenell, J. of Hydrology, 2000

Scaling in Minnesota KARST?

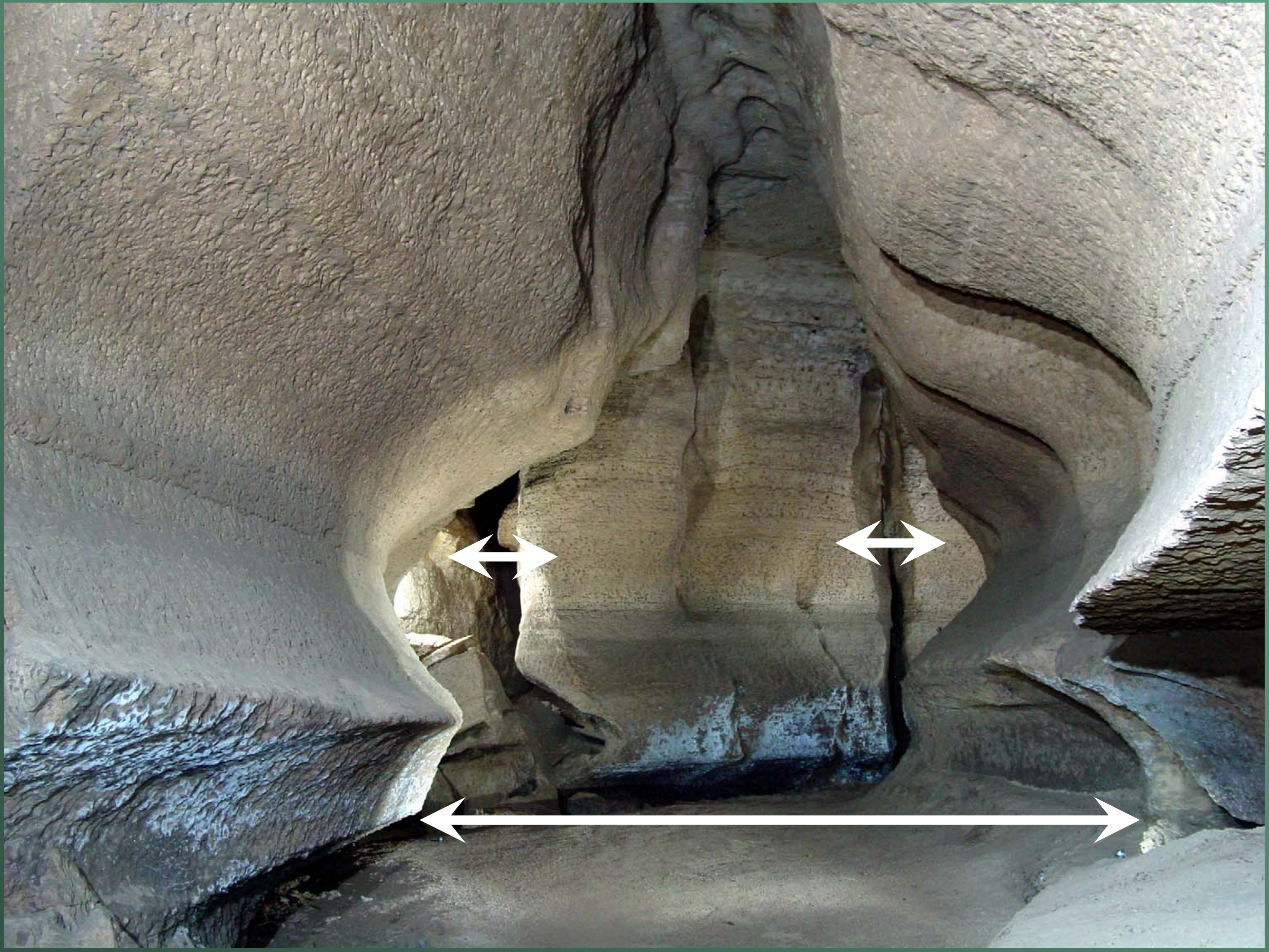
Upper Iowa River:

Drips in Mystery Cave:





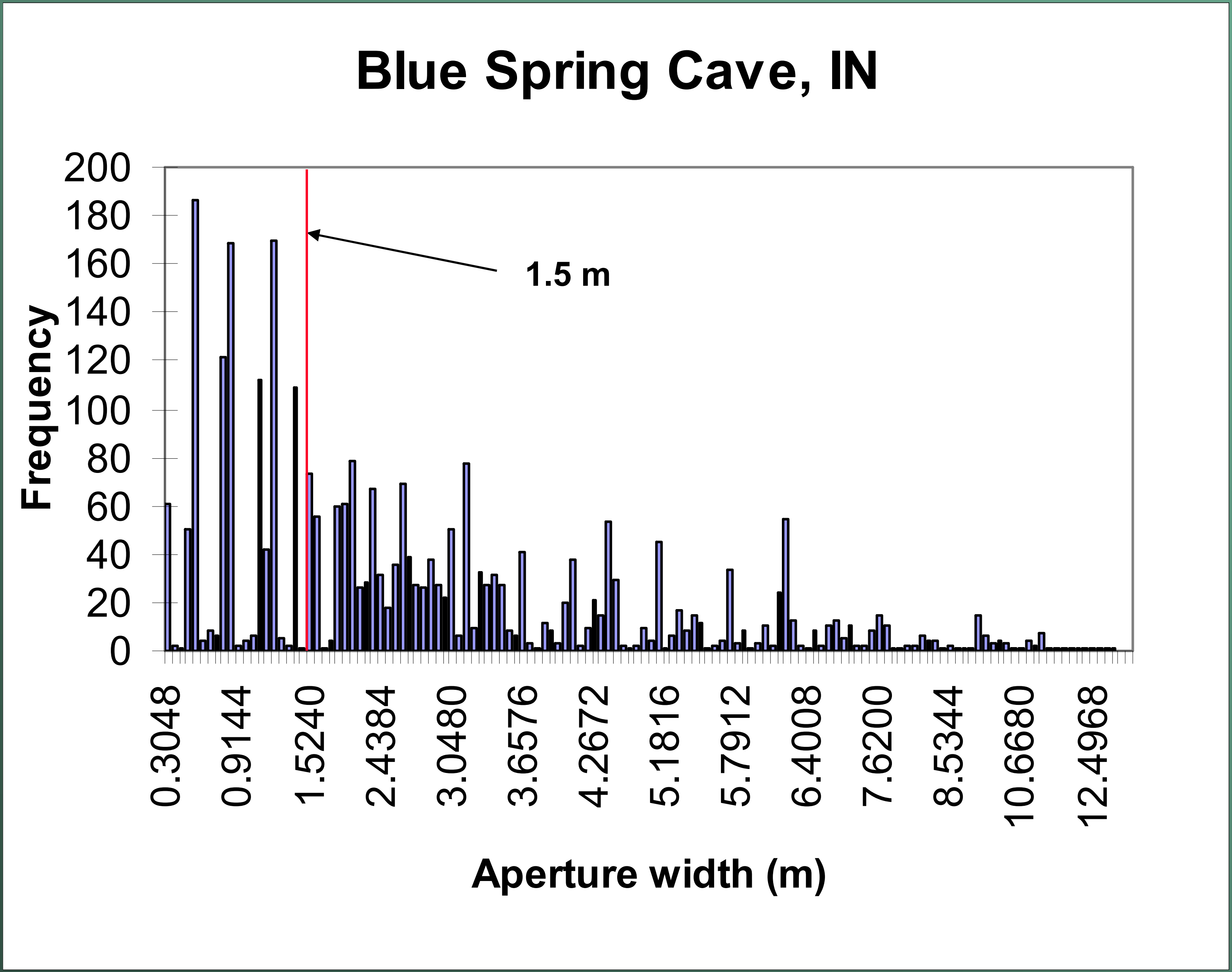
Why the abrupt breaks in recession slope?



Abrupt breaks in conduit dimension?

Photo by Allen Lewerer

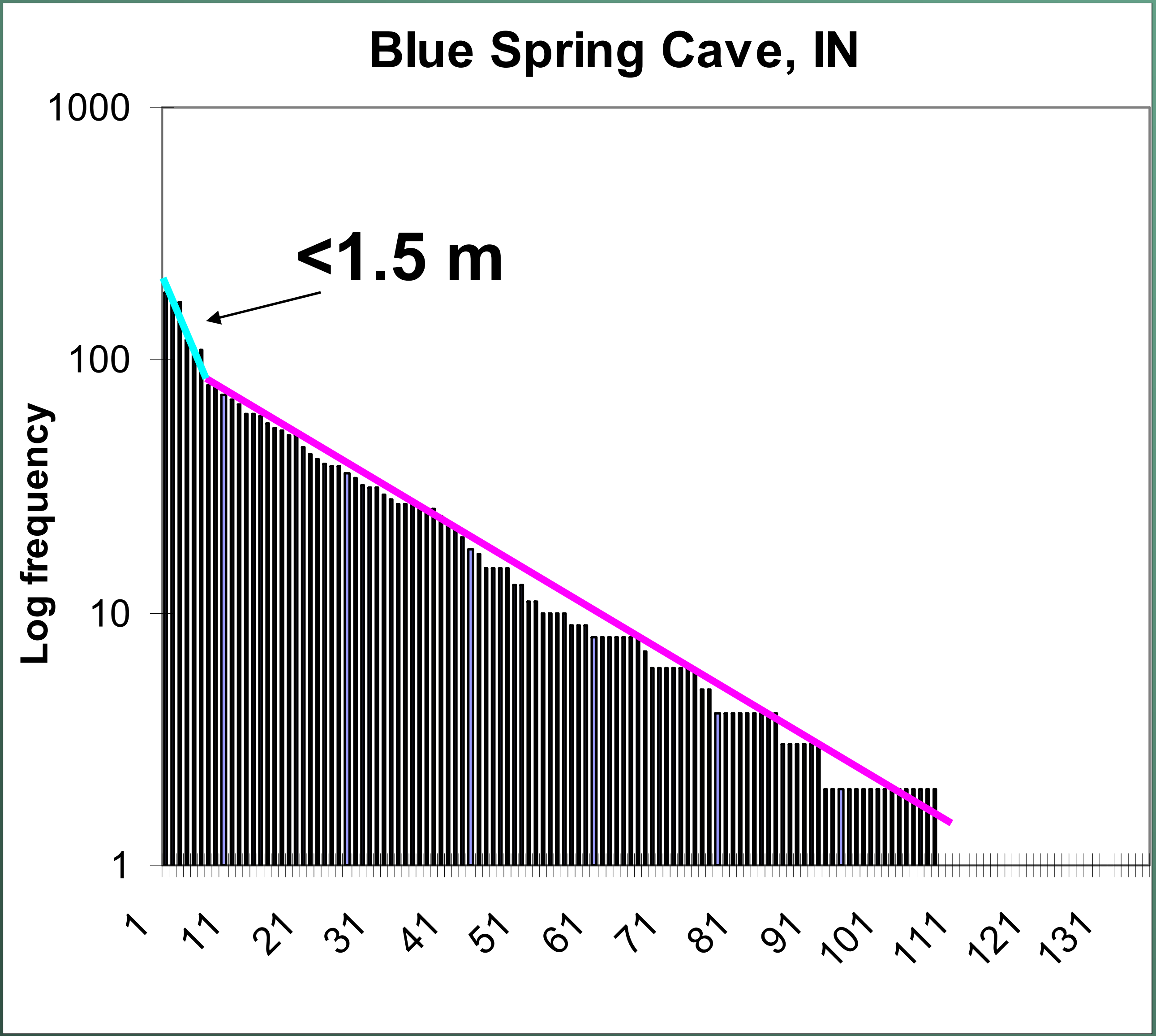
Conduit aperture distribution:



Data: Palmer and Palmer, personal comm.

Conduit aperture frequency:

Multiple fractal dimensions?



Data: Palmer and Palmer, personal comm.

Preferential flow is the norm

- Vadose zone: root casts, burrows, dessication cracks, rock fractures
- Interflow: permeability change across soil/bedrock interface, soil hardpans, calcrete
- Alluvium: sand & gravel channels/stringers
- Bedrock: fracture flow
- Karst: conduit flow
- (Mantle channel flow?)

What are some common patterns in hydrology?

- Recession slopes of hydrographs
- Hysteresis
- Diel periodicity
- Fractal networks
- Power-law relations in time series spectra

Linking chemistry to discharge

- Patterns in chemical data are as prevalent as patterns in physical hydrologic data
- Hysteresis
- Spatial distribution of chemical end-members
- Repetition in chemical “signatures” according to flow regimes

What lies ahead?

It may seem strange to end a review of modeling with an observation that future progress is very strongly linked to the acquisition of new data and to new experimental work but that, in our opinion, is the state of the science.

George Hornberger and Beth Boyer, 1995

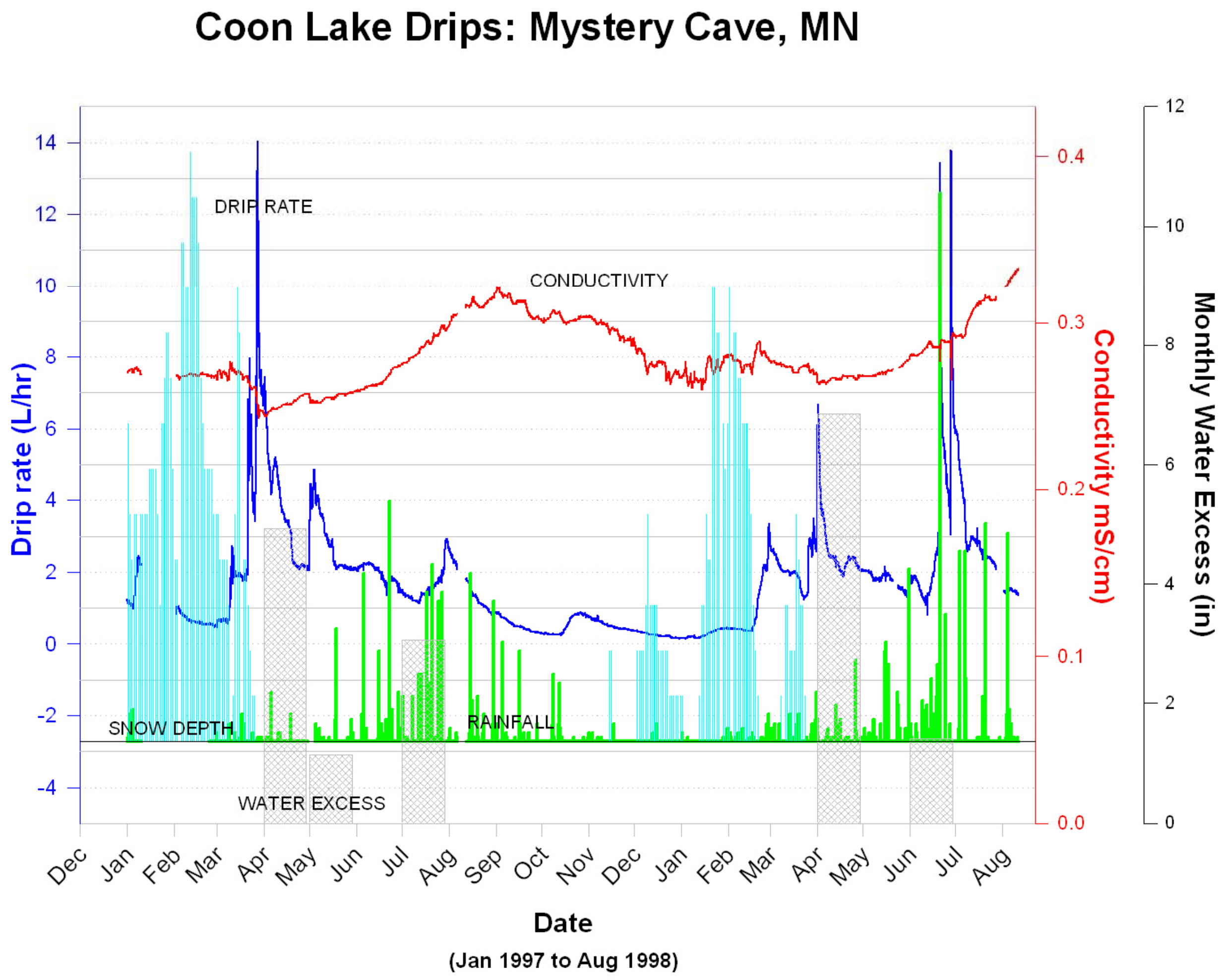
- High frequency data collection
- Wireless distributed smart sensors (“motes”)
- Data Based Modeling

A rebirth of empiricism in hydrology

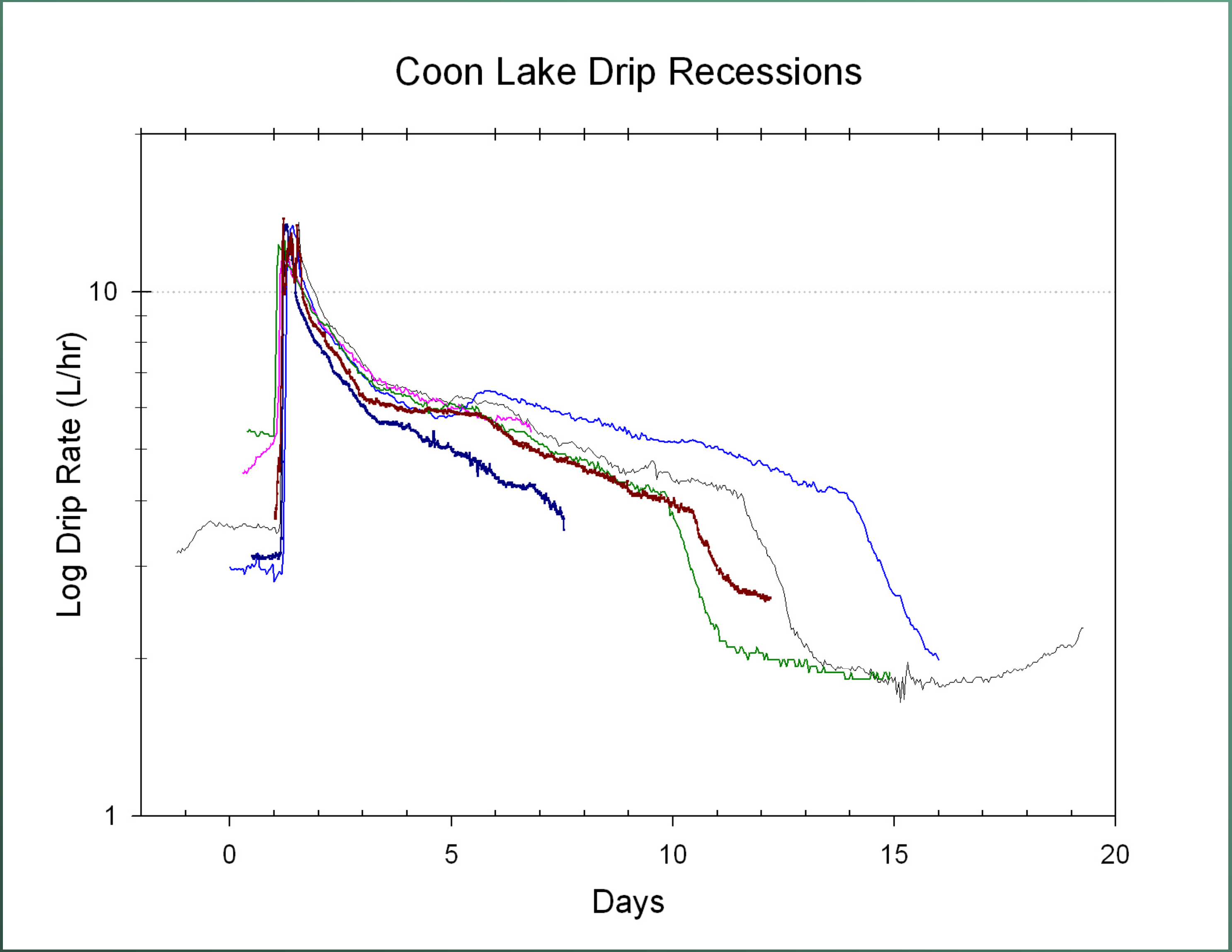
- Lumped parameter rainfall-runoff forecasting
- Kernal functions
- Convolution
- Artificial Neural Networks
- Lattice-Boltzmann models

THANK YOU

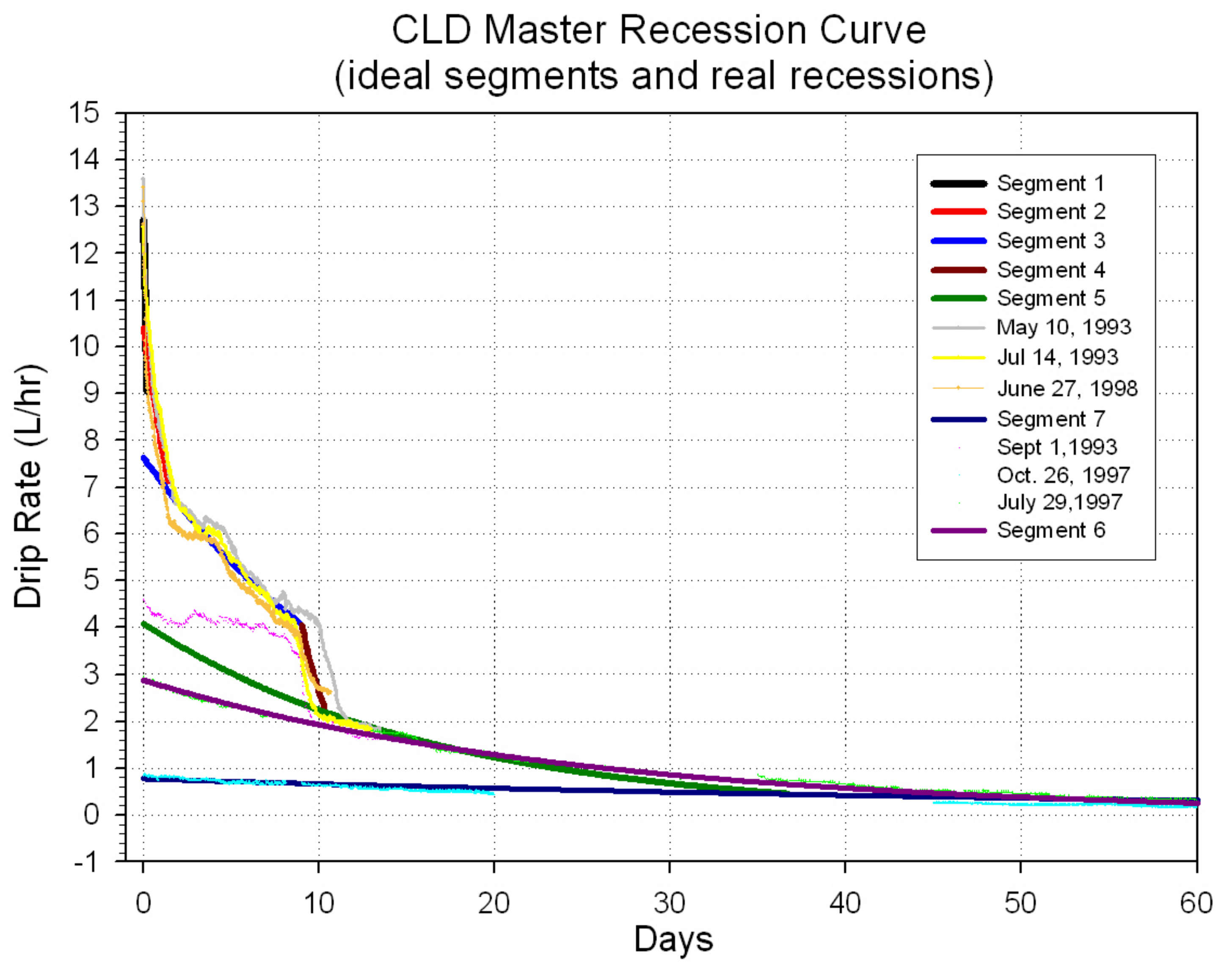
VADOSE ZONE PROCESSES IN KARST: Mystery Cave, MN



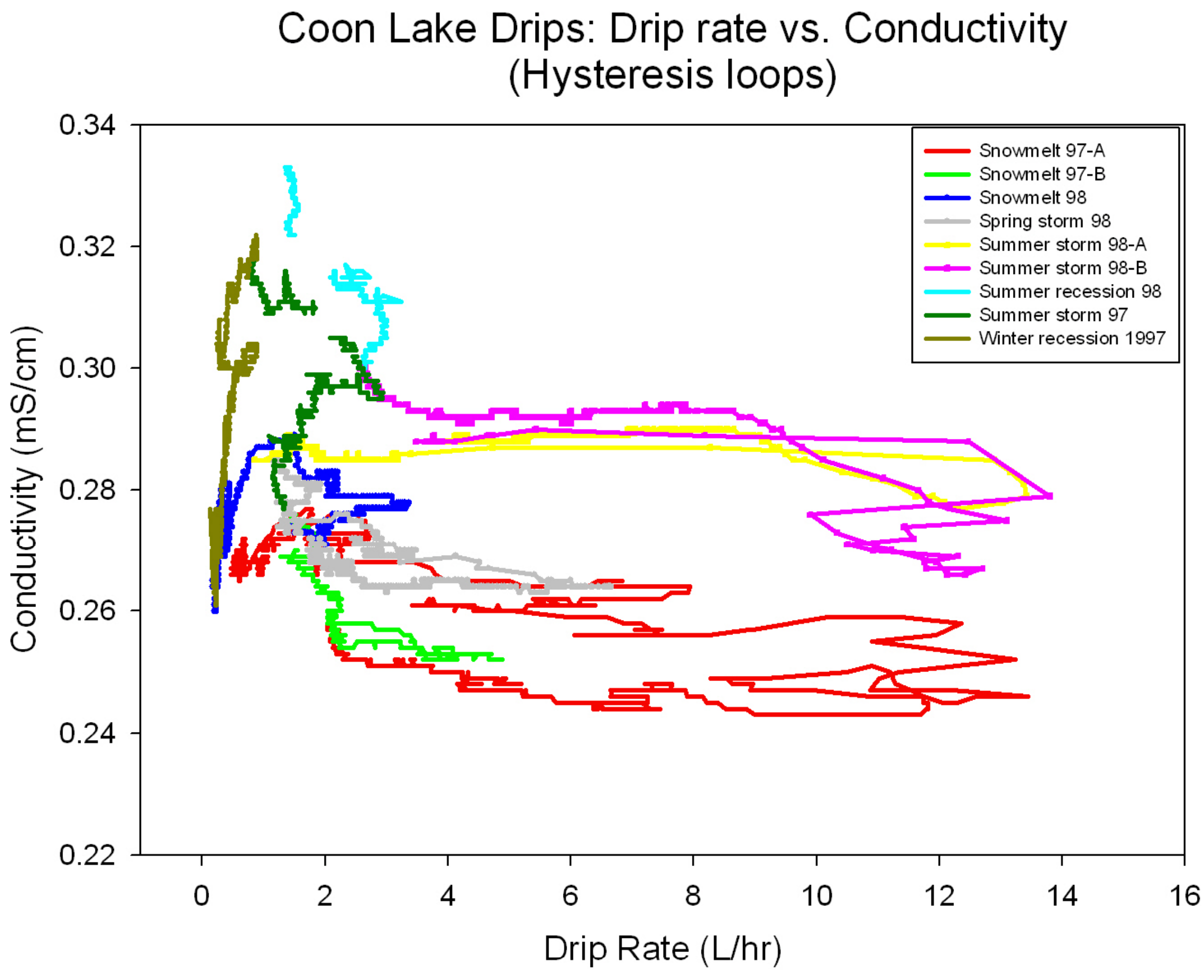
Coon Lake Drips: Recessions



Coon Lake Drips: Master Recession Curve



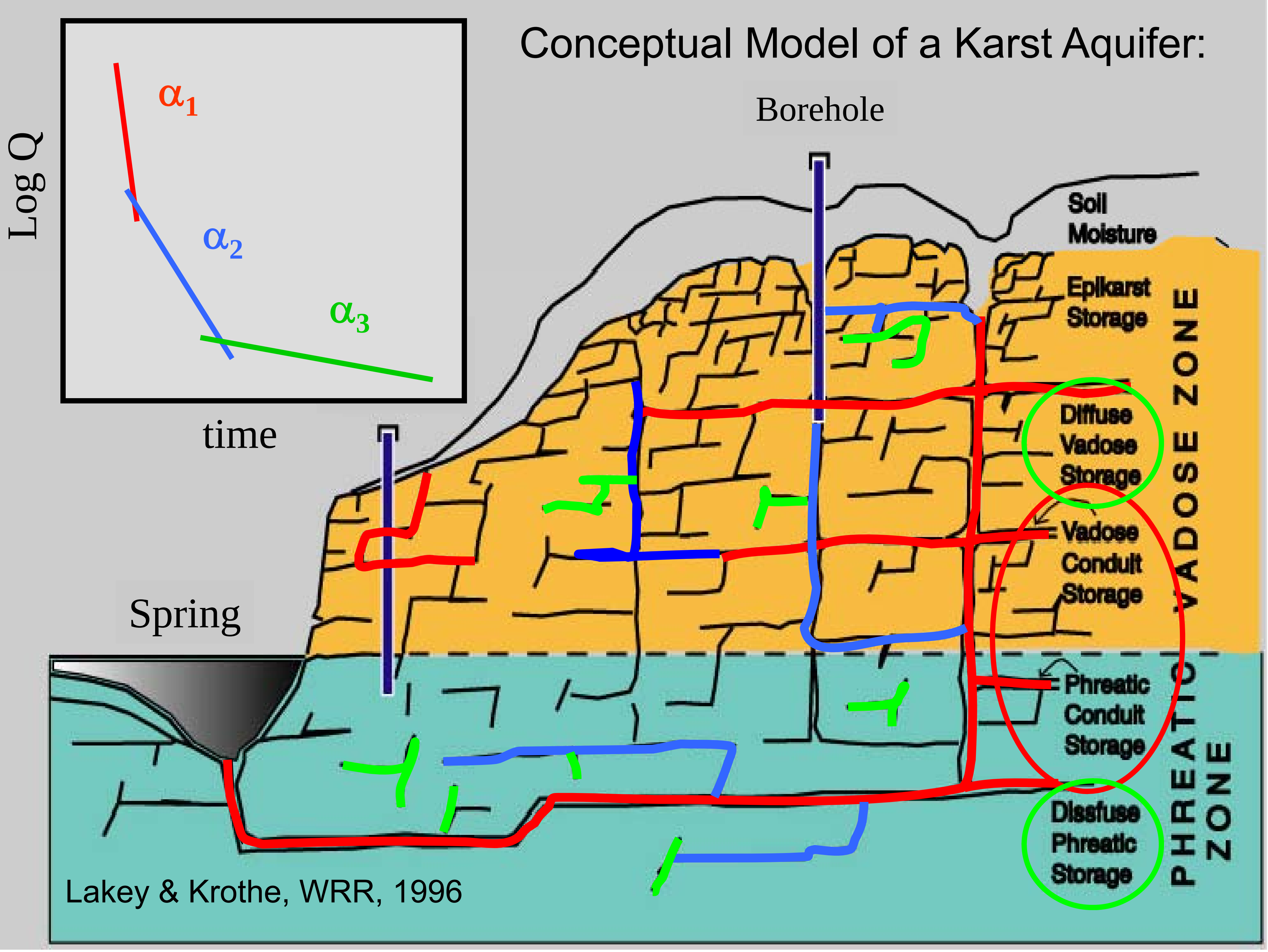
Hysteresis: Coon Lake Drips



Utility of Recession Analysis?

- Aquifer hydraulic parameters (or not)
- Flow regimes and aquifer storage volumes
- Characteristics of conduit geometry
- Identifying possible scaling effects

Conceptual Model of a Karst Aquifer:



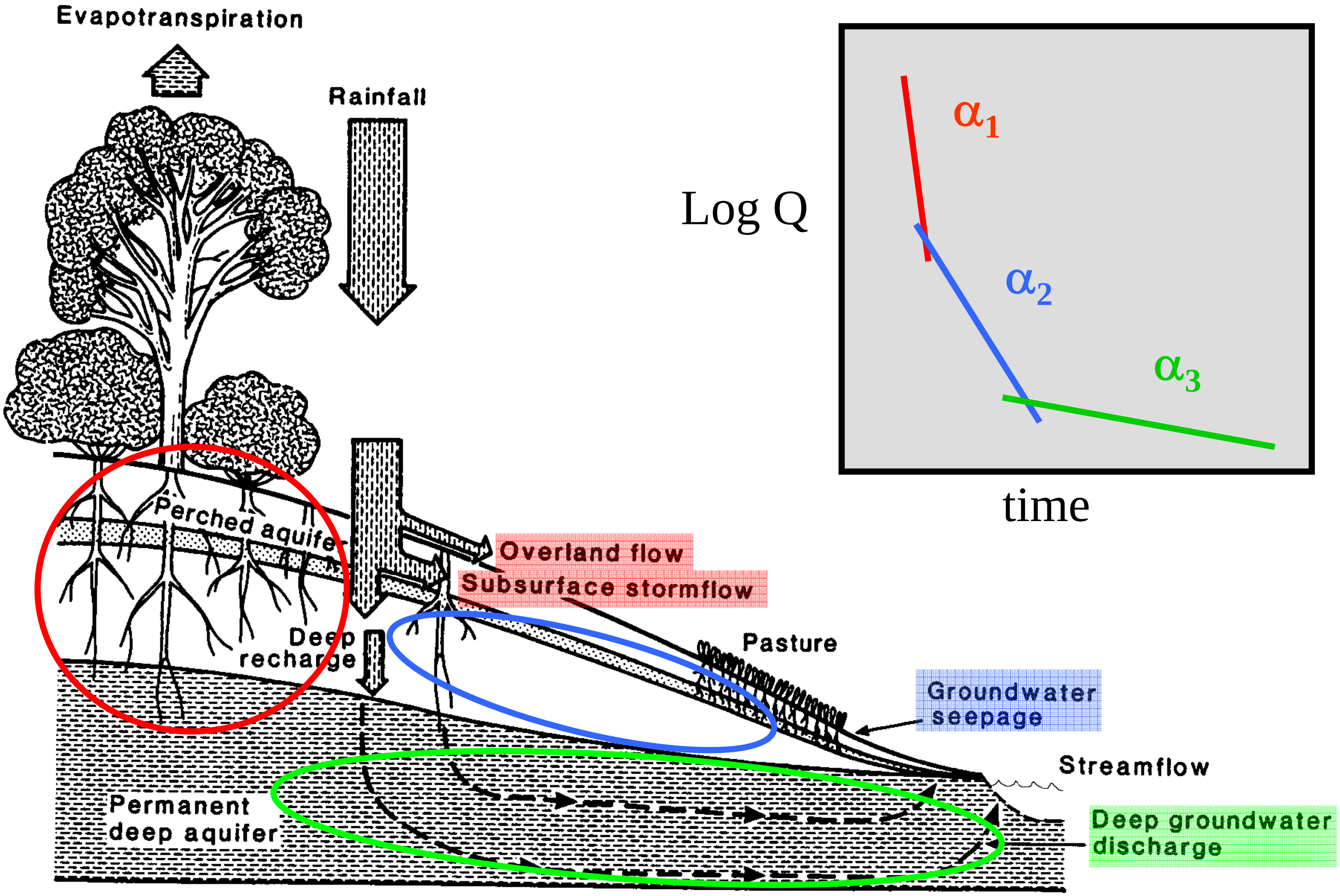
Lakey & Krothe, WRR, 1996

Streamflow Probability Density Function (pdf)

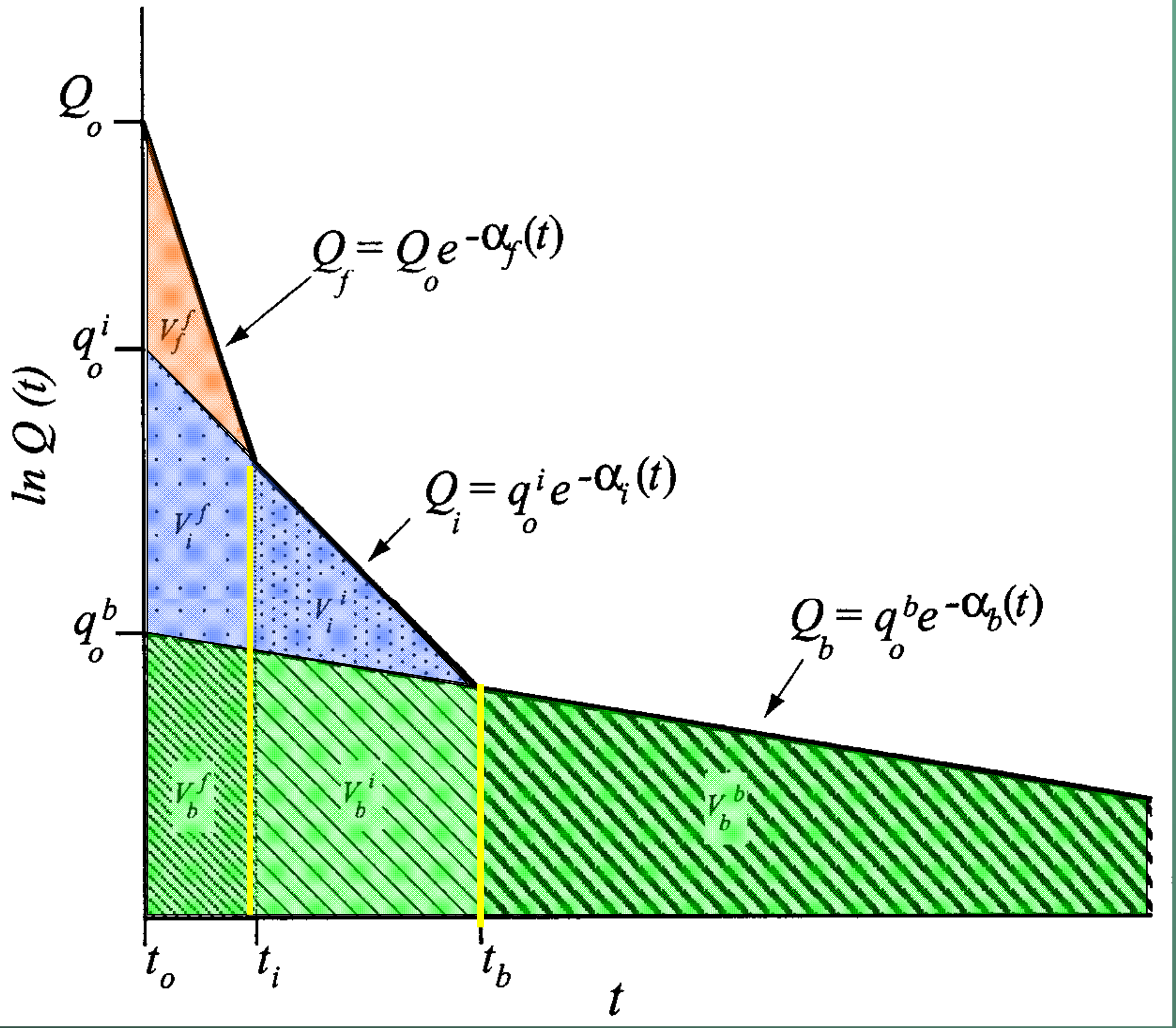
- Comparison between analytical and observed streamflow pdf's in the West Swan River catchment (47°, 14′ 40″, 93° 02′ 30″, Minnesota, USA) during the summer season. The pdf of the observed streamflows in the West Swan during the period 1963–1979 is shown by circles. The dashed line refers to the linear model of Botter et al. [2007a], while the nonlinear pdf derived in this paper (equation (19)) is reported by the solid line. The parameters used in the linear model can be found in the work by Botter et al. [2007c, Table 1]. The same parameters are employed also by the nonlinear model, except for the mean residence time in subsurface. The latter must be replaced by the parameters a and b, which are derived from the analysis of the recessions observed (in this case a = 2.88 and b = 0.8)

Physical & Probabilistic “Diffusion”

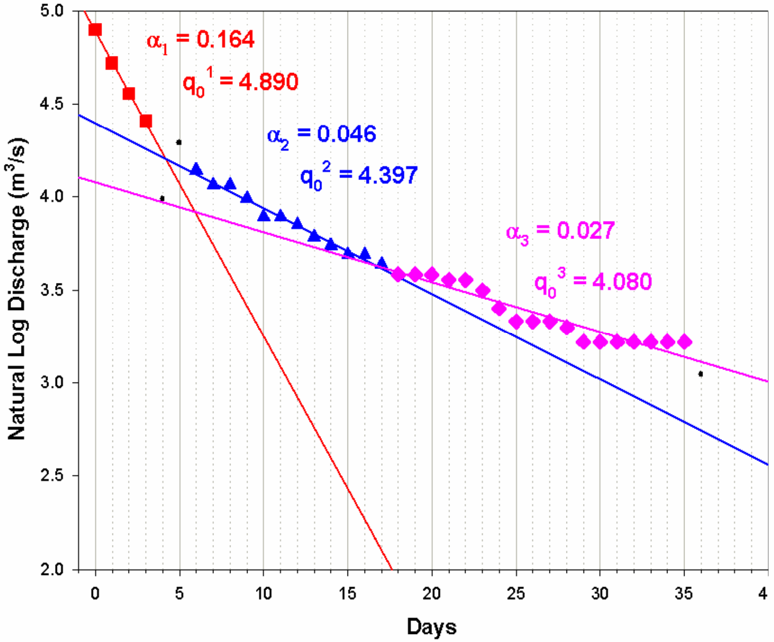
- Fourier and Laplace: separate approaches to similar conclusion
- Navier-Stokes: physical diffusion
- Chemical tracers: rapid peaks, long tails
- Tracer models: combined exponential and piston-flow models mimic travel times.
- Earliest response at springs is water displaced from stagnant conduits



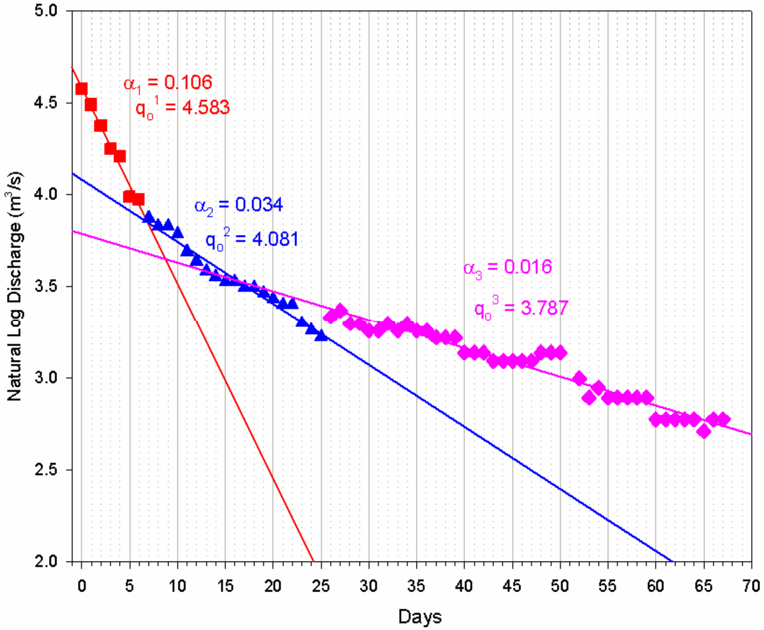
from Turner and Macpherson, 1990



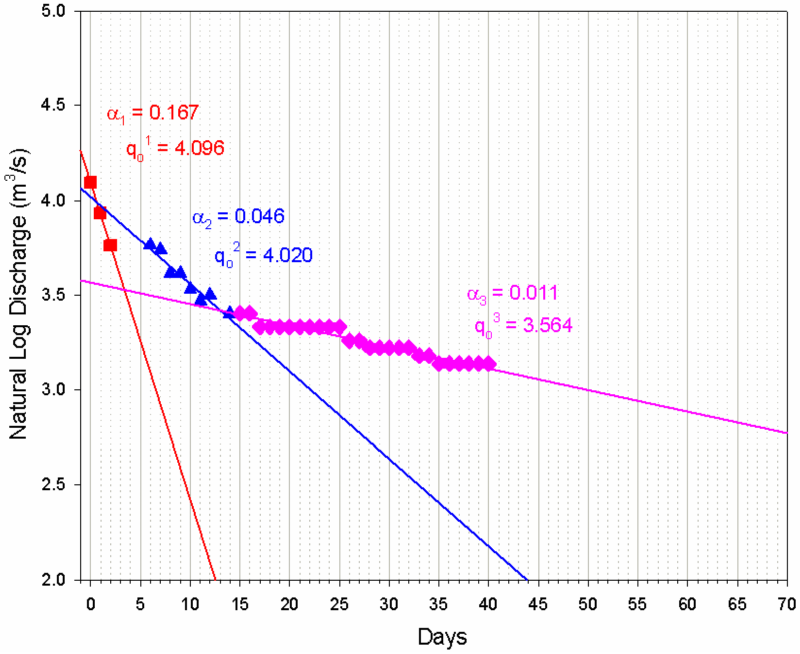
Q_o
q_o^i
q_o^b
$\ln Q(t)$
$Q_f = Q_o e^{-\alpha_f(t)}$
$Q_i = q_o^i e^{-\alpha_i(t)}$
$Q_b = q_o^b e^{-\alpha_b(t)}$
V_f^f
V_i^f
V_i^i
V_b^f
V_b^i
V_b^b
t_o
t_i
t_b
t



Timavo Discharge
Nov 8 - Dec 14,1998

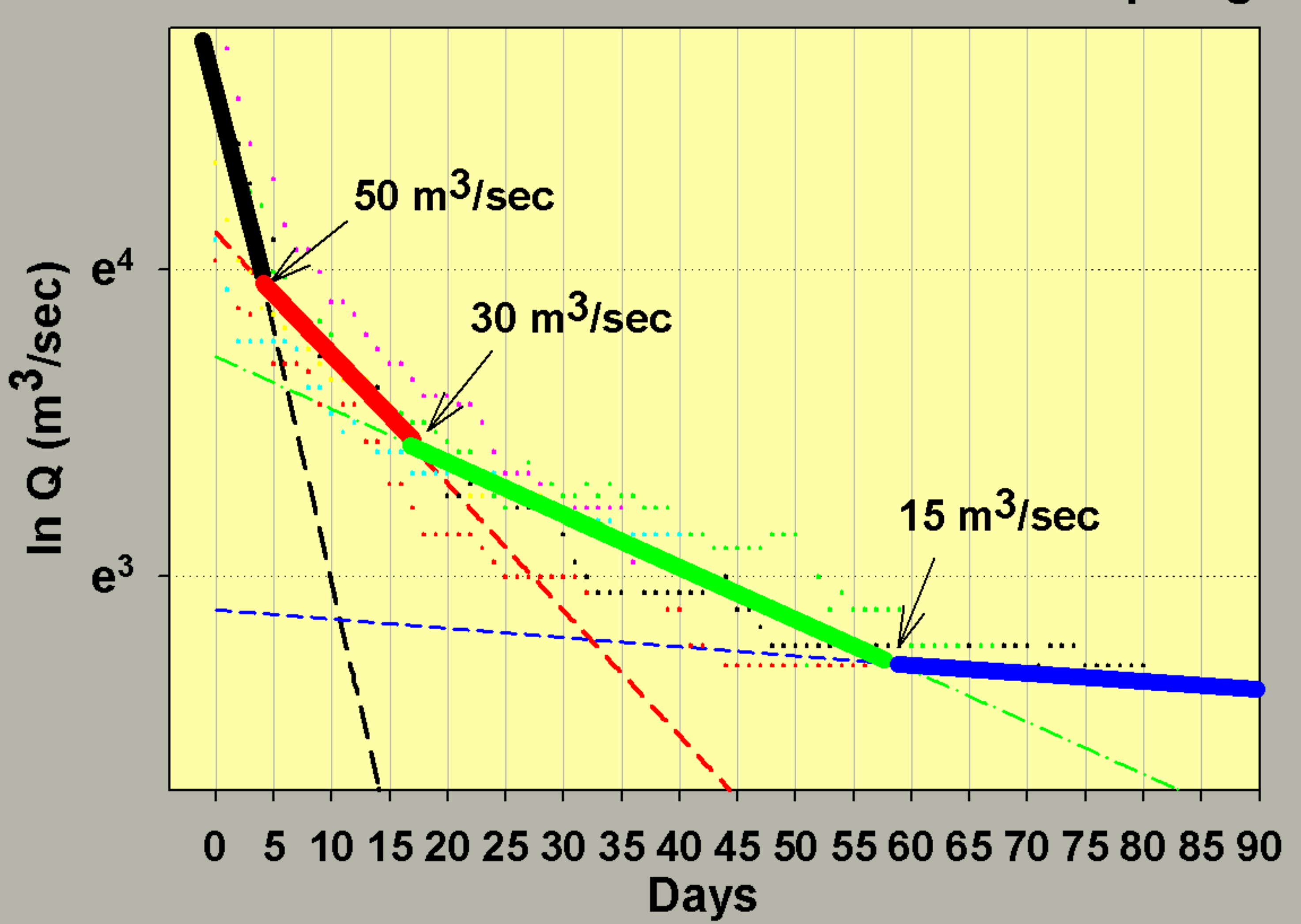


Timavo Discharge
April 23 - June 29,1999

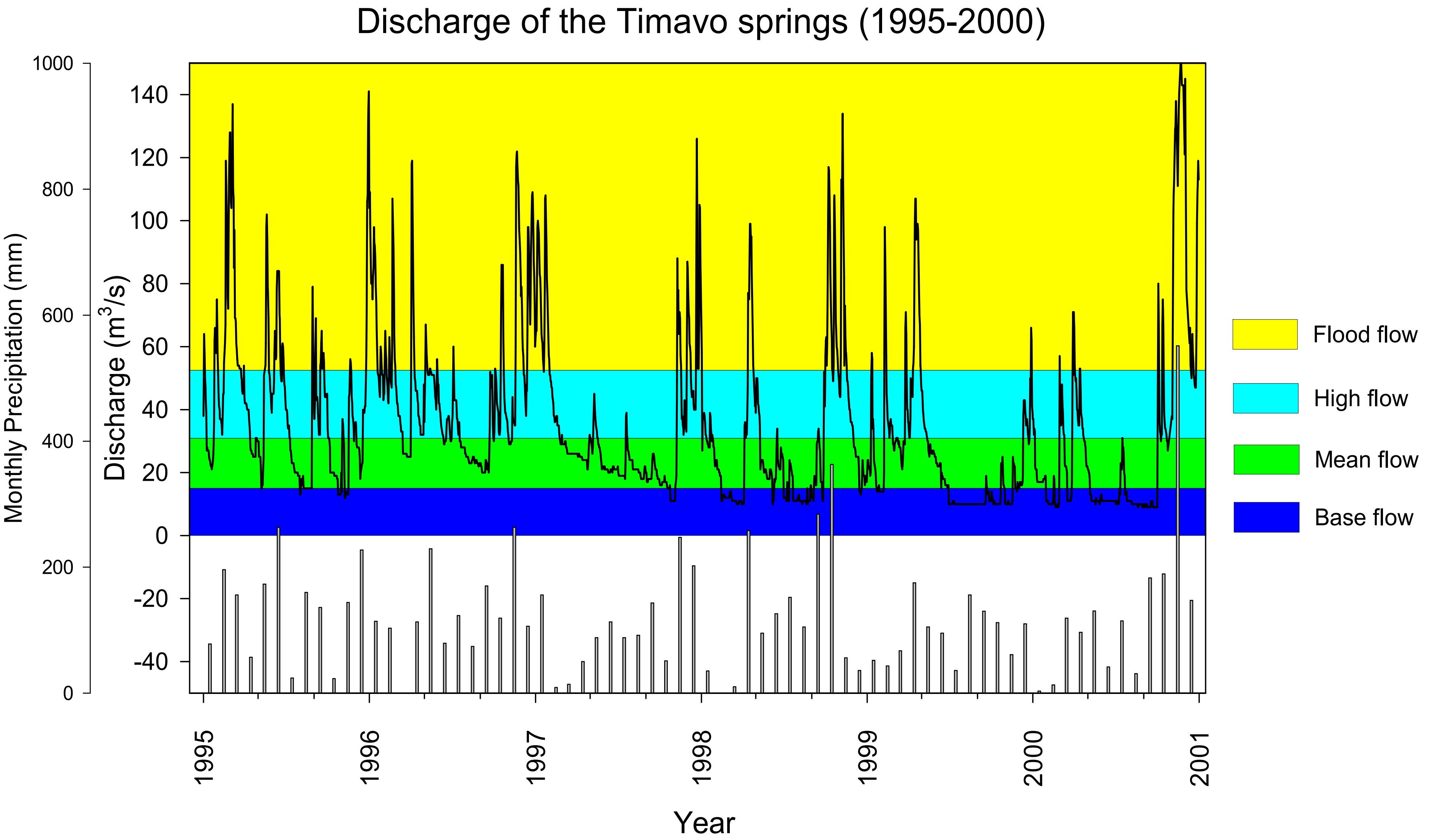


Timavo Discharge
July 4 - Sept. 9, 1996

Master Recession Curve of the Timavo springs



6-year Timavo discharge record



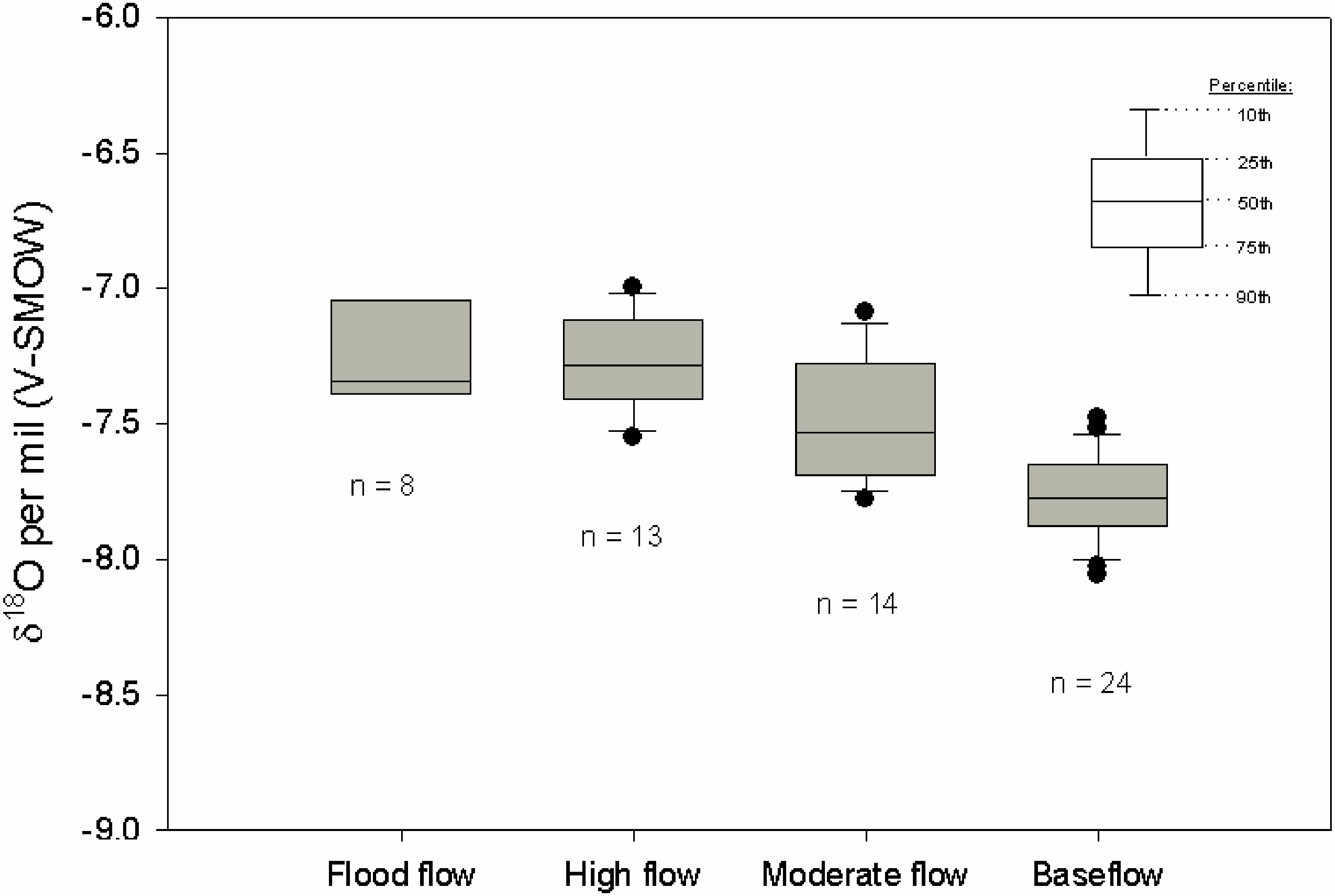
MASTER RECESSION CURVE

- Defines multiple flow regimes of each recession period in terms of multiple recession indices (i.e. transmissivities)

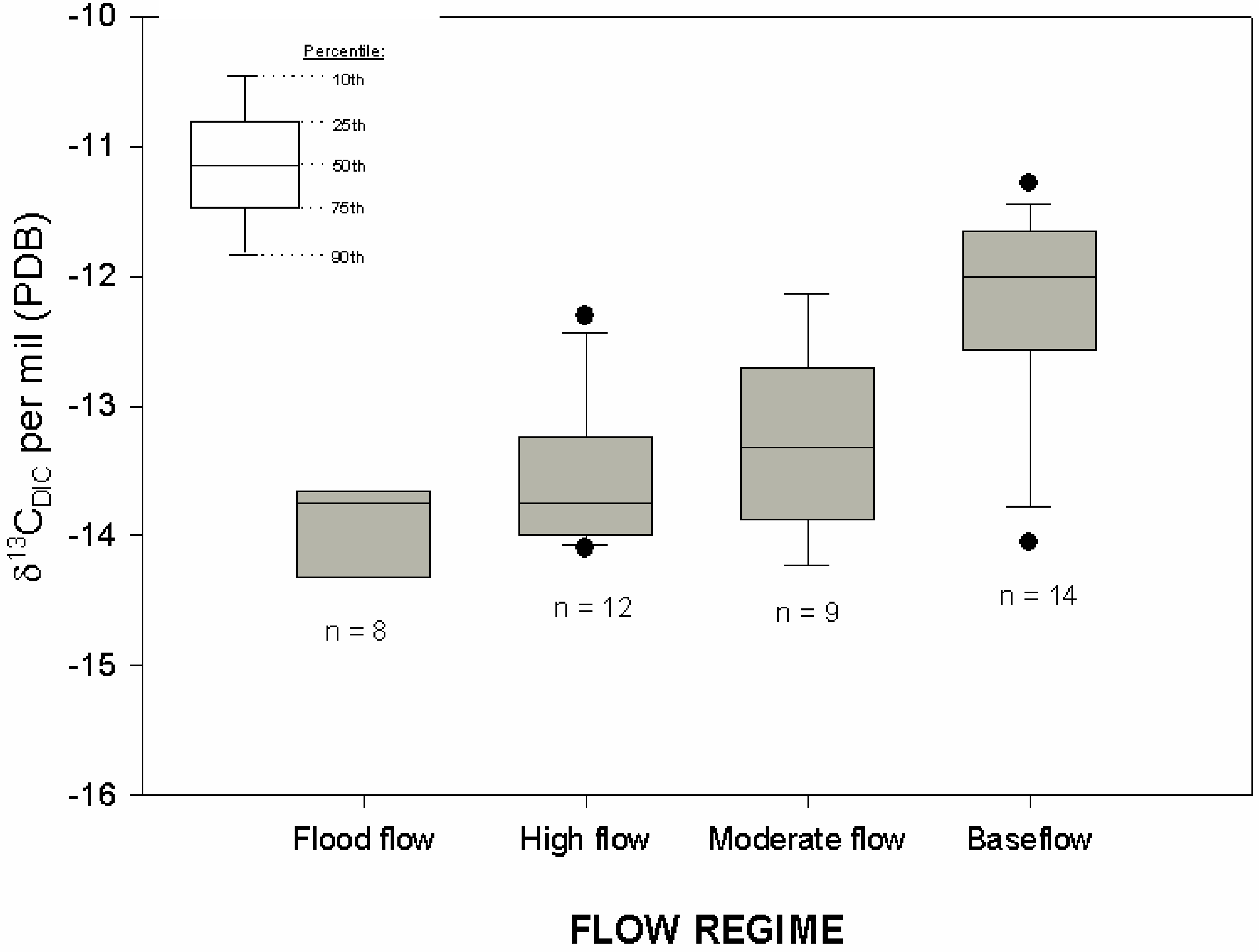
…but what can I do with it?

- Quantifiable, reproducible, and interpretable means of relating chemistry to discharge

Flow Regime $\delta^{18}O$ at Timavo



$\delta^{13}C_{DIC}$ at Timavo



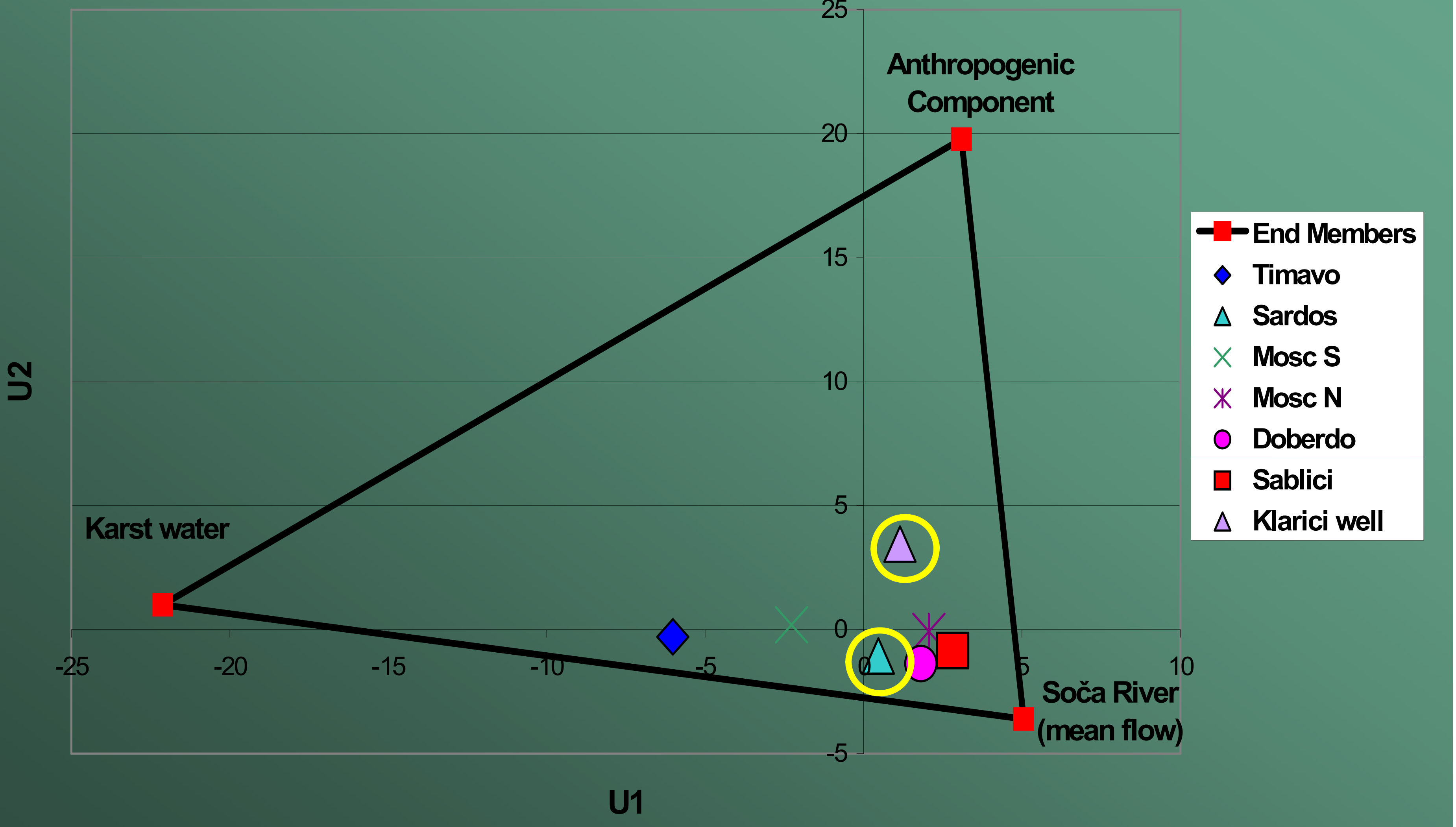
EMMA!

(End-Member Mixing Analysis)

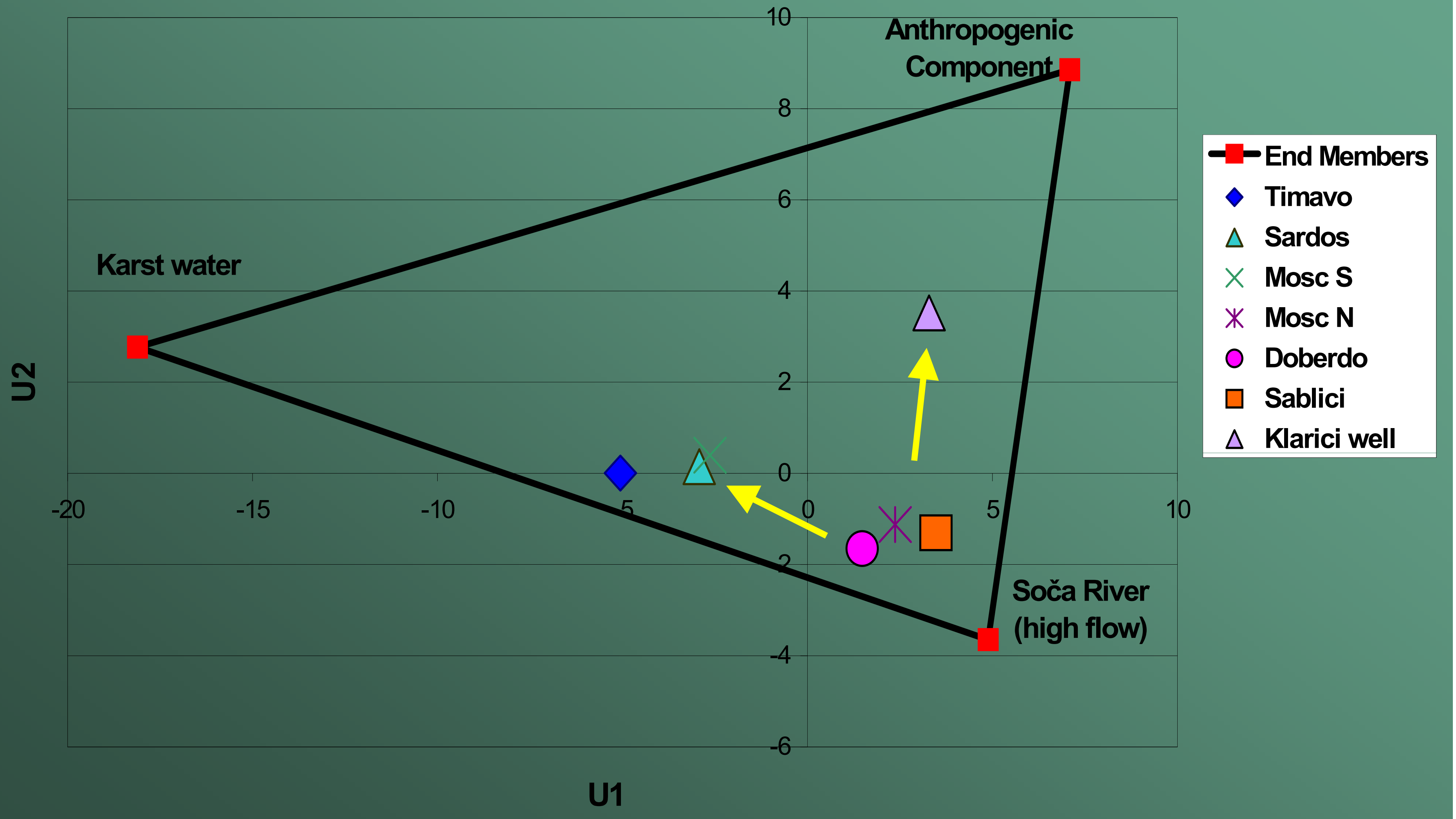
- **Group chemistry samples according to defined flow regimes**
- **Calculate relative contributions of end-members to measured stream chemistry within each flow regime**
- **Working within a subset of chemical data easier and more informative**

PC-space Mixing Diagram

Kras Springs, MEAN Flow Regime



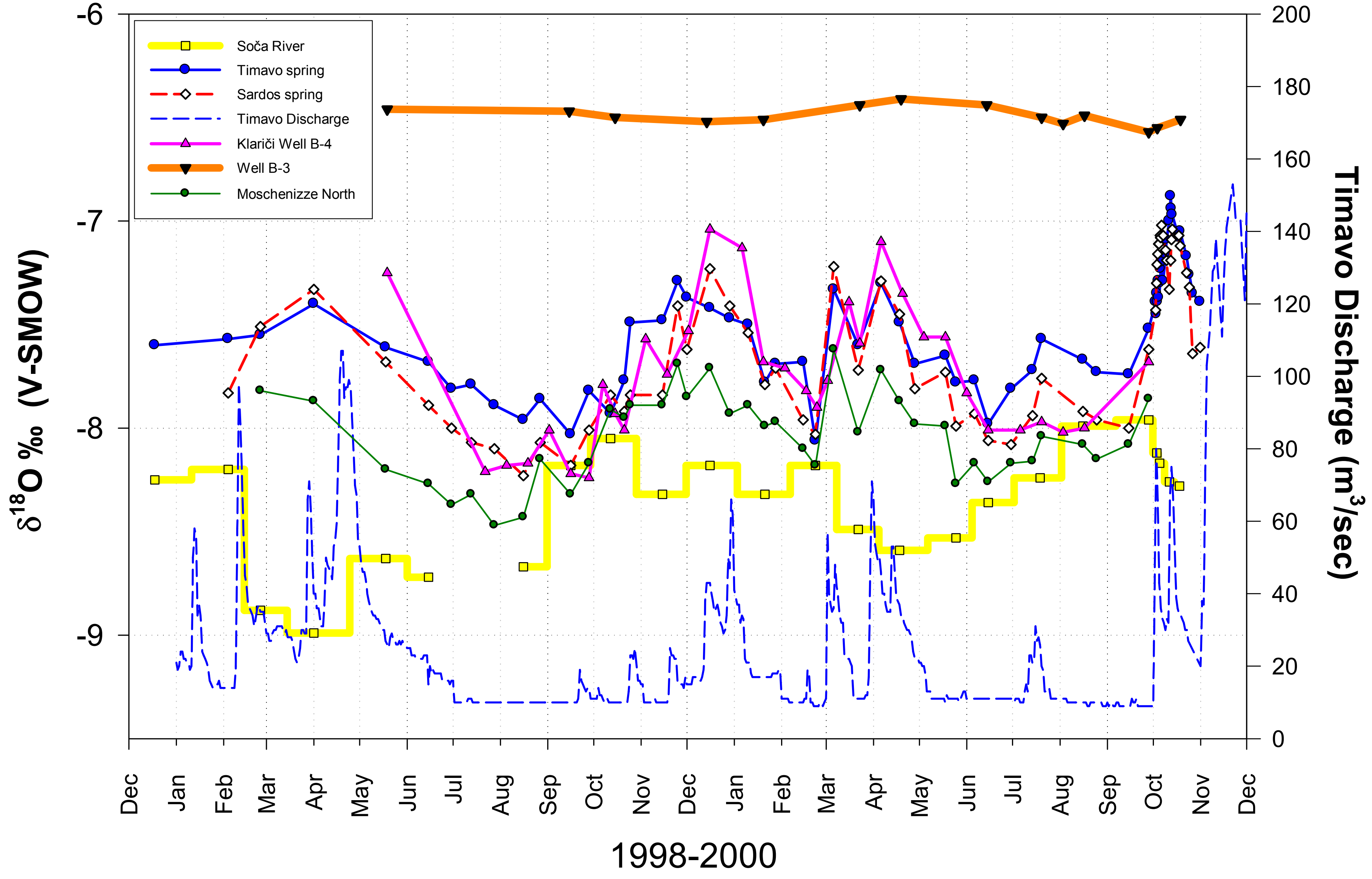
PC-space Mixing Diagram:
Kras Springs, HIGH Flow Regime



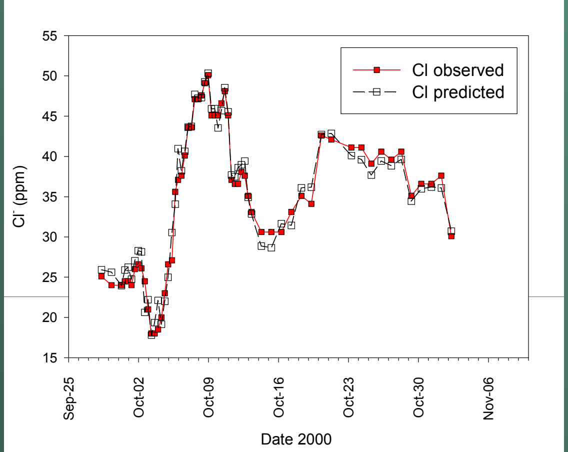
Importance of Event Sampling:

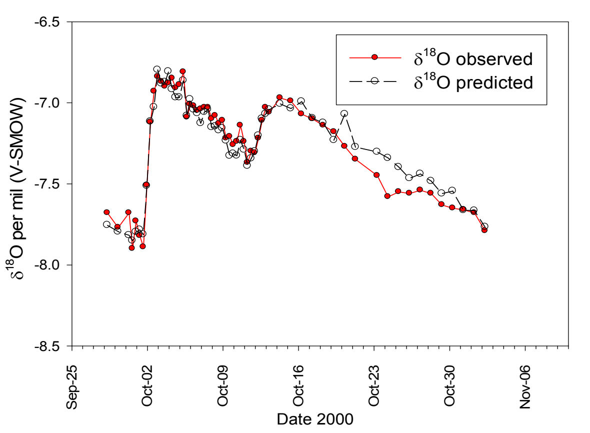
- High-frequency data collected over shorter time intervals can yield greater amount of useful information than monthly or even weekly monitoring

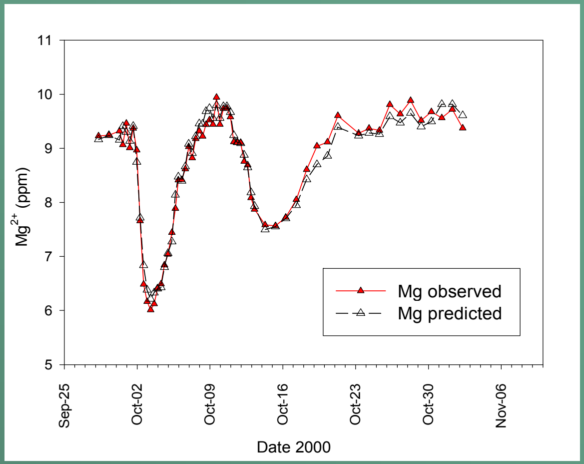
Oxygen isotopic compositions of Kras waters 1998-2000

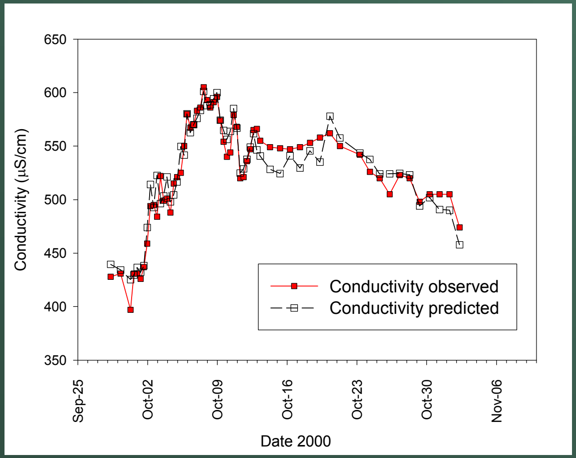


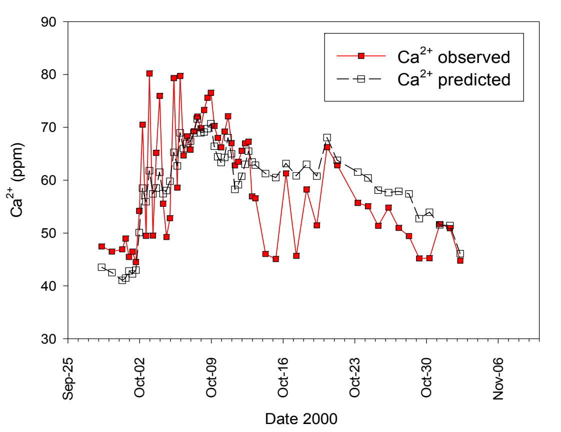
Measured vs. predicted chemistry and isotopic composition at Well B-4 during storm events of 2000

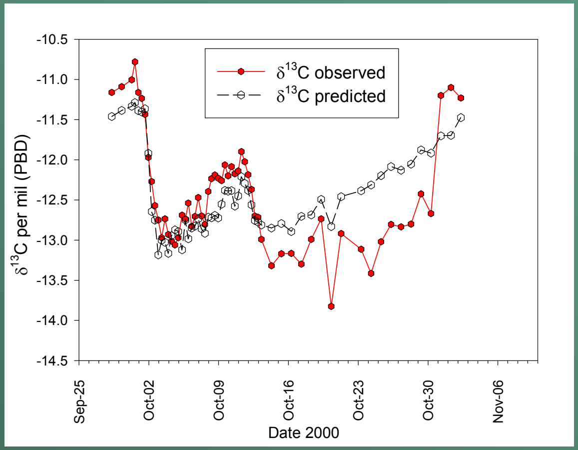












Representative Elementary Watershed (REW)

- Use of mono-valued characteristic functions (as in nearly all profile or hillslope scale hydrological models) is already a departure from our understanding of the physical principles that underlie hydrology.

- The challenge then is to find appropriate functional forms for representing the hysteretic storage-discharge relationship given (generally) very little information about the internal characteristics of the unit, very little observable data in the way of storage or discharge measurements at the unit scale, and no theoretical framework on which to base such a representation.

- Tracer experiments that suggest that in many small catchments, the hydrograph is dominated by the displacement of pre-event water. The difference can be illustrated simply within a simplified kinematic wave description of the flow processes but in reality is much more complex because of the effects of heterogeneities, immobile storage, fingering and preferential flows. The storage discharge response will be governed primarily by the celerities with which pressure effects are transmitted through the system. We still have much to learn about the details of this, particularly in unsaturated soils.

- These questions are the second most important problem in hydrology of the 21st Century. The *most* important is providing the techniques to measure integrated fluxes and storages at useful scales).

Beven, 2006