



New Tools for Water Quality Data Access and Trend Analysis

An overview of the USGS R Packages:

dataRetrieval and EGRET

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USGS

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Outline

Motivations for the package

**The WRTDS concept and examples
of results**

Overview of dataRetrieval

**How EGRET works, doing WRTDS
analysis and producing graphs and
tables**

From Ralph Keeling

The only way to figure out what is happening to our planet is to measure it,
and this means tracking changes decade after decade
and poring over the records.

Keeling, 2008, Recording Earth's vital signs, Science, p1771-1772

The challenge

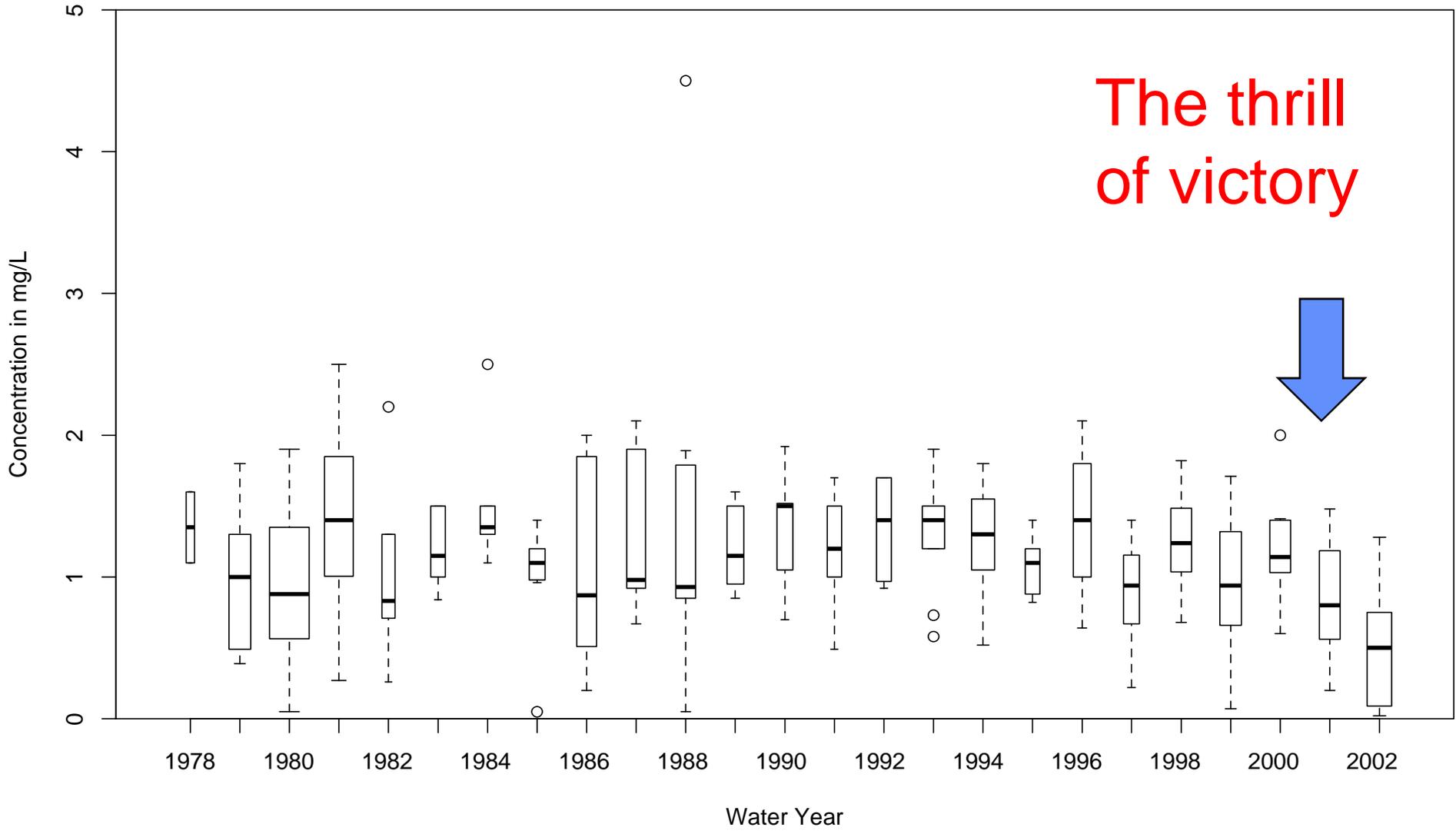
How do we come to understand what is happening to water quality in large watersheds.

Is it getting better or worse?

Can we develop ideas of causative factors and changes in processes?

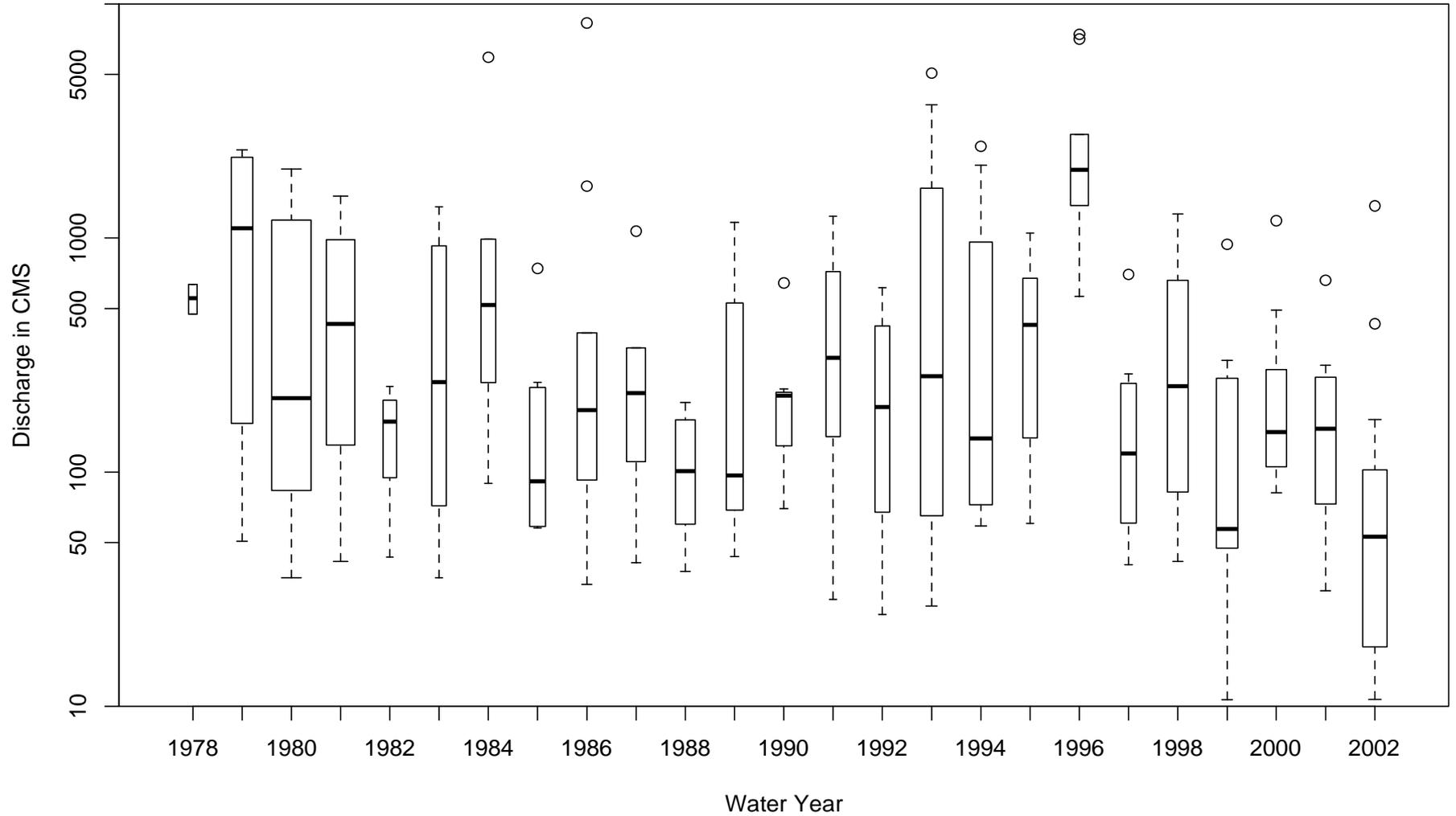
Can these be used to guide management choices?

Potomac River at Chain Bridge, Washington DC
Box plot of sample values by Water Year
Nitrate as N

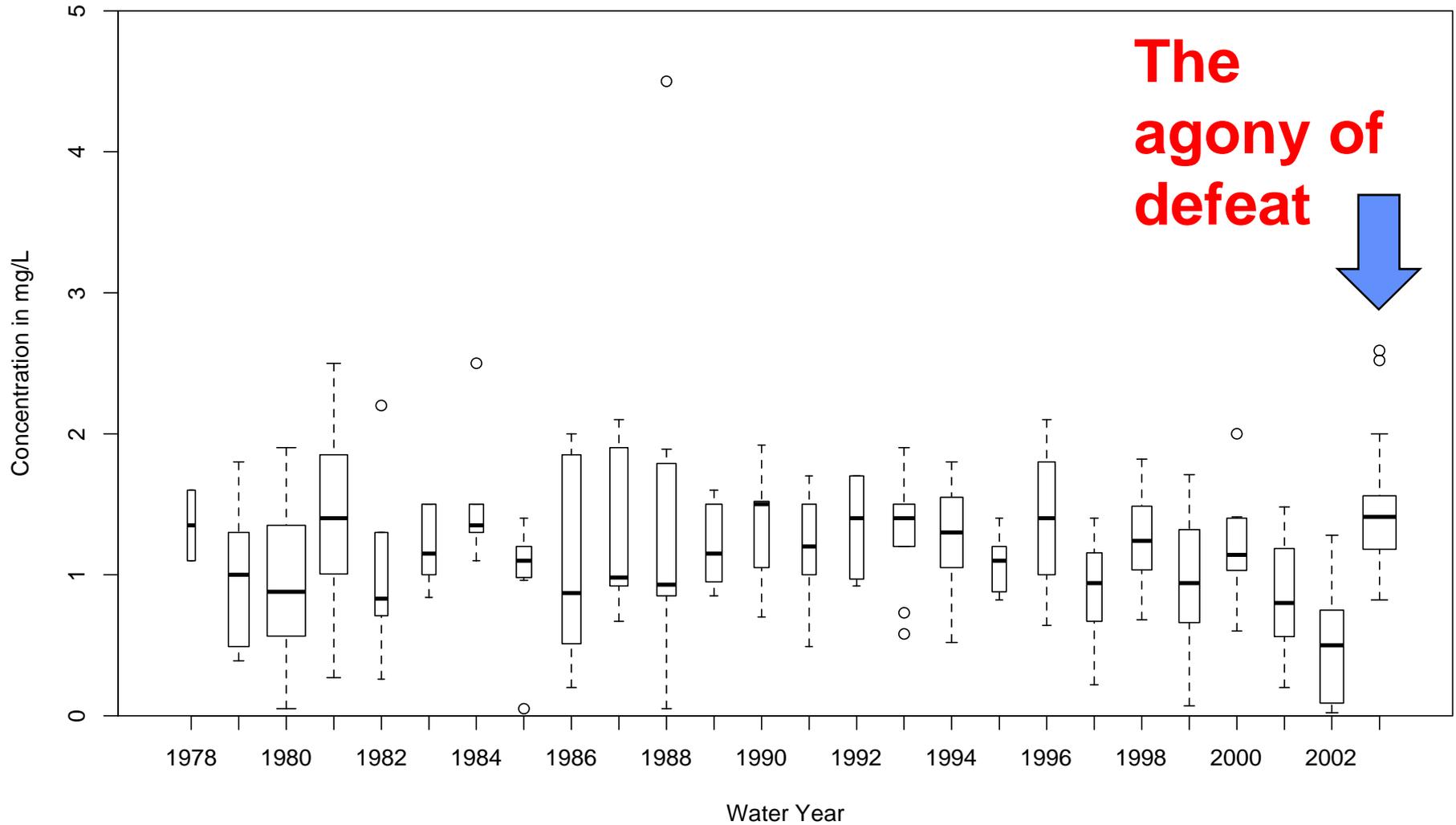


Data through September 2002

Potomac River at Chain Bridge, Washington DC
Boxplot of Discharge on Sampling Date by Water Year

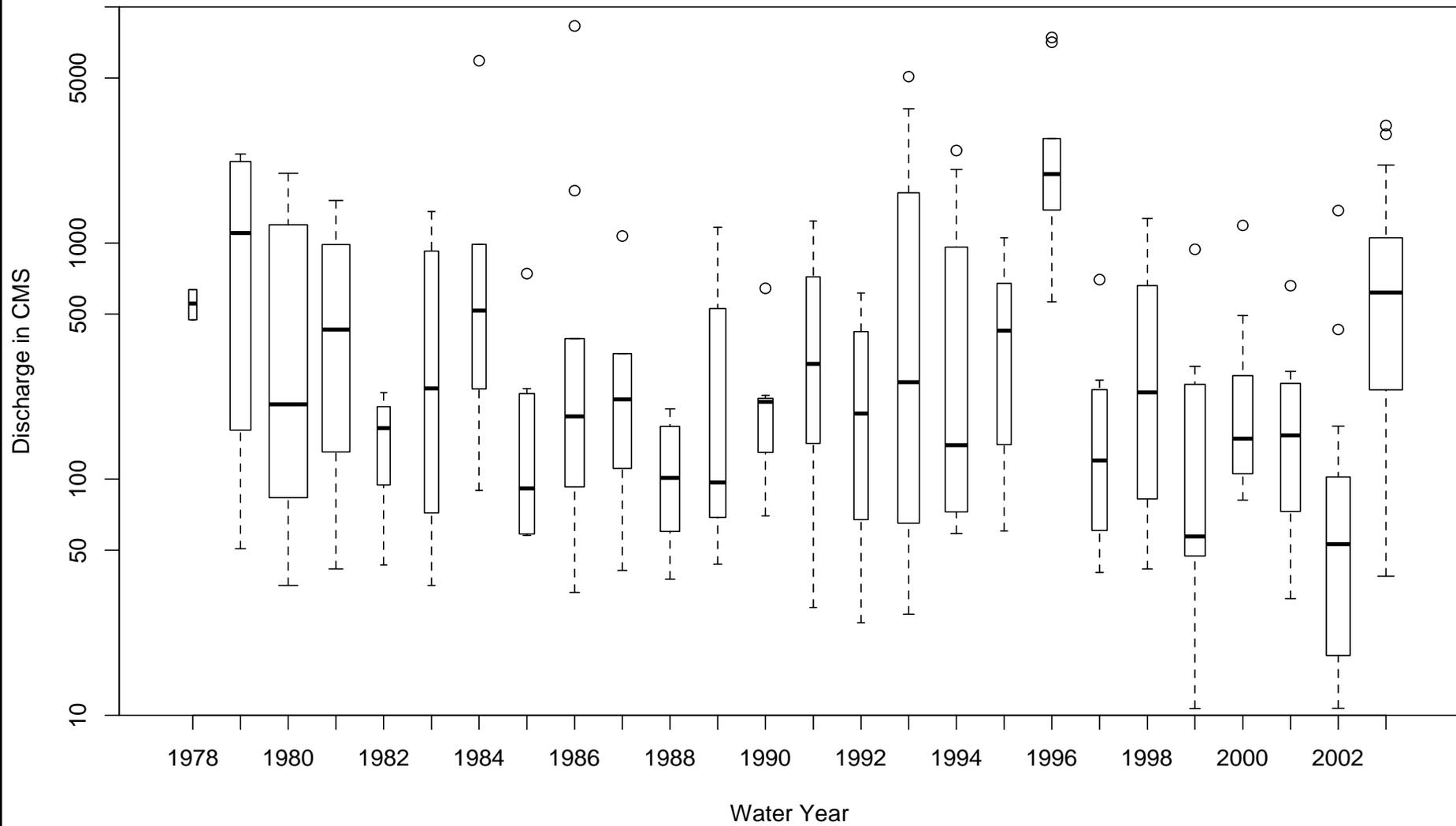


Potomac River at Chain Bridge, Washington DC
Box plot of sample values by Water Year
Nitrate as N



Data through September 2003

Potomac River at Chain Bridge, Washington DC
Boxplot of Discharge on Sampling Date by Water Year



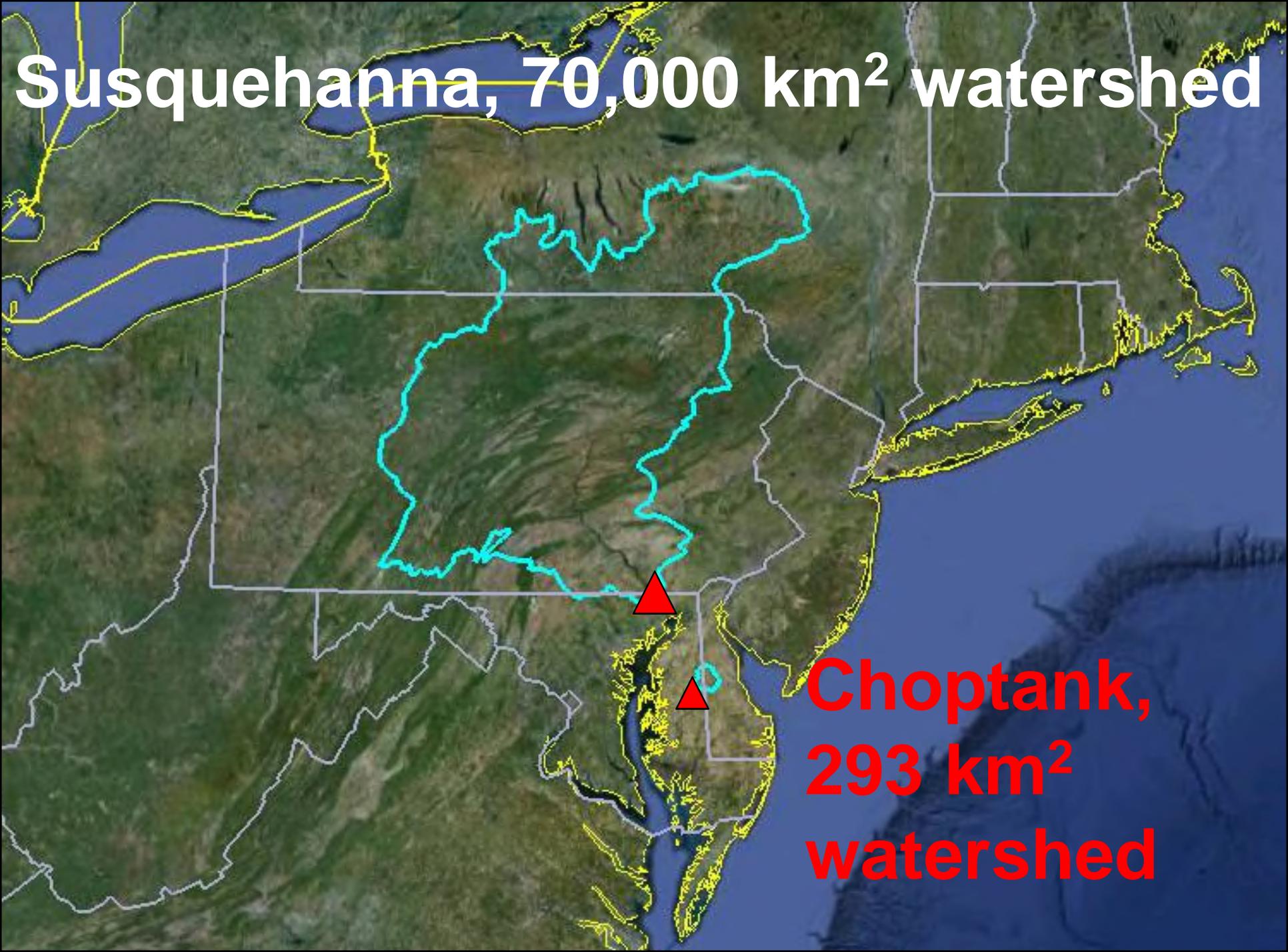
Motivations for the method

- Describe the evolving behavior of the watershed. No mathematical straight-jacket!!
- Estimate both concentration & flux (averages as well as trends).
- Estimate the actual history but also a flow-normalized history.
- Resolve a serious bias in flux estimates.
- Be quantitative but also exploratory.

Data requirements

- Low intra-day variability (not flashy)
- Requires a complete daily discharge record
- Intended for >200 samples, but has been used for some purposes with as few as 60 samples
- Water quality samples cover most of the discharge range
- For trend studies: 20+ years
- For average flux computations: 5 – 10 years.

Susquehanna, 70,000 km² watershed

A satellite-style map of the eastern United States showing the Susquehanna River watershed in blue and the Choptank River watershed in cyan. The Susquehanna watershed is significantly larger and extends further north and west. The Choptank watershed is a smaller tributary system located in the southern part of the Susquehanna watershed. Two red triangles mark specific locations within the Choptank watershed. State boundaries are shown as thin white lines.

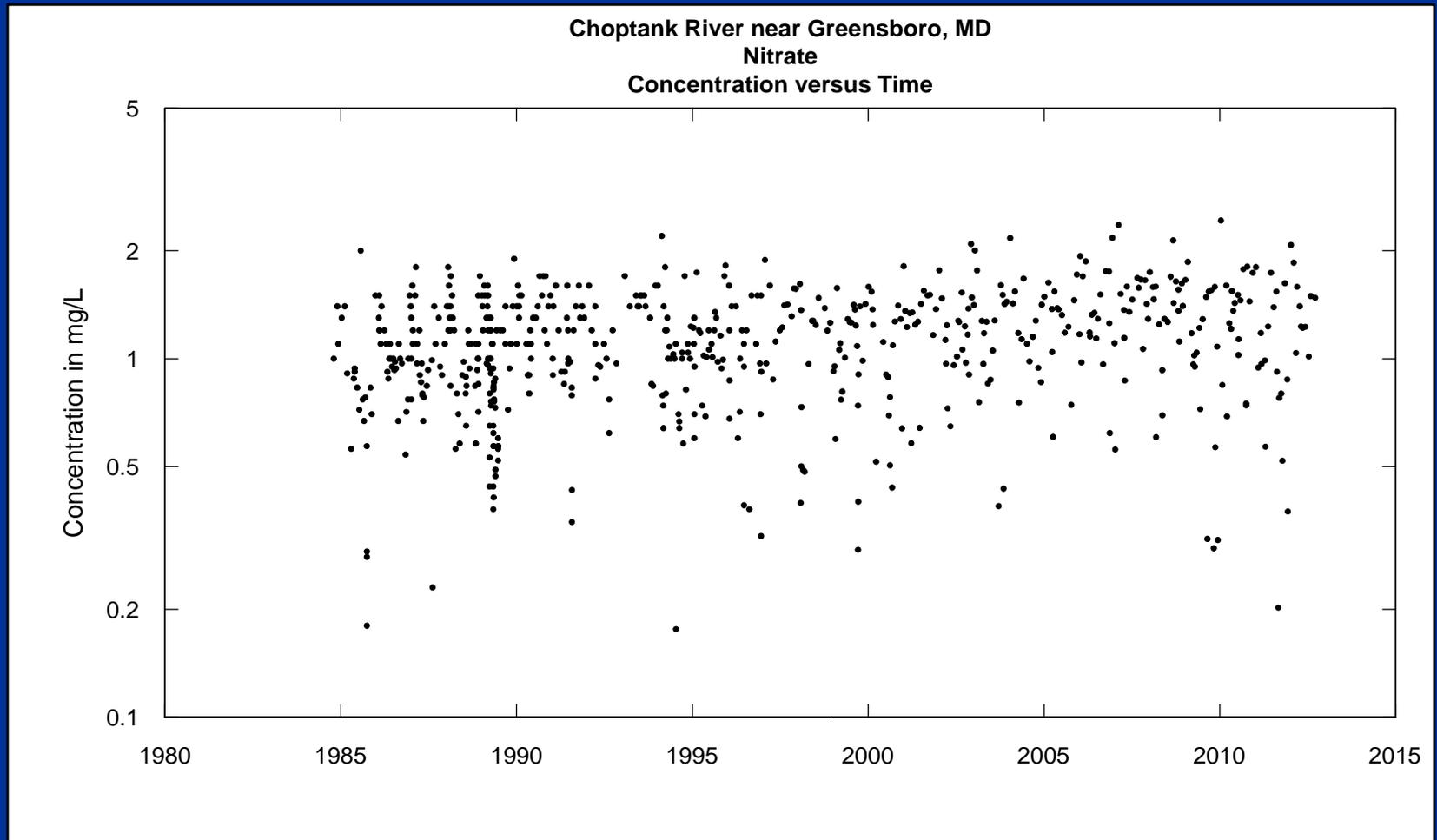
**Choptank,
293 km²
watershed**



**Choptank,
293 km²
watershed**

“Data without models are chaos, but models without data are fantasy”

Nesbit, Dlugokencky and Bousquet, *Science*, 31 January 2014, pp. 493-495



Use the data and a simple, highly-flexible smoothing model to decompose the data into 4 components.

1) Discharge related component

2) Seasonal component

3) Time trend

4) Random component

**Weighted Regressions on Time,
Discharge and Season (WRTDS)**

Locally Weighted Regression

For any location in time - discharge space (t and Q) we assume that concentration (c) follows this model

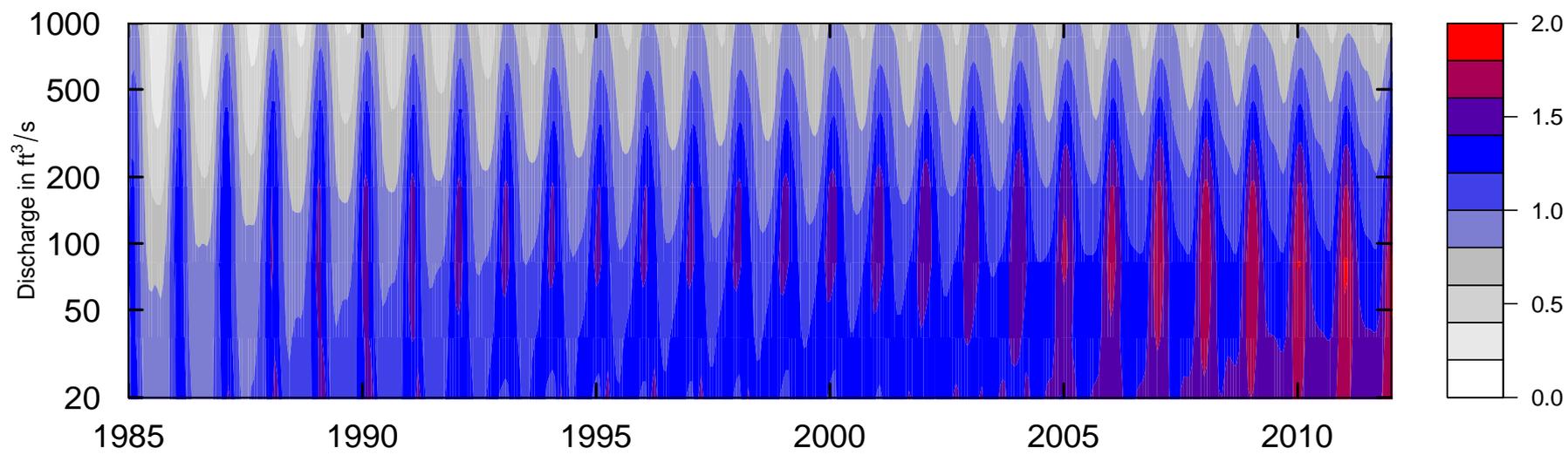
$$\ln(c) = \beta_0 + \beta_1 \cdot t + \beta_2 \cdot \ln(Q) + \beta_3 \cdot \sin(2\pi t) + \beta_4 \cos(2\pi t) + \varepsilon$$

But the coefficients should be smoothly changing as we move through the space

Use weighted regression at many points in that space. The weight on each sample is determined by its “relevance” to that particular point in the space.

WRTDS view of the evolving behavior of nitrate

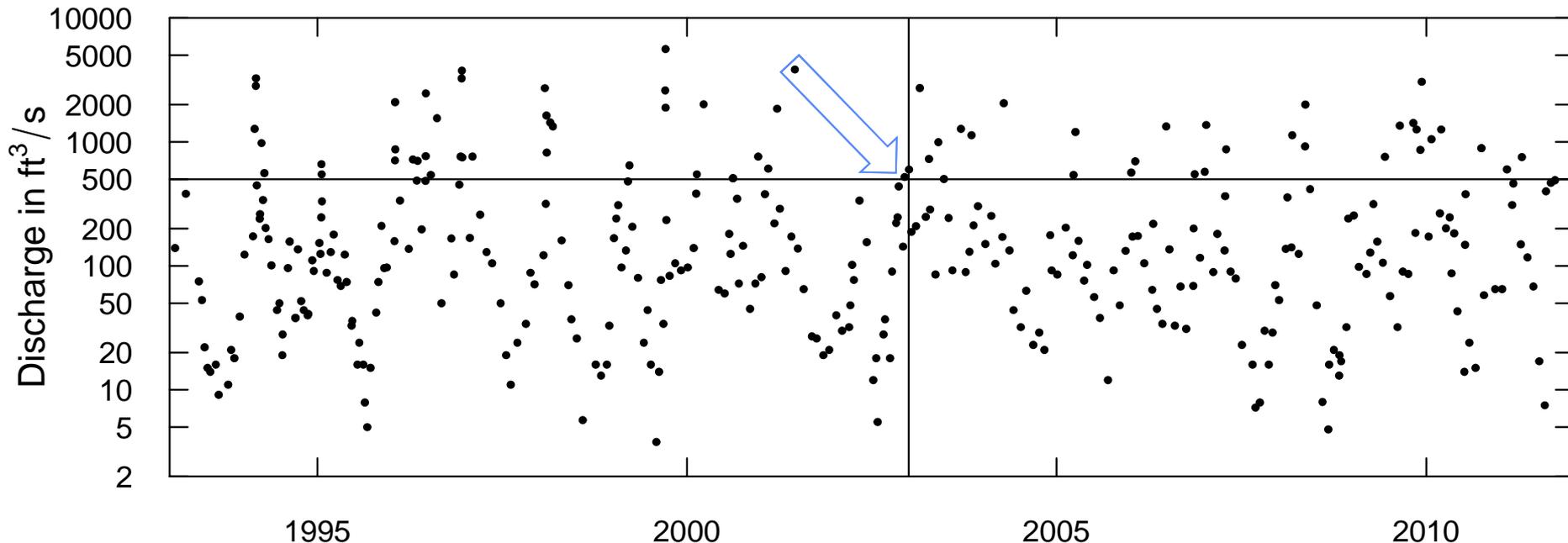
Choptank River near Greensboro, MD Nitrate plus Nitrite, Filtered, as N
Estimated Concentration Surface in Color



How is this surface created?

Every dot is a data point from 1993 to 2012
Let's say we want to use the data to estimate the expected value of concentration for January 1, 2003 at Q=500 cfs

Choptank River near Greensboro, MD Nitrate plus Nitrite, filtered, as N
Locations of all available data

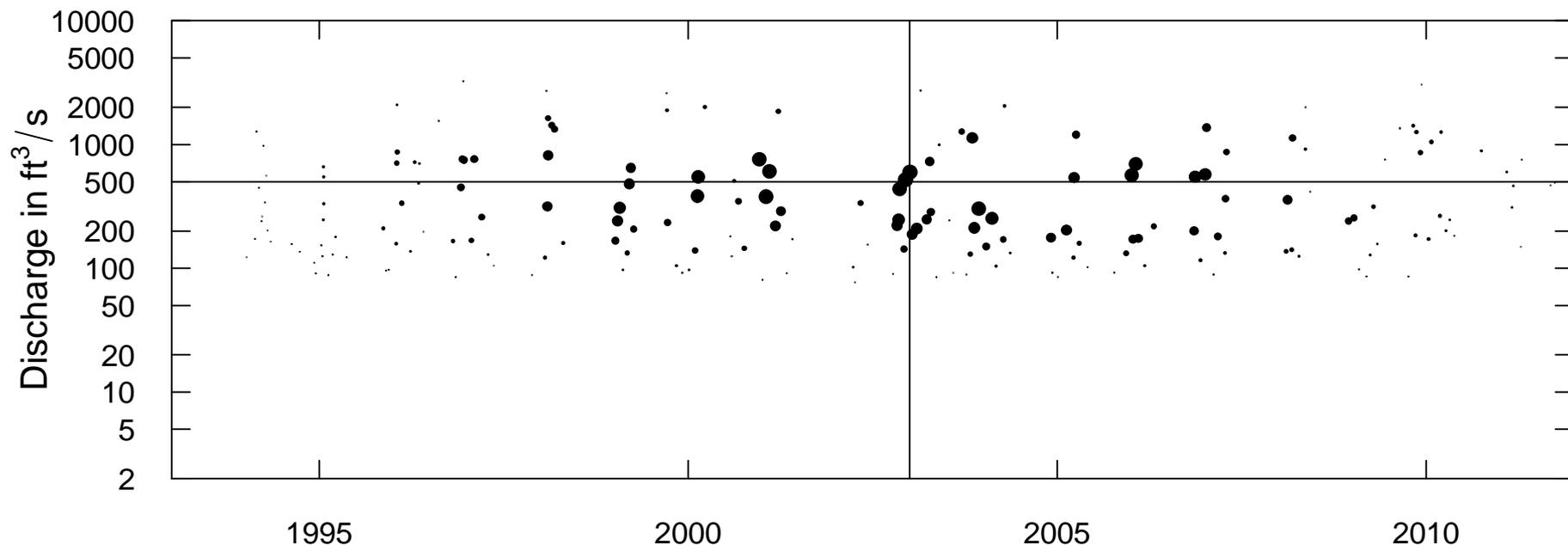


How do we set the weights for the regression?

These are the same points we just saw, but the radius of the dot is proportional to weight assigned to that point for purposes of estimating concentration for January 1, 2003 at Q=500 cfs

The weight depends on distance in: time, log discharge, and season from January 1, 2003 at Q = 500 cfs

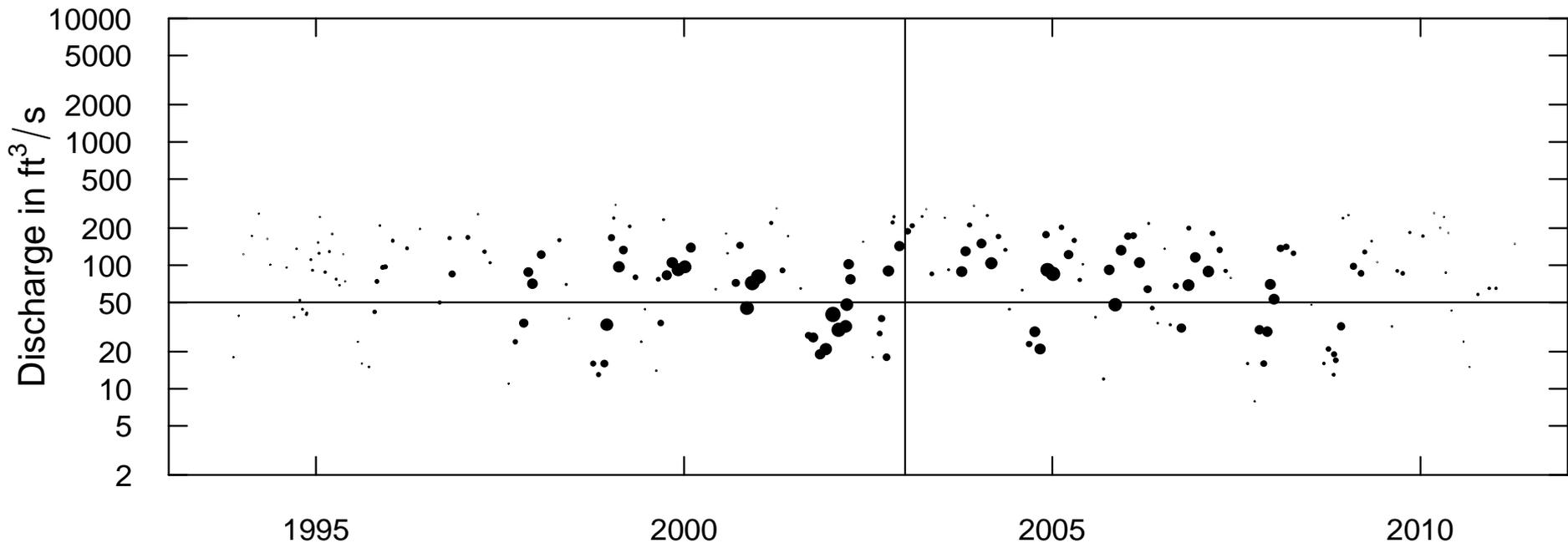
Choptank River near Greensboro, MD Nitrate plus Nitrite, filtered, as N
Locations of all available data



What if we wanted to make an estimate for January 1, 2003 but for $Q = 50$ cfs

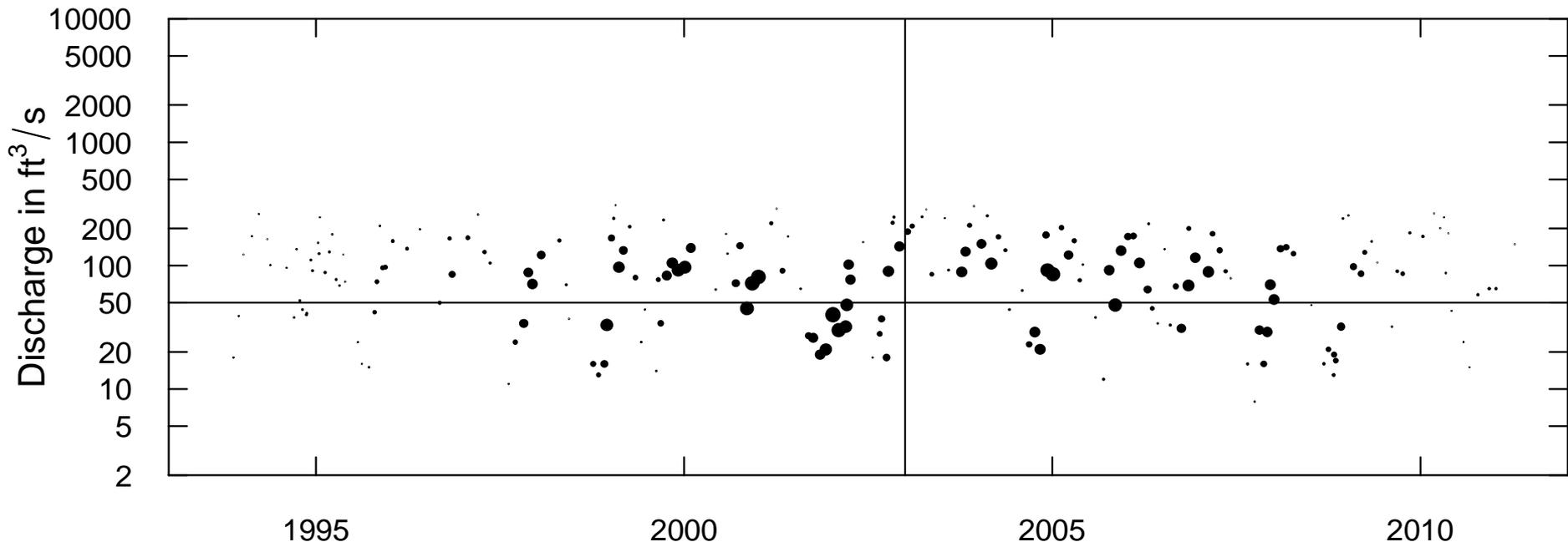
Redo the weights for distance from that point

Choptank River near Greensboro, MD Nitrate plus Nitrite, filtered, as N
Locations of all available data



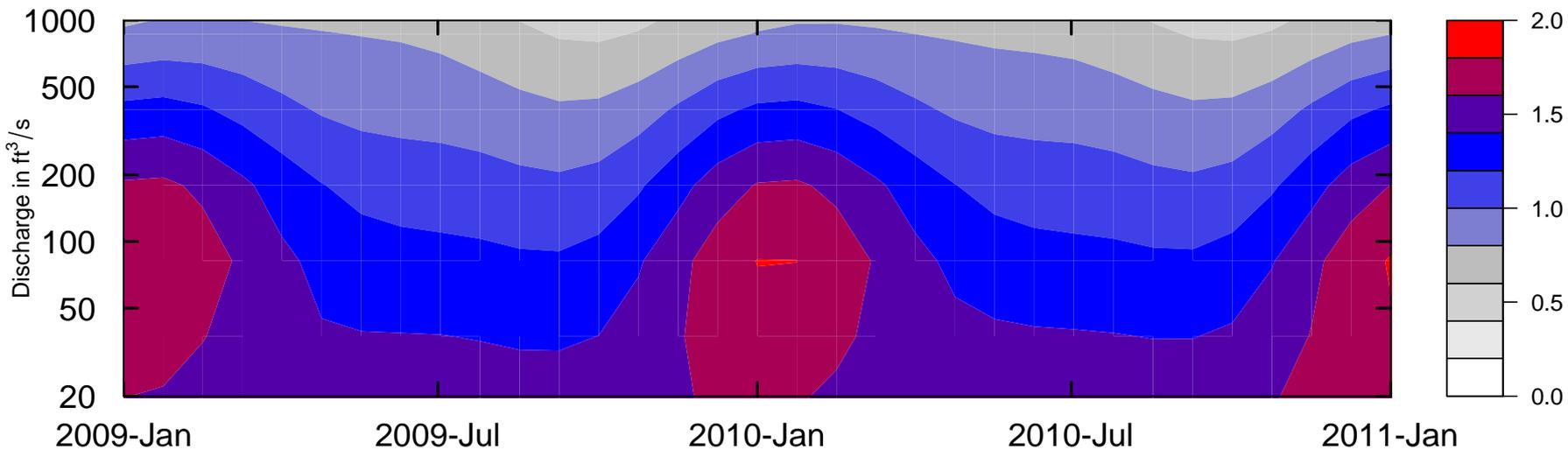
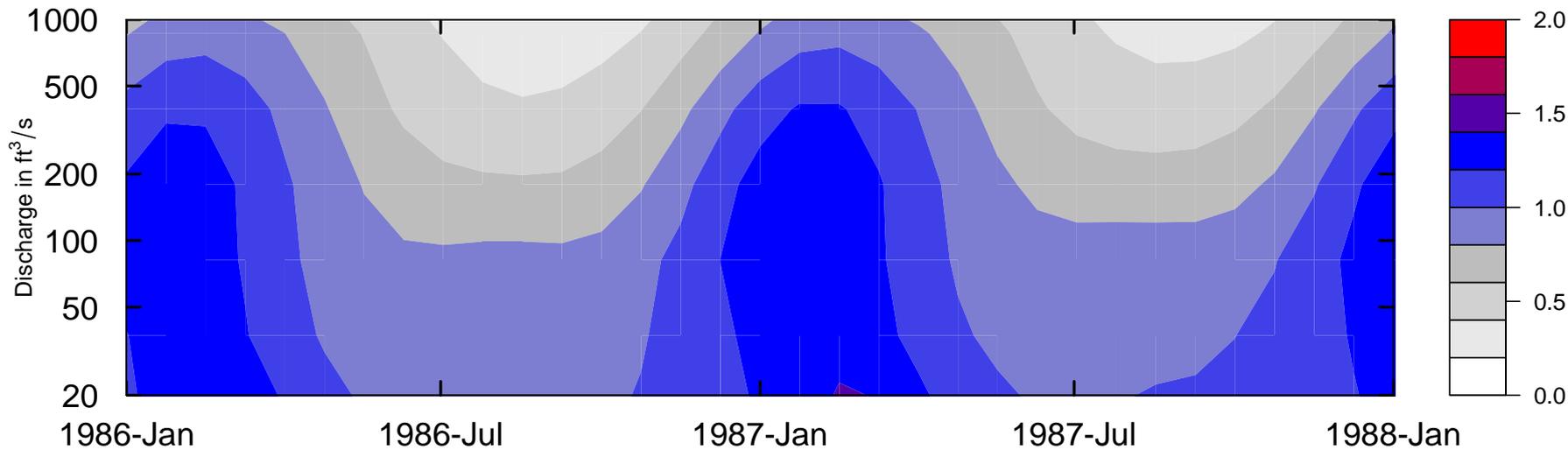
To organize the work, lets make estimates for a fine mesh of points in this space. We will do it at 14 Q values and 177 time values, for a grid of 2,478 points.

Choptank River near Greensboro, MD Nitrate plus Nitrite, filtered, as N
Locations of all available data



Here are two, more detailed looks at this surface

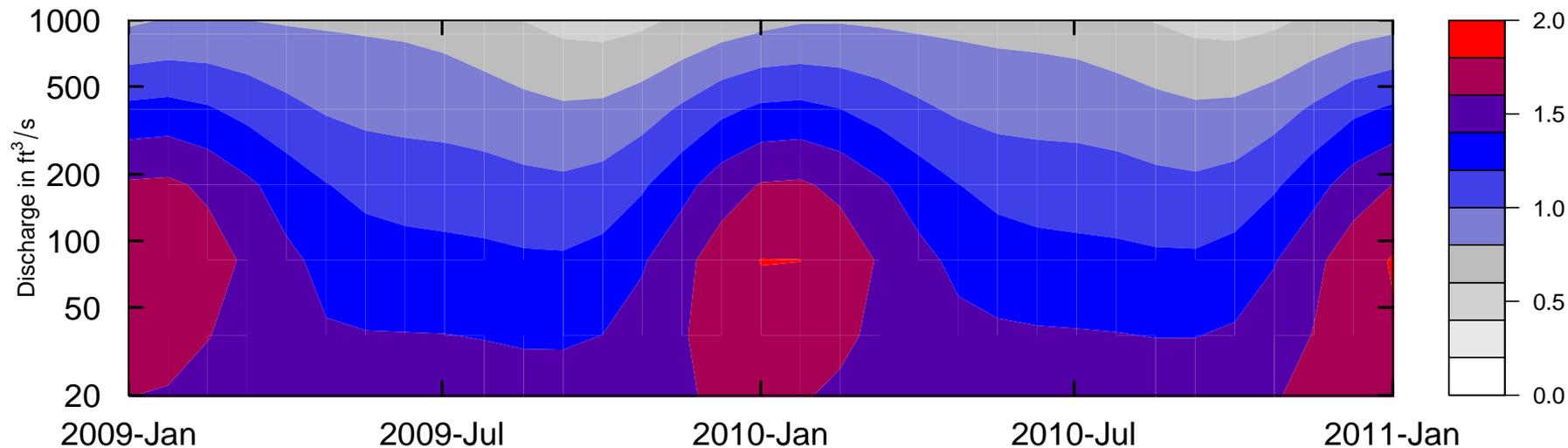
Choptank River near Greensboro, MD Nitrate plus Nitrite, Filtered, as N
Estimated Concentration Surface in Color



Now, for every one of 10,227 days in the record from 1985 through 2012:

We can use the date and the observed discharge to compute the expected value of concentration.

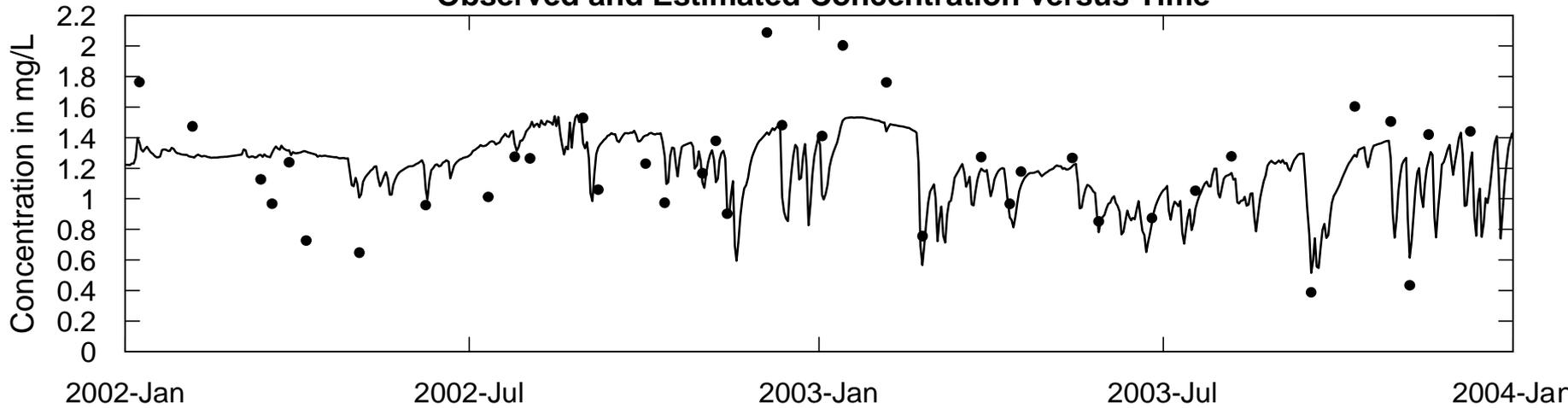
From that value we can compute the expected value of flux.



Then we can sum these estimates by year to compute estimates of annual mean concentration & annual mean flux

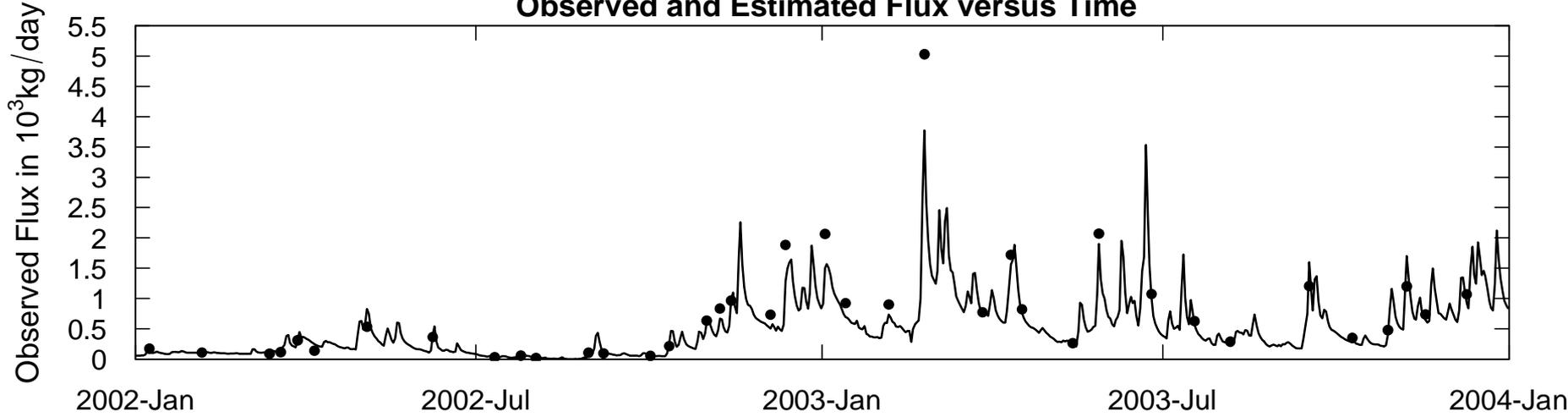
Choptank River near Greensboro, MD
Nitrate

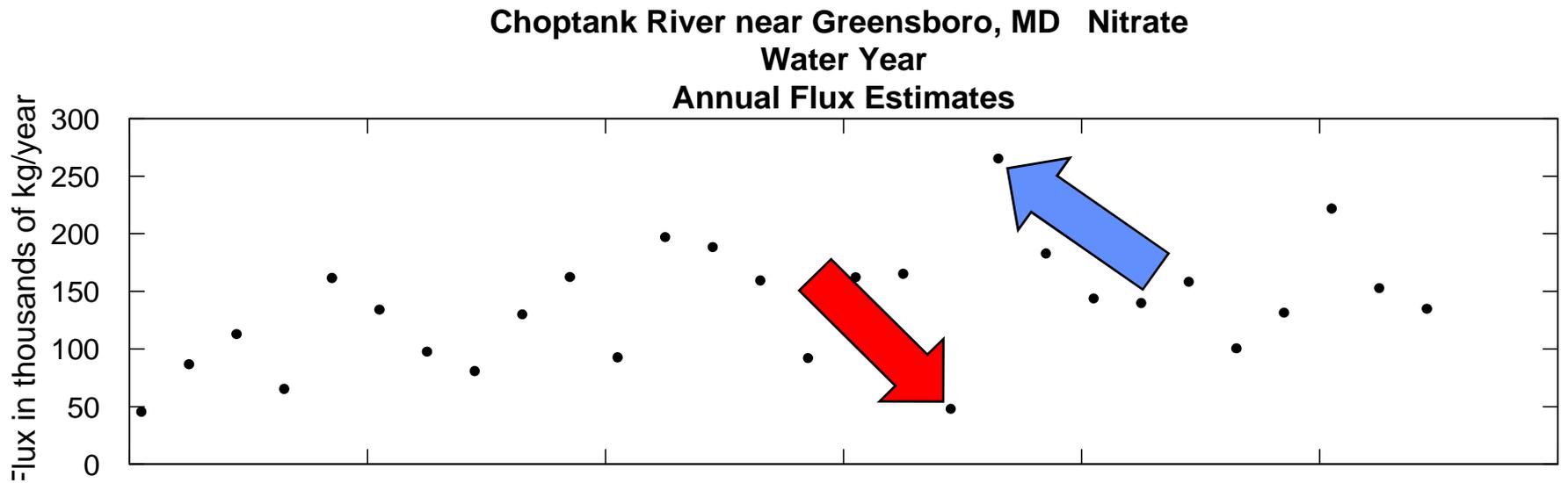
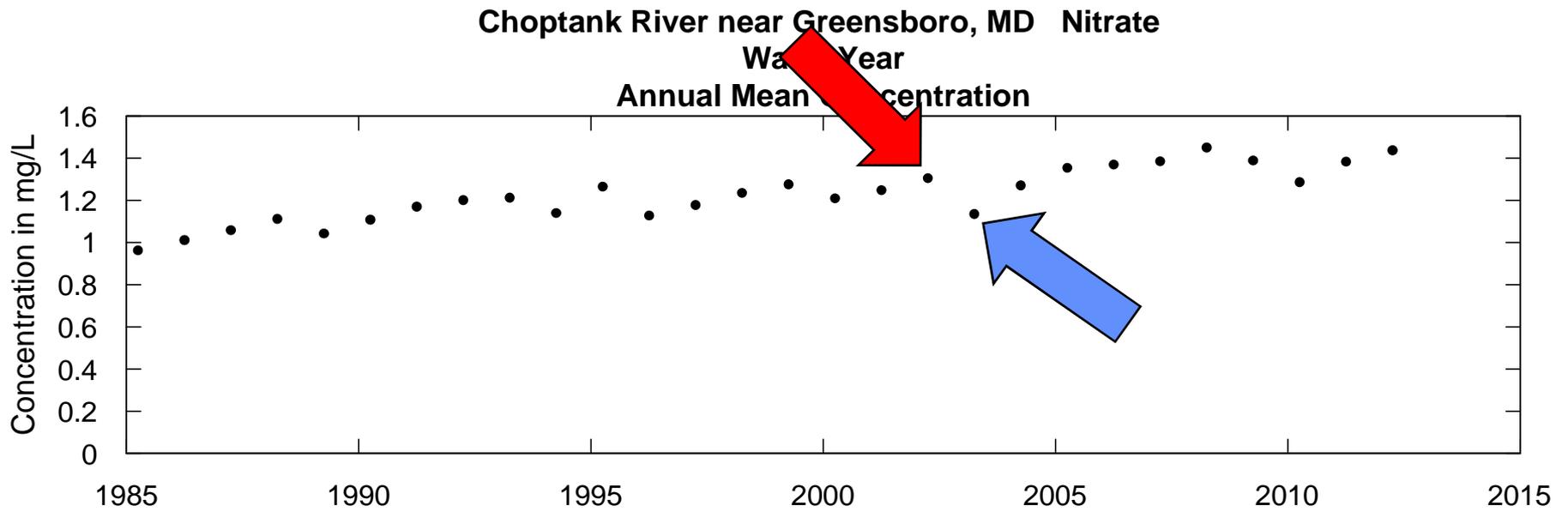
Observed and Estimated Concentration versus Time



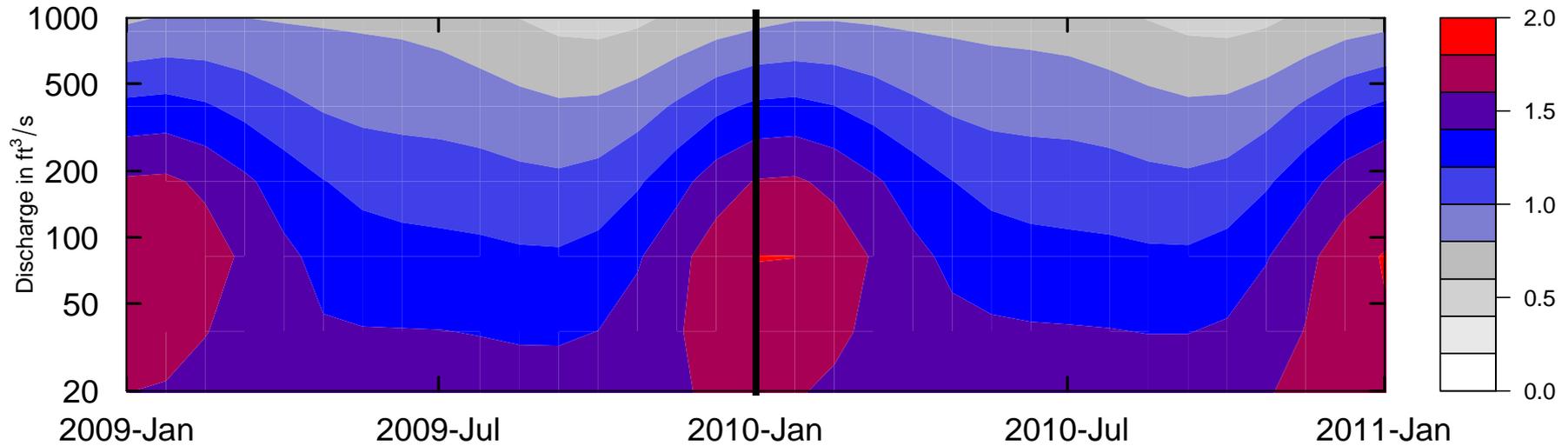
Choptank River near Greensboro, MD
Nitrate

Observed and Estimated Flux versus Time





Can we filter out this flow-driven variation to see the underlying change?



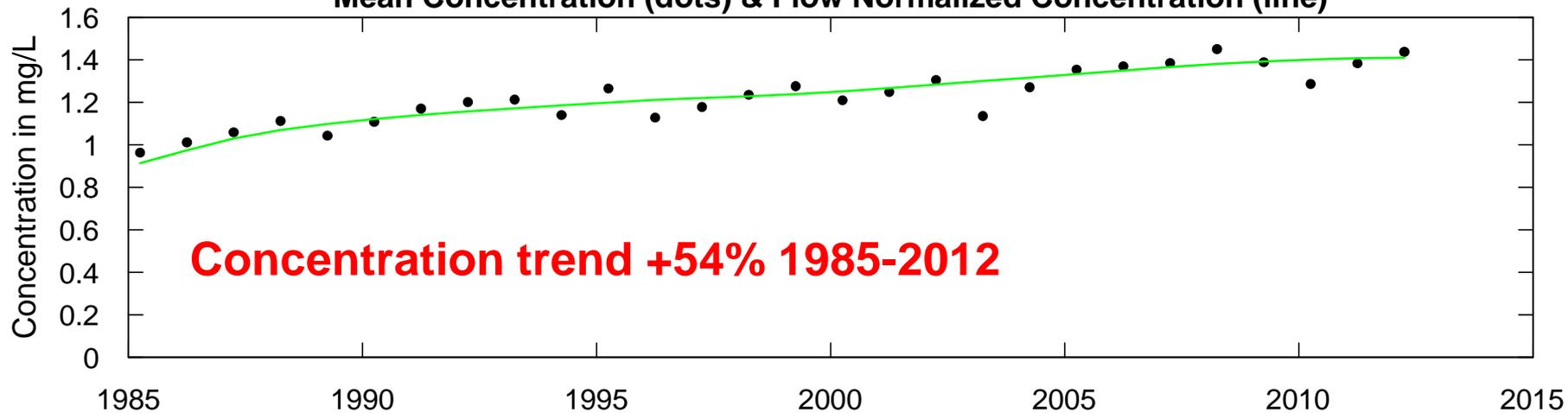
**The “flow normalized concentration” on any given day is:
 $c=f(Q,T)$ integrated over the probability distribution of Q
 for that day of the year.**

**Flow normalized flux is just $c \times Q$ integrated over
 discharge.**

**Sum those over the year to get annual flow-normalized
 mean concentration and flux.**

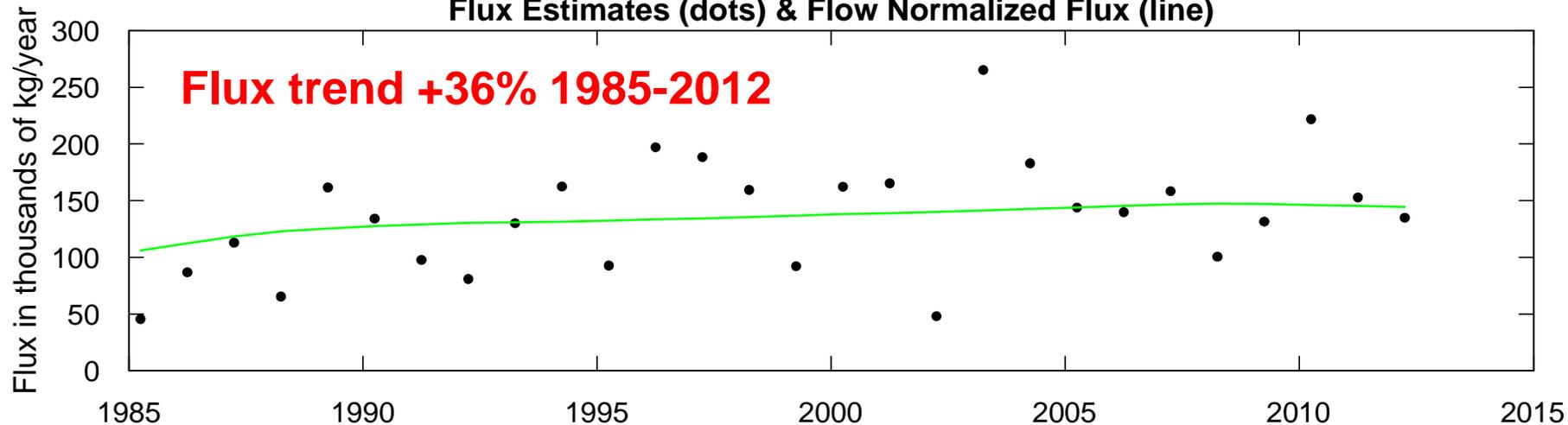
Choptank River near Greensboro, MD Nitrate
Water Year

Mean Concentration (dots) & Flow Normalized Concentration (line)

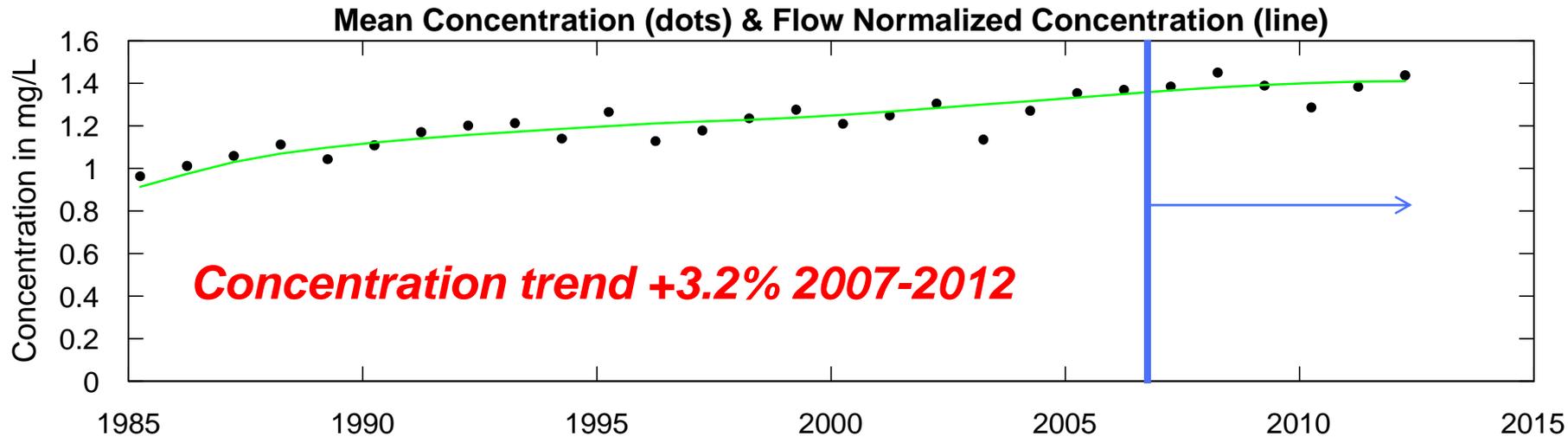


Choptank River near Greensboro, MD Nitrate
Water Year

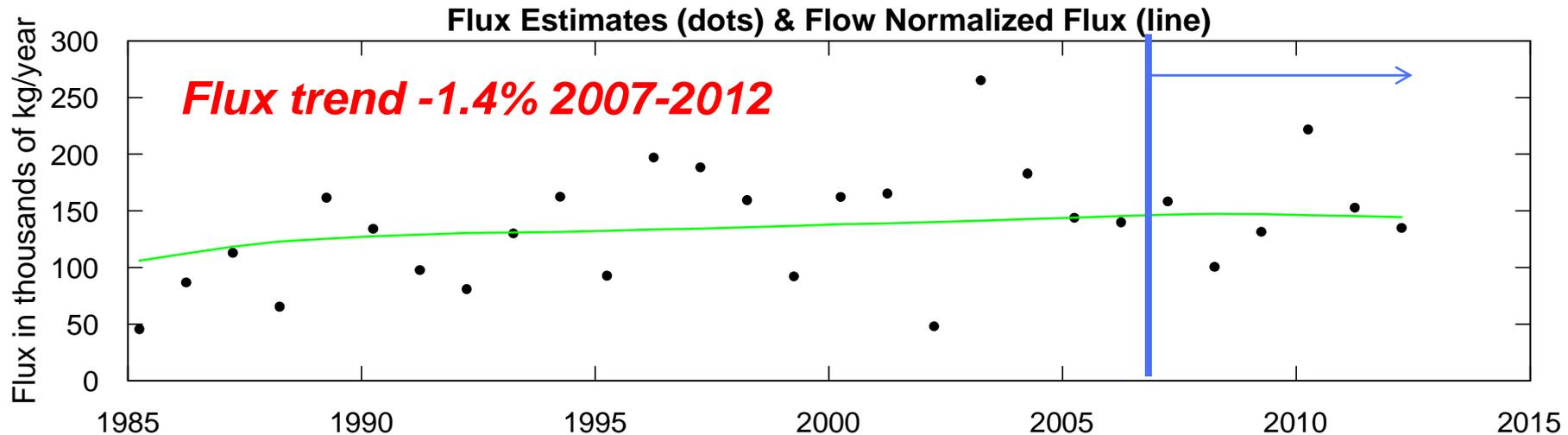
Flux Estimates (dots) & Flow Normalized Flux (line)



Choptank River near Greensboro, MD Nitrate
Water Year



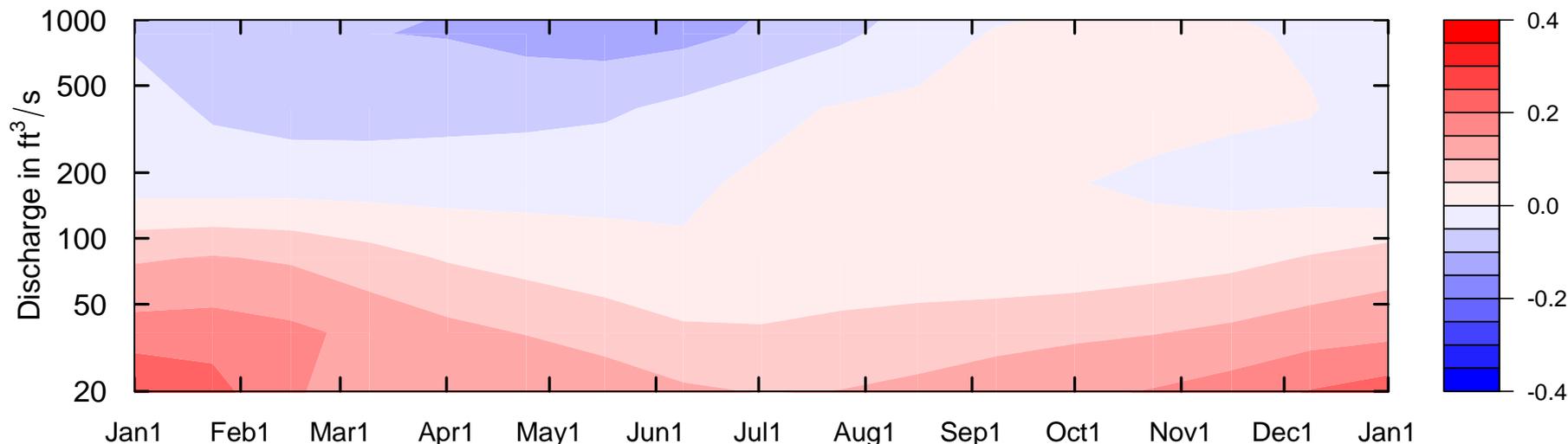
Choptank River near Greensboro, MD Nitrate
Water Year



Look at changes in just the last few years.

This is a graphic of differences 2007 to 2012

Choptank River near Greensboro, MD Nitrate plus Nitrite, Filtered, as N
Estimated Concentration change from 2007 to 2012



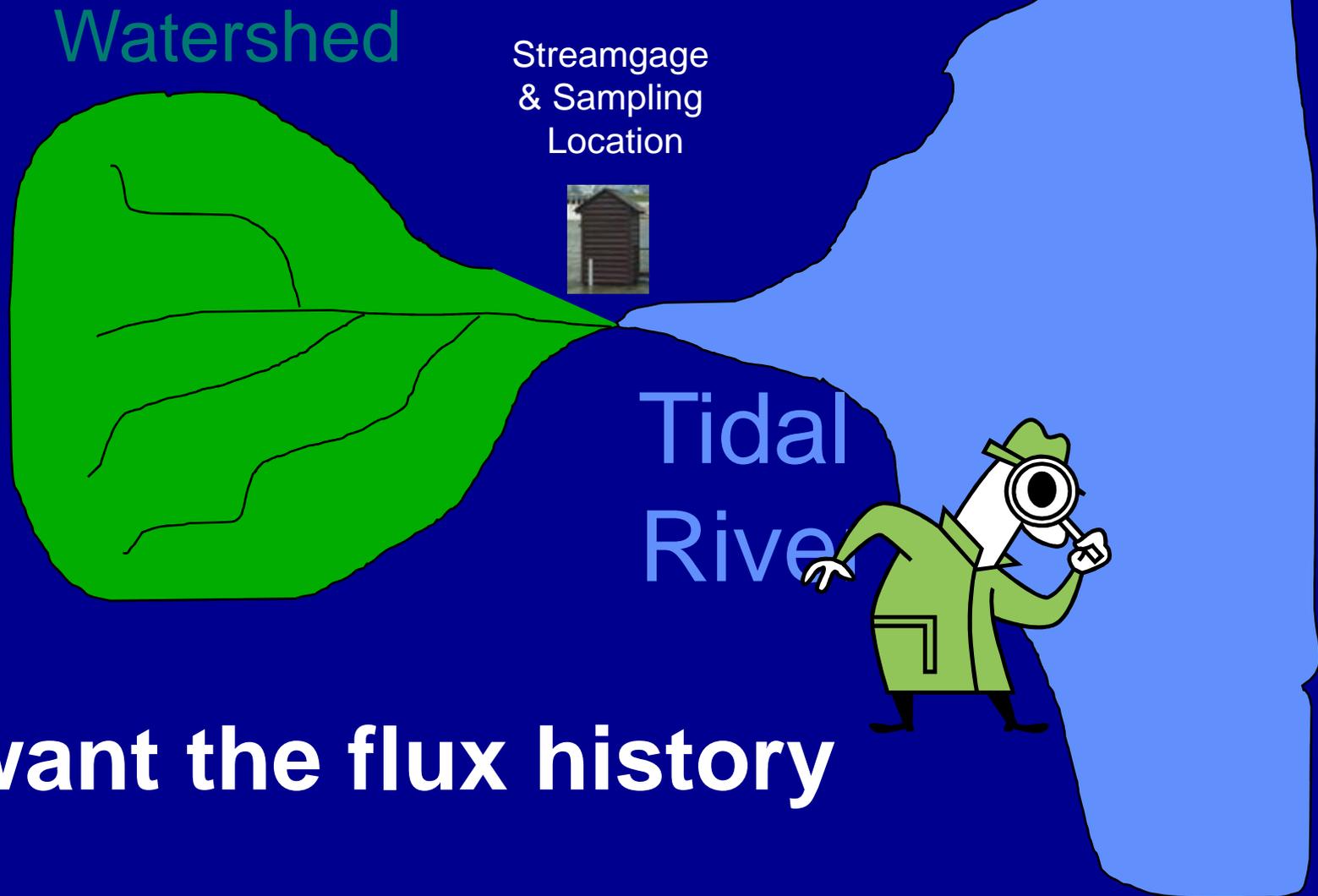
Hypothesis, cover crops are helping at higher flows particularly in the winter. Low flows are still responding to legacy of nitrate enriched groundwater.

Why all this complexity?

Different products for different purposes

- Concentration versus flux
- Actual history versus flow-normalized history

For understanding impact on the estuary ecosystem



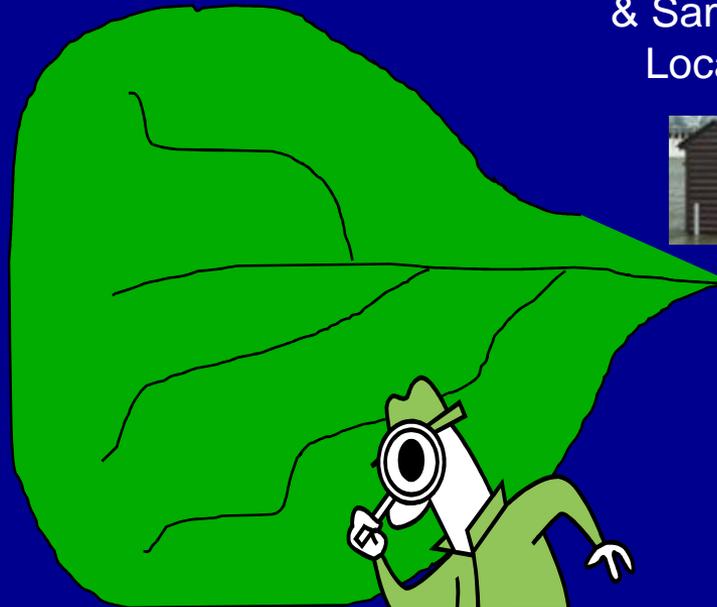
We want the flux history

For understanding progress in the watershed

Estuary

Watershed

Streamgage
& Sampling
Location



Tida
River

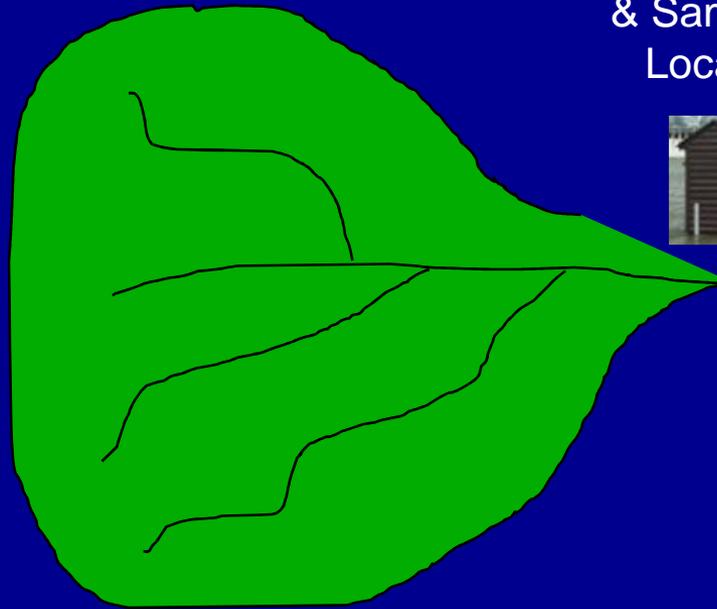
We want the flow-normalized flux history

For understanding the changes in the rivers

Estuary

Watershed

Streamgage
& Sampling
Location

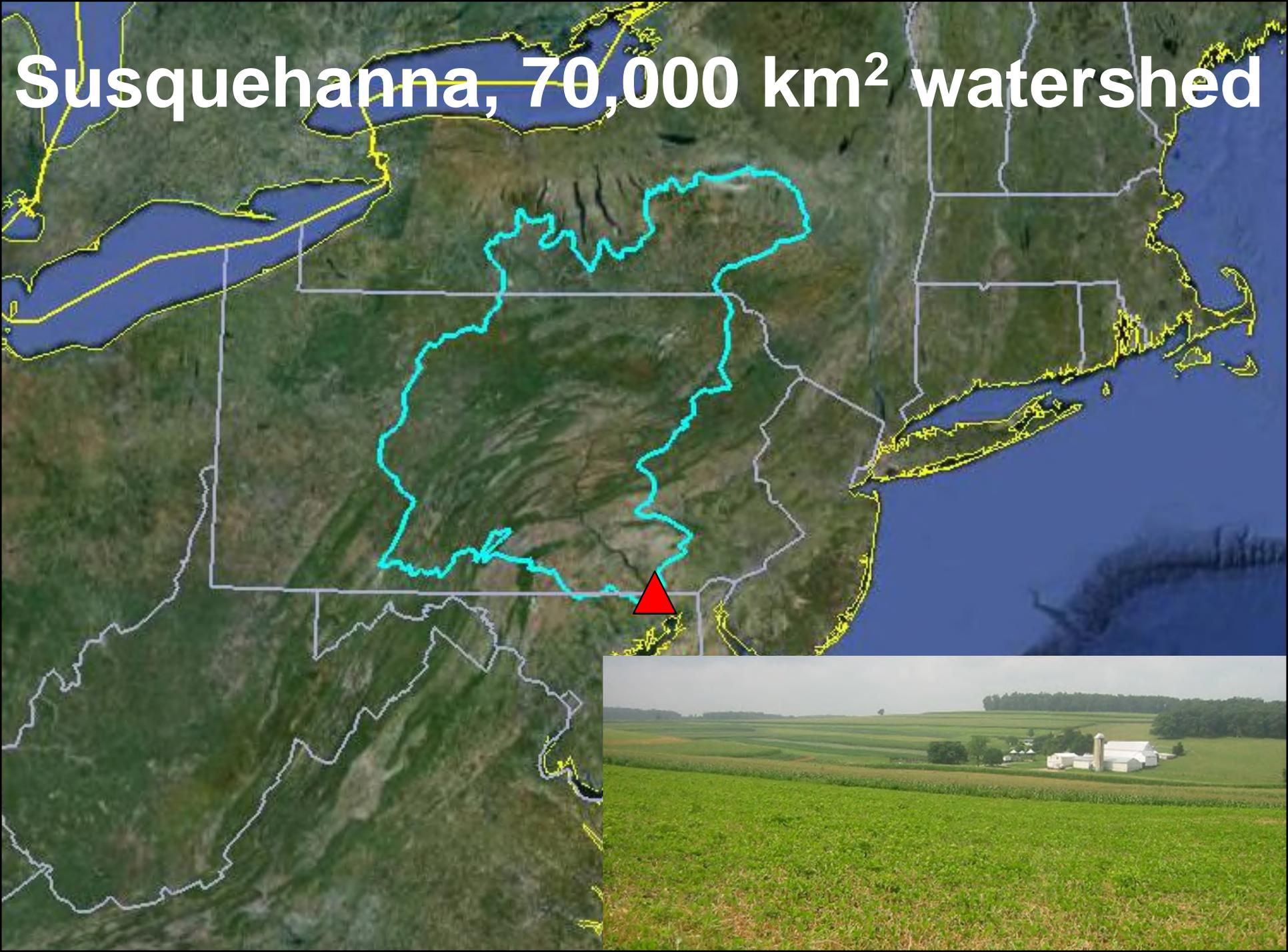


Tidal
River



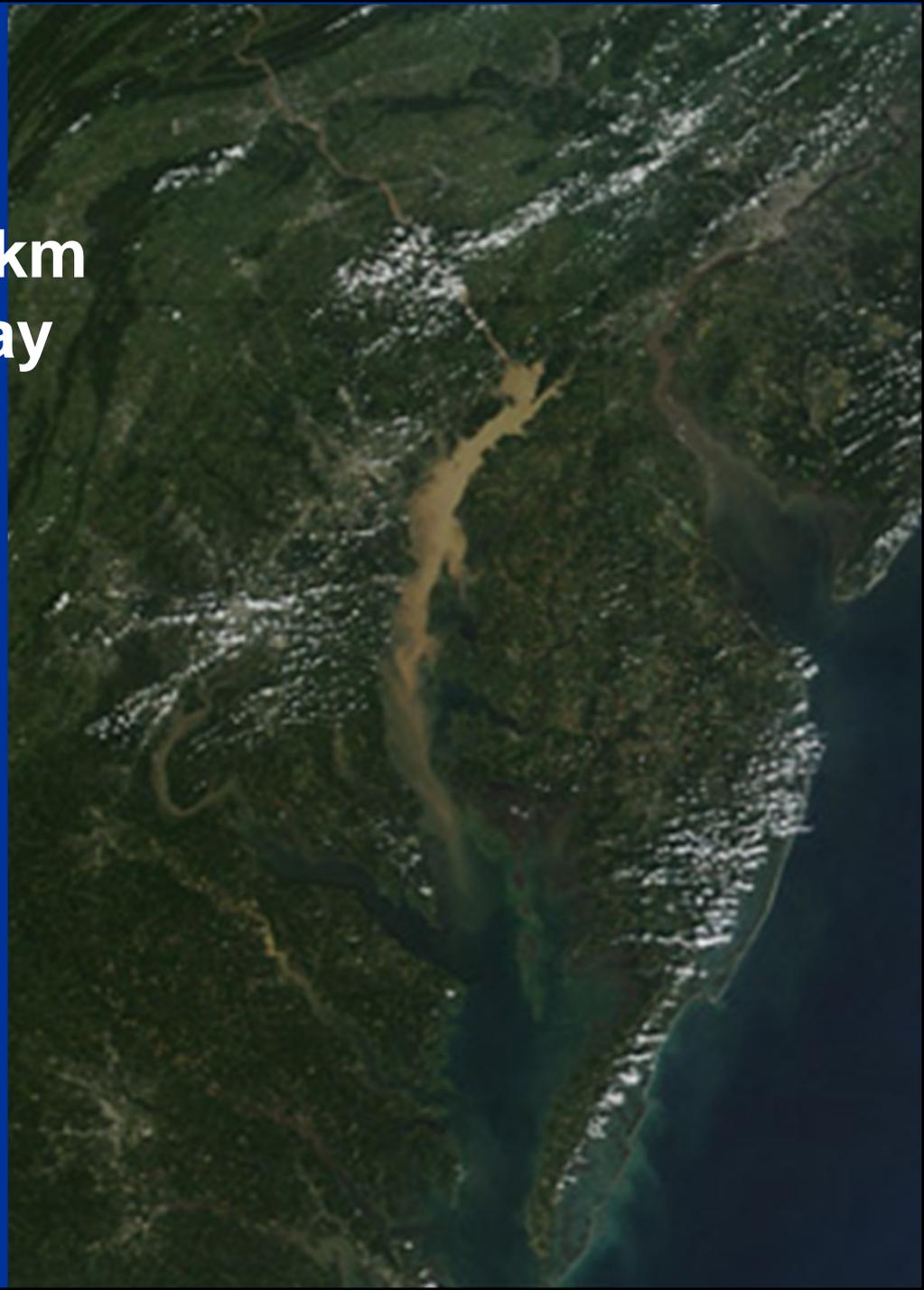
We want the concentration history

Susquehanna, 70,000 km² watershed

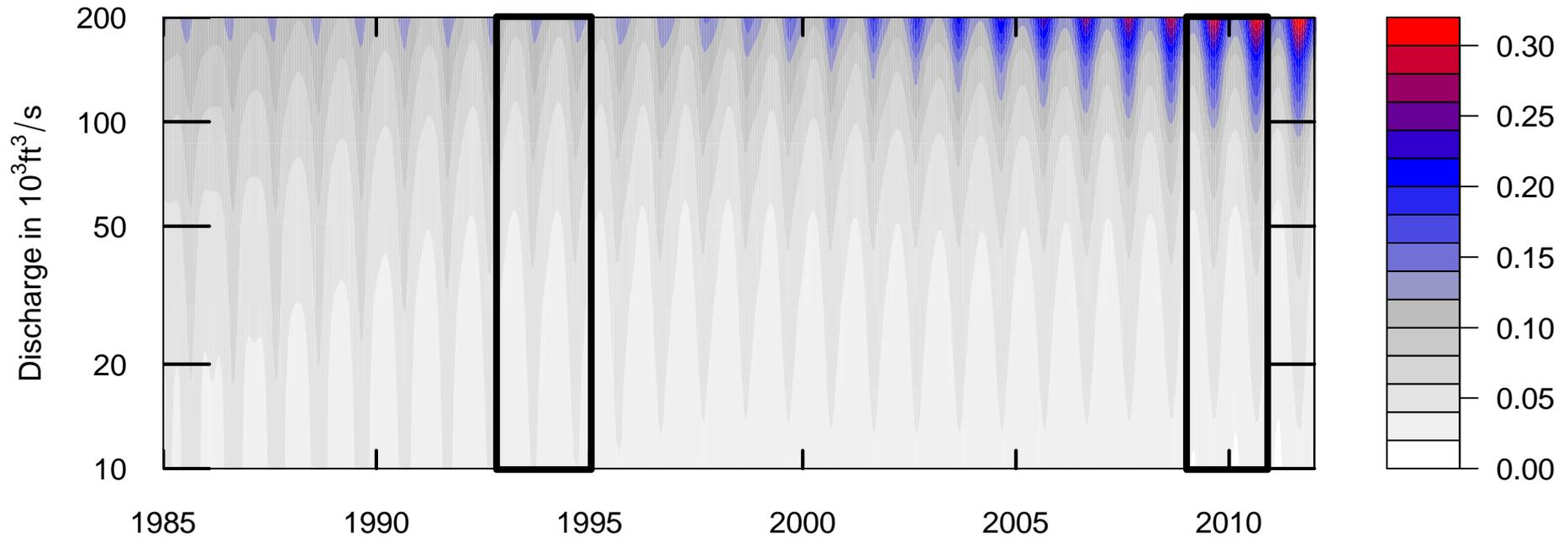


**Sediment plume from
Susquehanna watershed
Plume extends over 150 km
down the Chesapeake Bay
Carrying:
Sediment,
Phosphorus,
Nitrogen**

**From the watershed and
from storage in
Conowingo Reservoir**



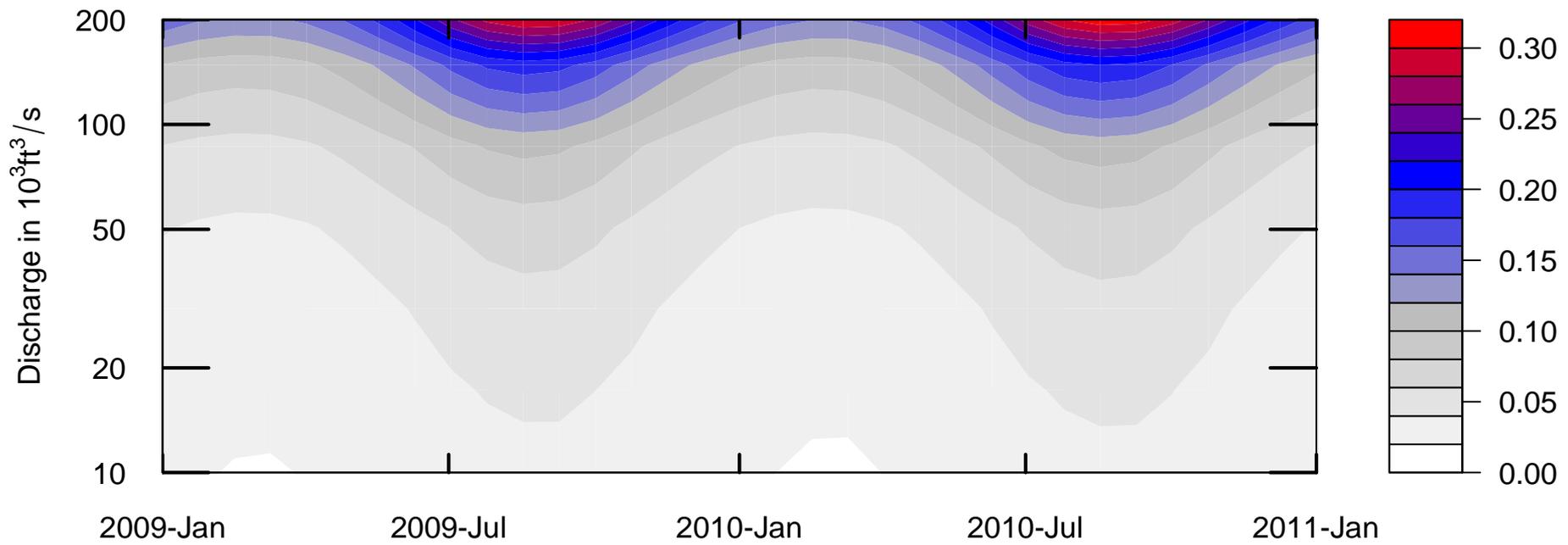
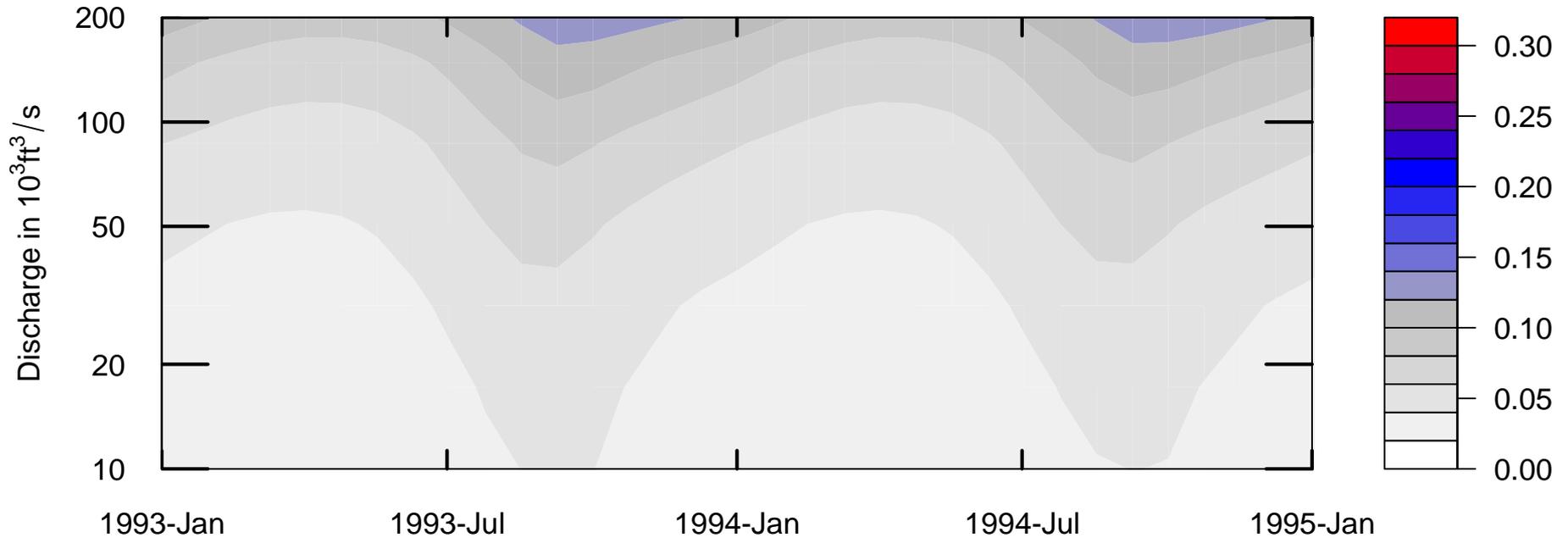
Susquehanna River at Conowingo, MD Total Phosphorus Estimated Concentration Surface in Color



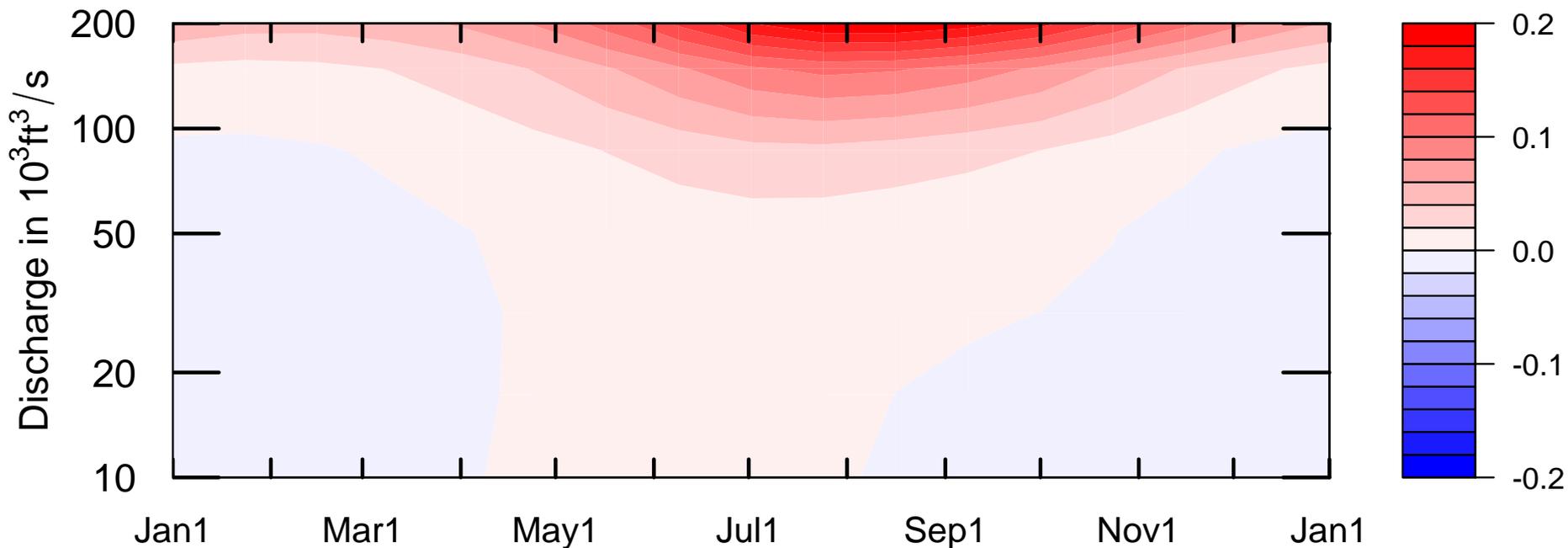
Conowingo Dam during
Tropical Storm Lee,
September 2011,
Reservoir is rapidly filling,
Trap efficiency in decline



Susquehanna River at Conowingo, MD Total Phosphorus Estimated Concentration Surface in Color

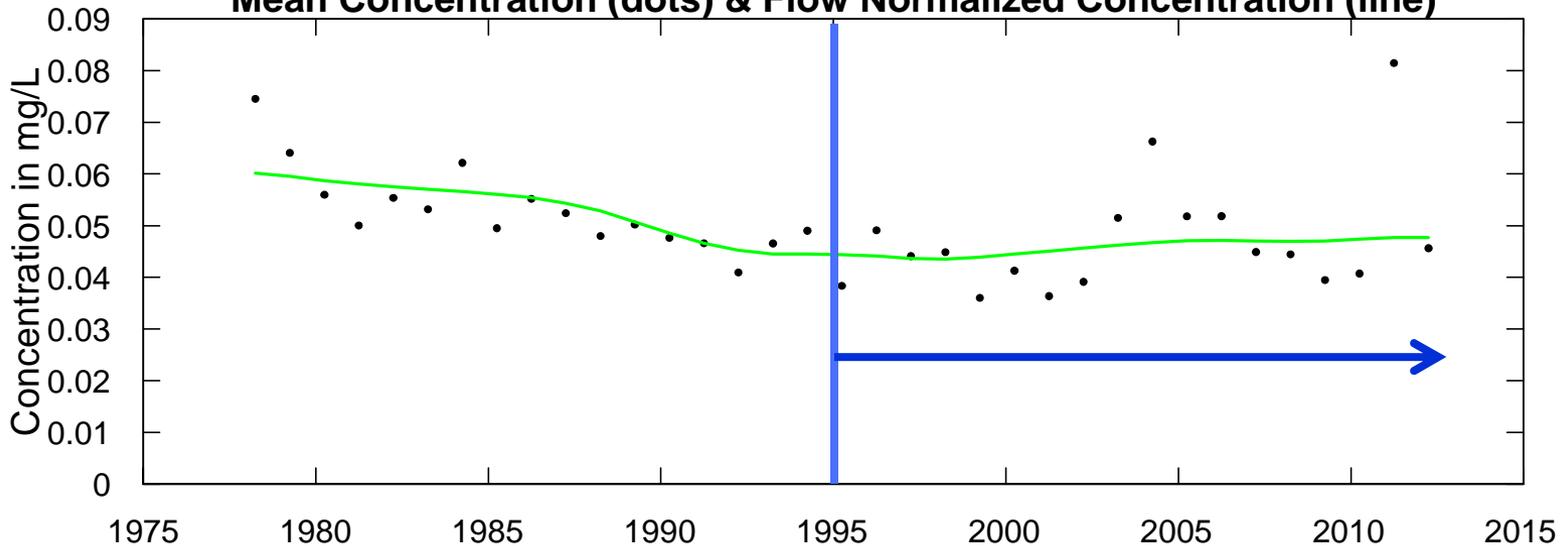


Susquehanna River at Conowingo, MD Total Phosphorus Estimated Concentration change from 1995 to 2011



Susquehanna River at Conowingo, MD Total Phosphorus Water Year

Mean Concentration (dots) & Flow Normalized Concentration (line)

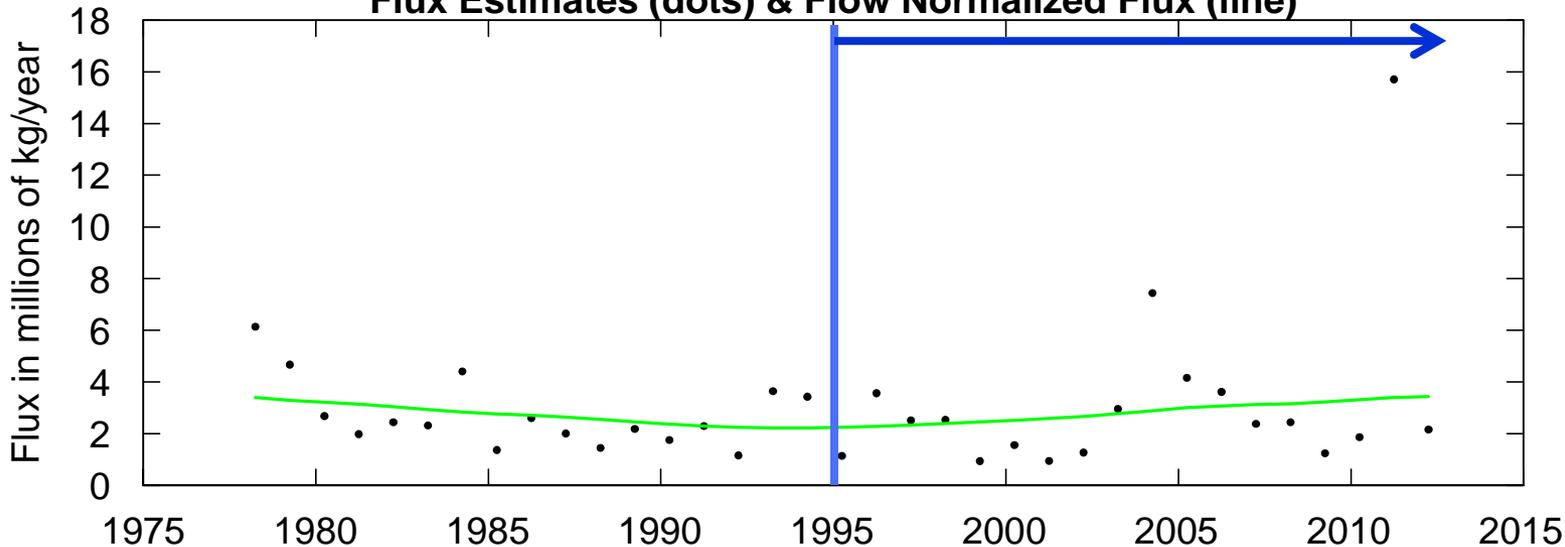


**Change
from
1995-2012**

0.4%/yr

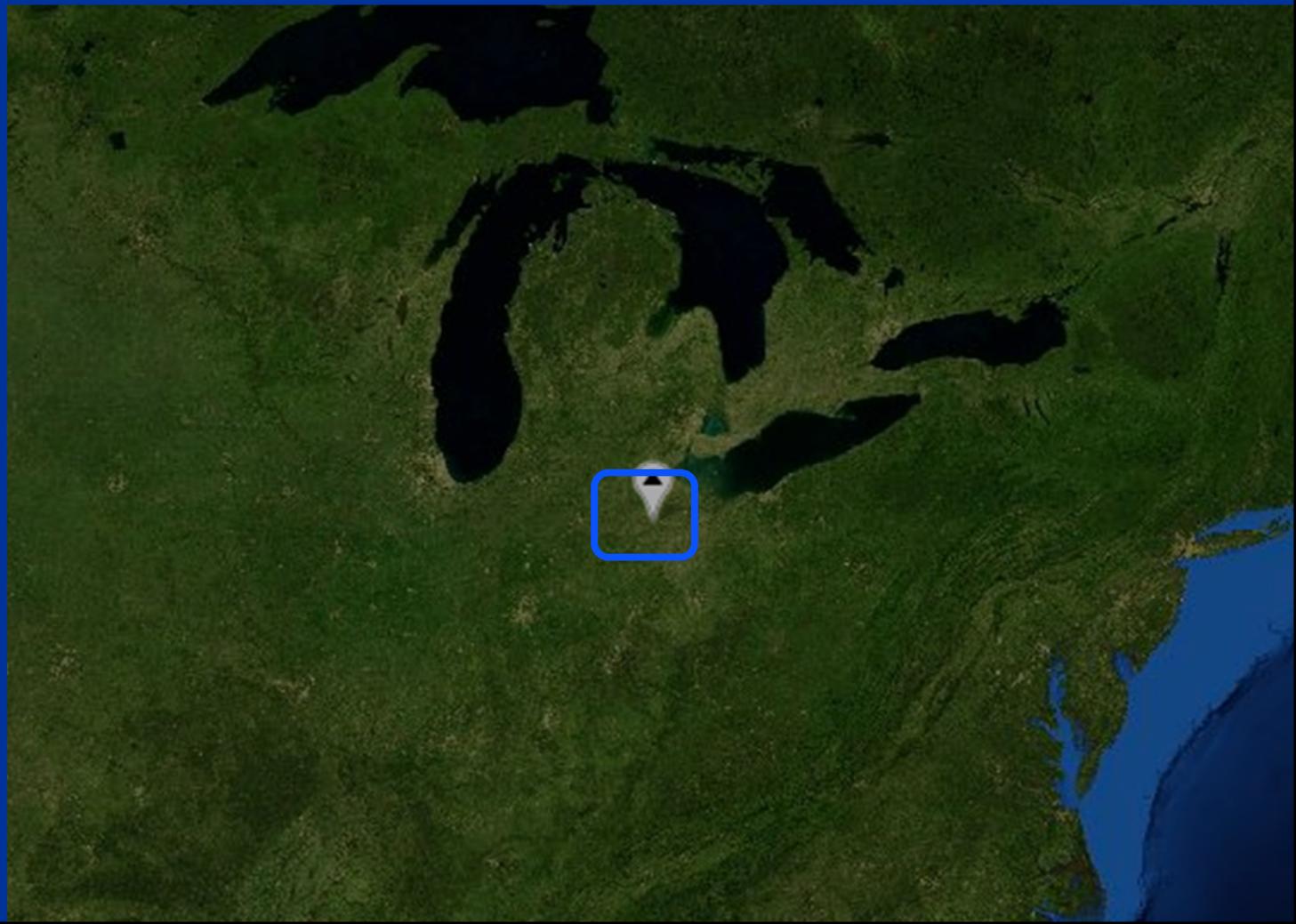
Susquehanna River at Conowingo, MD Total Phosphorus Water Year

Flux Estimates (dots) & Flow Normalized Flux (line)



3.1%/yr

Maumee River – 16,000 km² Tributary to Lake Erie

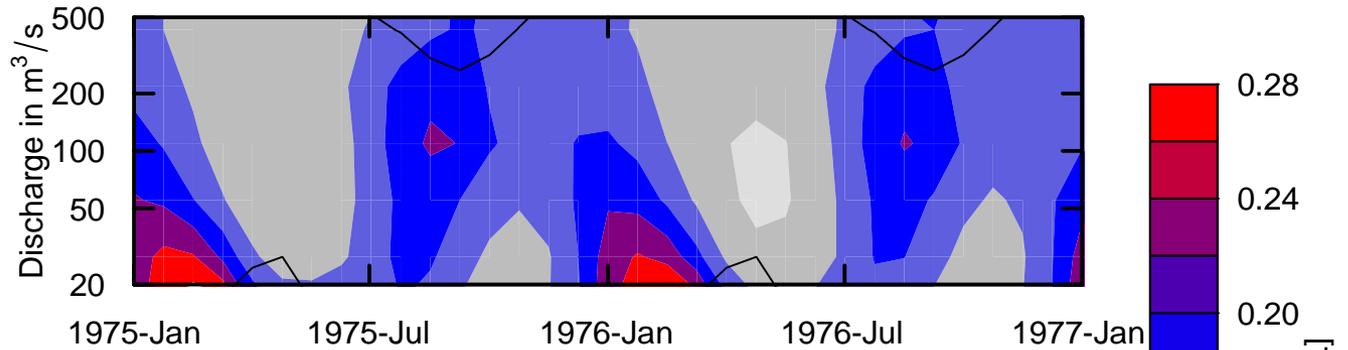


Cyanobacter – Lake Erie

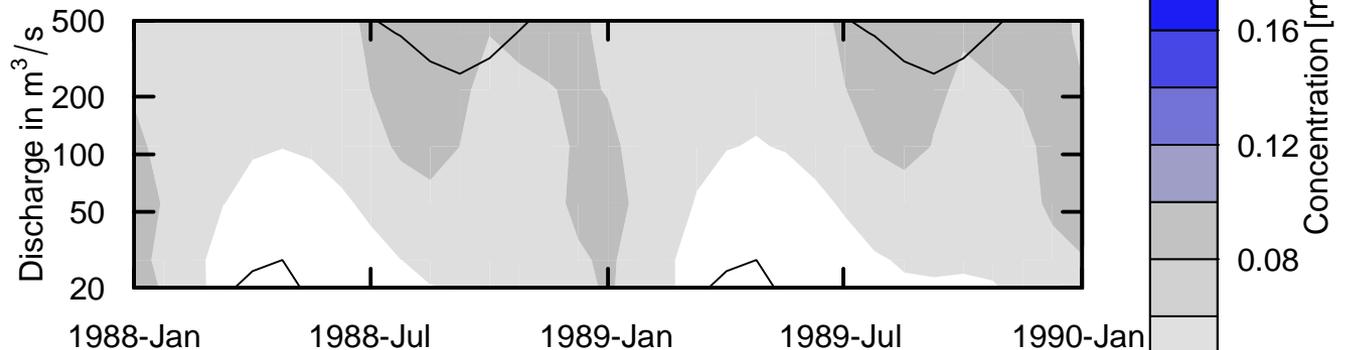


Dissolved Reactive Phosphorus, Maumee River, at Waterville, OH

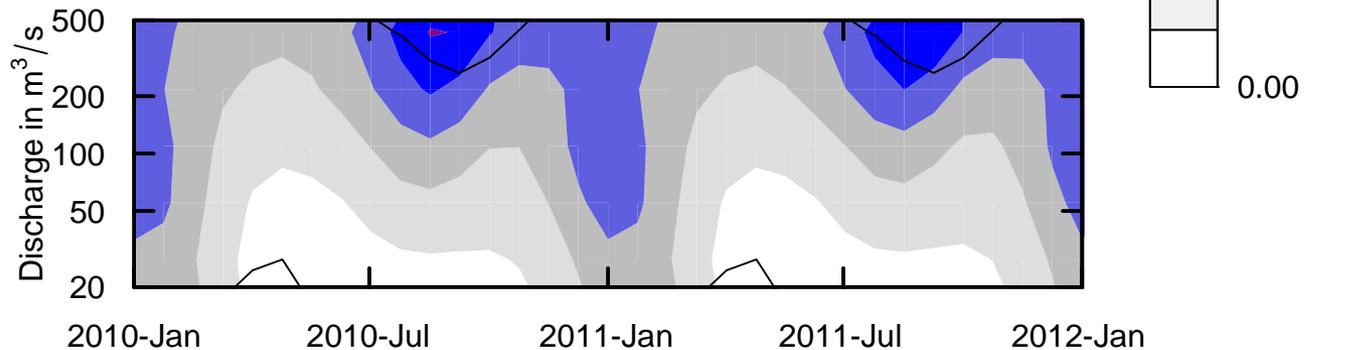
Mid 1970's



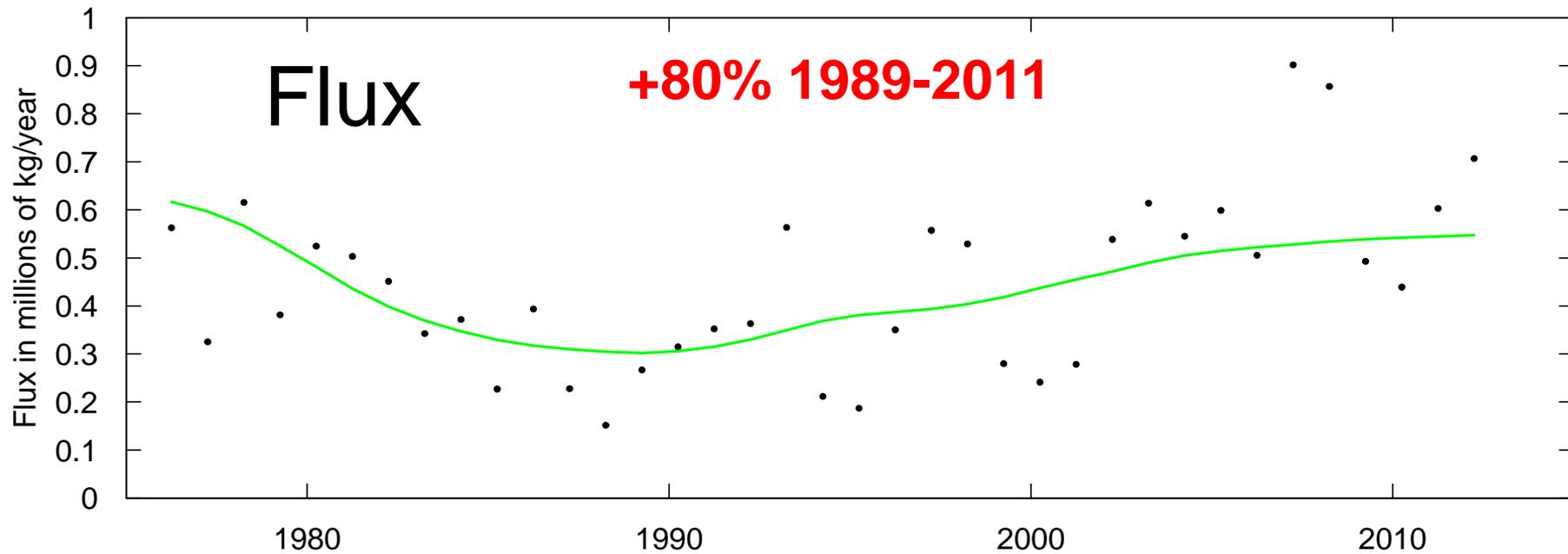
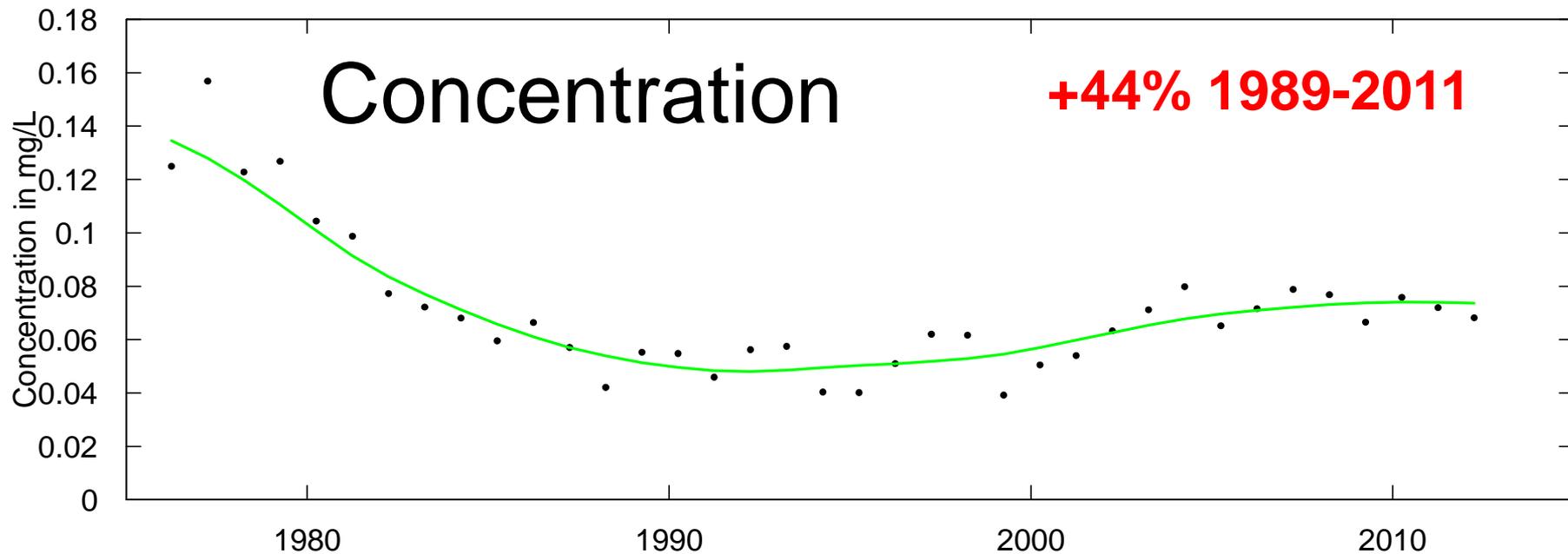
Late 1980's



Early 2010's



Dissolved Reactive Phosphorus, Maumee River, at Waterville, OH



dataRetrieval & EGRET (Exploration and Graphics for RivEr Trends)

- **dataRetrieval: ingests the data from multiple sources and puts them in a form suitable for analysis by EGRET or generic use of R**
- **EGRET includes the WRTDS computations: for trend analysis, flux computation, and exploration**
- **Also includes analysis of streamflow trends**
- **Produces a wide range of graphical and tabular outputs**

dataRetrieval

- Can acquire data from web services (USGS or Storet) as well as from user-supplied files
- Includes capability for sample data, daily discharge, other daily values, sensor data, and meta data about site and parameter
- Structures the data to be conveniently used by the EGRET software

Getting Started

- Need to install R (freely downloaded from <http://cran.us.r-project.org/>)
- Next install the EGRET & dataRetrieval packages & the other R packages they depend on:
- In R, run the following commands:
 - `install.packages(c("zoo", "survival", "stringr", "fields", "spam", "XML", "Rcurl", "plyr", "reshape2"))`
 - `install.packages("dataRetrieval", repos=http://usgs-r.github.com, type="both")`
 - `install.packages("EGRET", repos="http://usgs-r.github.com", type="both")`

Getting Started 2

- Then each time packages are used, they need to be loaded, using the commands
`library(dataRetrieval)`
`library(EGRET)`
- Once this is done you will have access to help and to the package vignettes.
- To get help with a function (such as the function `getSampleData`) just type `?getSampleData`

How can we enter data

- **For the water quality sample data**
 - From USGS web services
 - From EPA-Storet web services
 - From a user supplied file
- **For the daily discharge data**
 - From USGS web services
 - From a user supplied file
- **For the meta-data**
 - From USGS web services
 - From user entries

```

> library(dataRetrieval)
> library(EGRET)
> siteID <- "01491000"
> parameter_cd <- "00631"
> startDate <- "1979-09-01"
> endDate <- "2011-09-30"
> Sample <- getSampleData(siteID,parameter_cd,startDate,endDate)
> summary(Sample)

```

```

> library(dataRetrieval)
> library(EGRET)
> siteID <- "01491000"
> parameter_cd <- "00631"
> startDate <- "1979-09-01"
> endDate <- "2011-09-30"
> Sample <- getSampleData(siteID, parameter_cd, startDate, endDate)
> summary(Sample)

```

Date	ConcLow	ConcHigh	Uncen	ConcAve	Julian	Month
Min. :1979-09-25	Min. :0.176	Min. :0.050	Min. :0.0000	Min. :0.025	Min. :47383	Min. : 1.00
1st Qu.:1989-01-06	1st Qu.:0.880	1st Qu.:0.880	1st Qu.:1.0000	1st Qu.:0.880	1st Qu.:50775	1st Qu.: 3.00
Median :1994-03-15	Median :1.100	Median :1.100	Median :1.0000	Median :1.100	Median :52668	Median : 6.00
Mean :1995-05-23	Mean :1.124	Mean :1.122	Mean :0.9985	Mean :1.122	Mean :53102	Mean : 6.07
3rd Qu.:2002-05-29	3rd Qu.:1.400	3rd Qu.:1.400	3rd Qu.:1.0000	3rd Qu.:1.400	3rd Qu.:55665	3rd Qu.: 9.00
Max. :2011-09-29	Max. :2.430	Max. :2.430	Max. :1.0000	Max. :2.430	Max. :59075	Max. :12.00
	NA's :1					
Day	DecYear	MonthSeq	SinDY	CosDY		
Min. : 2.00	Min. :1980	Min. :1557	Min. : -1.00000	Min. : -0.999963		
1st Qu.: 82.25	1st Qu.:1989	1st Qu.:1669	1st Qu.: -0.63727	1st Qu.: -0.672949		
Median :157.00	Median :1994	Median :1731	Median : 0.17928	Median : 0.000000		
Mean :169.03	Mean :1995	Mean :1745	Mean : 0.08233	Mean : 0.003879		
3rd Qu.:256.75	3rd Qu.:2002	3rd Qu.:1830	3rd Qu.: 0.78412	3rd Qu.: 0.722117		
Max. :364.00	Max. :2012	Max. :1941	Max. : 1.00000	Max. : 0.999668		

```

> length(Sample$Date)
[1] 654
> |

```

```
> Daily <- getDVData(siteID,"00060",startDate,endDate)
```

```
>
>
> Daily <- getDVData(siteID,"00060",startDate,endDate)
There are 11718 data points, and 11718 days.
> summary(Daily)
      Date          Q          Julian      Month          Day          DecYear
Min.   :1979-09-01  Min.   : 0.00991  Min.   :47359  Min.   : 1.000  Min.   : 1.0  Min.   :1980
1st Qu.:1987-09-08  1st Qu.: 0.93446  1st Qu.:50288  1st Qu.: 4.000  1st Qu.: 93.0  1st Qu.:1988
Median :1995-09-15  Median : 2.40693  Median :53218  Median : 7.000  Median :184.0  Median :1996
Mean   :1995-09-15  Mean   : 4.08210  Mean   :53218  Mean   : 6.529  Mean   :183.9  Mean   :1996
3rd Qu.:2003-09-22  3rd Qu.: 4.61565  3rd Qu.:56147  3rd Qu.:10.000  3rd Qu.:275.0  3rd Qu.:2004
Max.   :2011-09-30  Max.   :246.35656  Max.   :59076  Max.   :12.000  Max.   :366.0  Max.   :2012

      MonthSeq      Qualifier          i          LogQ          Q7          Q30
Min.   :1557      Length:11718  Min.   : 1  Min.   : -4.61412  Min.   : 0.01808  Min.   : 0.09606
1st Qu.:1653      Class :character  1st Qu.: 2930  1st Qu.: -0.06779  1st Qu.: 0.99109  1st Qu.: 1.17609
Median :1749      Mode  :character  Median : 5860  Median : 0.87835  Median : 2.55661  Median : 2.87133
Mean   :1749                                Mean   : 5860  Mean   : 0.76602  Mean   : 4.08154  Mean   : 4.08059
3rd Qu.:1845                                3rd Qu.: 8789  3rd Qu.: 1.52945  3rd Qu.: 4.91095  3rd Qu.: 5.68036
Max.   :1941                                Max.   :11718  Max.   : 5.50678  Max.   :84.00395  Max.   :25.47478
                                     NA's   :6      NA's   :29

> length(Daily$Q)
[1] 11718
> |
```

Censored values

All concentration data are treated as intervals.

- Let's say reported concentration is 1 mg/L
- We code this as: `ConcLow = 1.0` and `ConcHigh = 1.0`
- The interval for this data point is then 1.0 to 1.0

- For a value reported as “less than 1.0 mg/L”
- We code this as: `ConcLow = NA` and `ConcHigh = 1.0`
- The interval for this data point is then 0.0 to 1.0

All of the “weighted regressions” in WRTDS are really “survival regression” (the function `survreg` in R) which is design for data reported as an interval.

Censored values and compound analytes

Sometimes an analyte of interest is the sum of two or more measured analytes. Here is a real example for Total Nitrogen in the Susquehanna River, Maryland, April 27, 1988.

- The rule is: Compute Total N as Ammonia plus organic N, unfiltered + Nitrate plus nitrite, filtered

The two analyte values were reported as <0.2 and 0.9 mg/L respectively. Therefore, this data point has $\text{ConcLow} = 0.9$ and $\text{ConcHigh} = 1.1$.

- The conventional left-censored approach calls this $(0, 1.1)$
- WRTDS calls this $(0.9 \text{ to } 1.1)$

For Non-USGS data from the Water Quality Portal

```
> siteID <- "IL_EPA_WQX-BPK-07"  
> characteristicName <- "Inorganic nitrogen (nitrate and nitrite)"  
> startDate <- "2005-01-01"  
> endDate <- "2012-01-01"  
> Sample <- getSTORETSampleData(siteID,characteristicName,startDate,endDate)  
> summary(Sample)
```

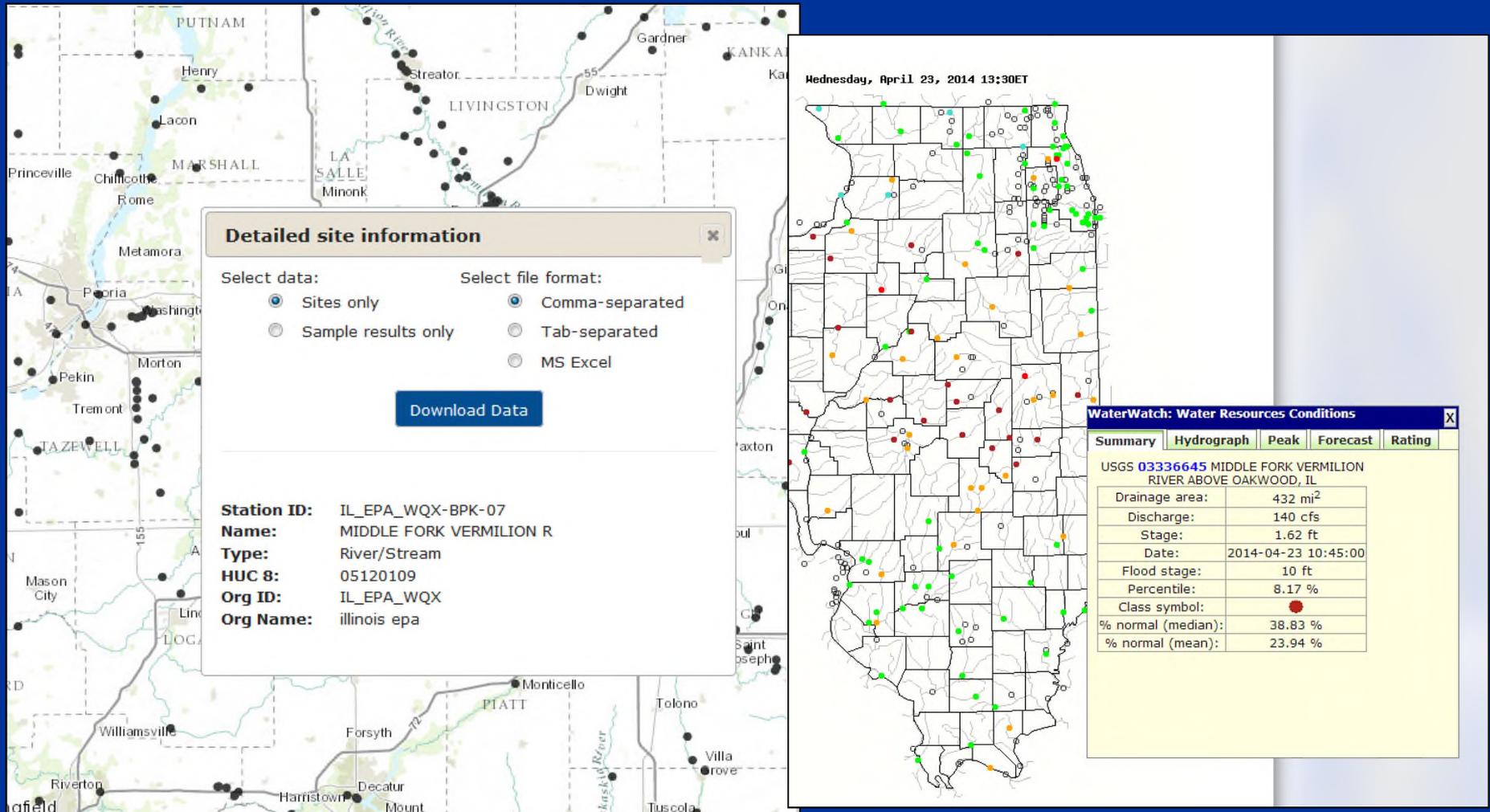
```
> siteID <- "IL_EPA_WQX-BPK-07"  
> characteristicName <- "Inorganic nitrogen (nitrate and nitrite)"  
> startDate <- "2005-01-01"  
> endDate <- "2012-01-01"  
> Sample <- suppresswarnings(getSTORETSampleData(siteID,characteristicName,startDate,endDate))  
> summary(Sample)
```

Date	ConcLow	ConcHigh	Uncen	ConcAve	Julian
Min. :2005-01-24	Min. : 0.041	Min. : 0.0180	Min. :0.0	Min. : 0.0090	Min. :56636
1st Qu.:2009-02-08	1st Qu.: 3.658	1st Qu.: 0.1905	1st Qu.:1.0	1st Qu.: 0.1905	1st Qu.:58112
Median :2010-01-07	Median : 5.205	Median : 4.5950	Median :1.0	Median : 4.5950	Median :58446
Mean :2009-05-21	Mean : 4.834	Mean : 3.8710	Mean :0.8	Mean : 3.8692	Mean :58215
3rd Qu.:2011-03-03	3rd Qu.: 6.560	3rd Qu.: 6.2250	3rd Qu.:1.0	3rd Qu.: 6.2250	3rd Qu.:58866
Max. :2011-11-28	Max. :11.400	Max. :11.4000	Max. :1.0	Max. :11.4000	Max. :59135

Month	Day	DecYear	MonthSeq	SinDY	CosDY
Min. : 1.000	Min. : 10.0	Min. :2005	Min. :1861	Min. : -0.997643	Min. : -0.99908
1st Qu.: 4.000	1st Qu.: 96.5	1st Qu.:2009	1st Qu.:1910	1st Qu.: -0.742051	1st Qu.: -0.69469
Median : 6.500	Median :184.0	Median :2010	Median :1921	Median : -0.008572	Median : -0.16188
Mean : 6.425	Mean :179.5	Mean :2009	Mean :1913	Mean : -0.011740	Mean : -0.07631
3rd Qu.: 9.000	3rd Qu.:256.2	3rd Qu.:2011	3rd Qu.:1934	3rd Qu.: 0.739359	3rd Qu.: 0.62395
Max. :12.000	Max. :349.0	Max. :2012	Max. :1943	Max. : 0.998674	Max. : 0.98673

```
> length(Sample$Date)  
[1] 40
```

Find a nearby USGS streamgage that can provide appropriate discharge data to use with these water quality data



Retrieve daily discharge data

```
> siteID <- "03336645"
```

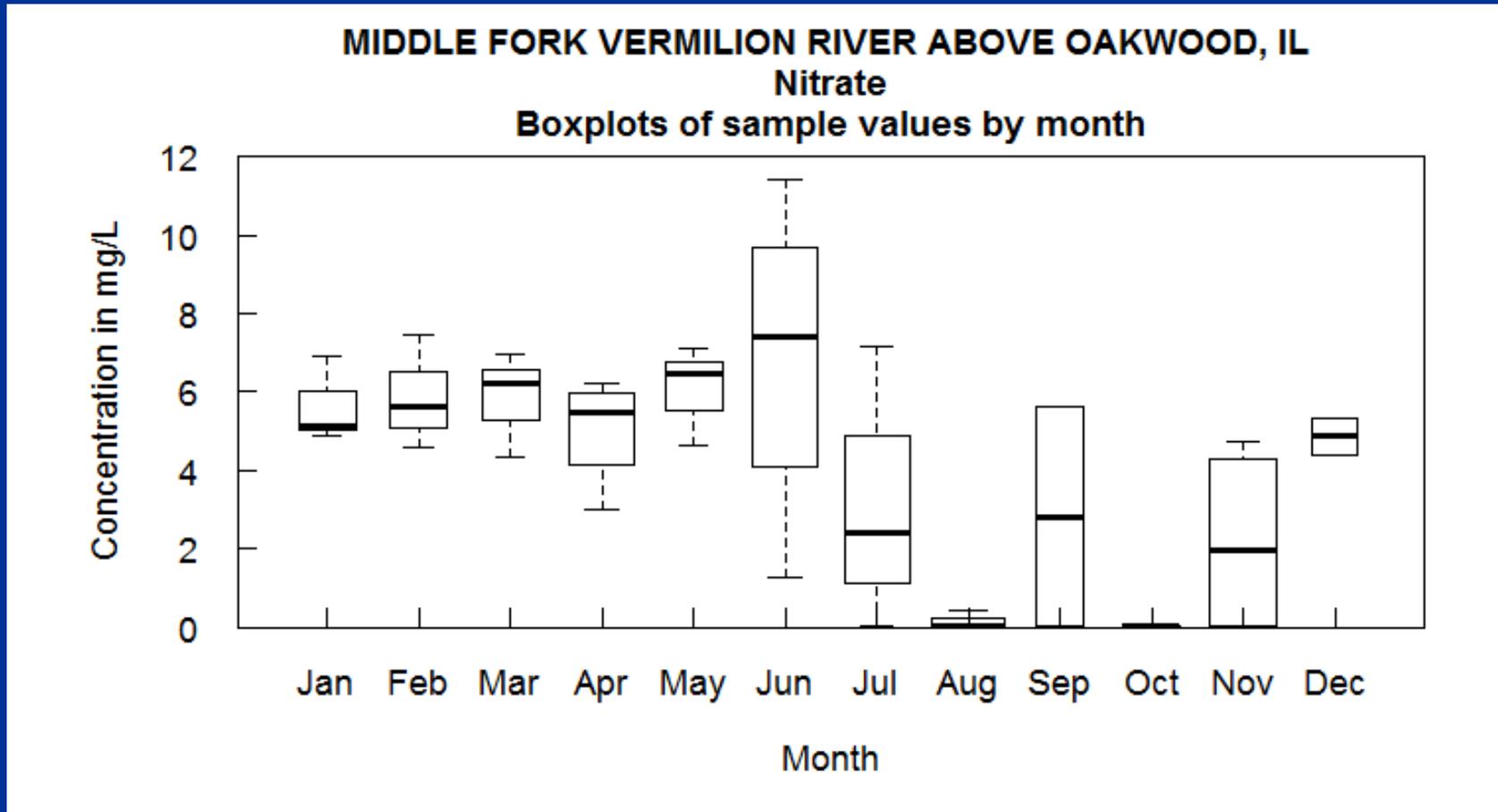
```
> Daily <- getDVDData(siteID,"00060",startDate,endDate)
```

```
>
> siteID <- "03336645"
> Daily <- getDVDData(siteID,"00060",startDate,endDate)
There are 2557 data points, and 2557 days.
> summary(Daily)
      Date                Q                Julian                Month                Day                DecYear                MonthSeq
Min.   :2005-01-01   Min.   : 0.1727   Min.   :56613   Min.   : 1.000   Min.   : 1.0   Min.   :2005   Min.   :1861
1st Qu.:2006-10-02   1st Qu.: 1.4725   1st Qu.:57252   1st Qu.: 4.000   1st Qu.: 93.0   1st Qu.:2007   1st Qu.:1882
Median :2008-07-02   Median : 4.6723   Median :57891   Median : 7.000   Median :184.0   Median :2009   Median :1903
Mean   :2008-07-02   Mean   :12.2350   Mean   :57891   Mean   : 6.522   Mean   :183.7   Mean   :2009   Mean   :1903
3rd Qu.:2010-04-02   3rd Qu.:12.4877   3rd Qu.:58530   3rd Qu.:10.000   3rd Qu.:275.0   3rd Qu.:2010   3rd Qu.:1924
Max.   :2012-01-01   Max.   :322.8120   Max.   :59169   Max.   :12.000   Max.   :366.0   Max.   :2012   Max.   :1945

      qualifier                i                LogQ                Q7                Q30
Length:2557   Min.   : 1   Min.   : -1.7560   Min.   : 0.1905   Min.   : 0.2219
Class :character   1st Qu.: 640   1st Qu.: 0.3869   1st Qu.: 1.6768   1st Qu.: 2.3293
Mode  :character   Median :1279   Median : 1.5416   Median : 5.2548   Median : 7.6092
                Mean   :1279   Mean   : 1.4538   Mean   :12.2107   Mean   :11.9463
                3rd Qu.:1918   3rd Qu.: 2.5247   3rd Qu.:14.1463   3rd Qu.:19.9598
                Max.   :2557   Max.   : 5.7771   Max.   :151.2524   Max.   :55.4217
                NA's   :6   NA's   :29

> length(Daily$Q)
[1] 2557
>
>
>
```

Data can then be used for EGRET or other analysis this plot > boxConcMonth()

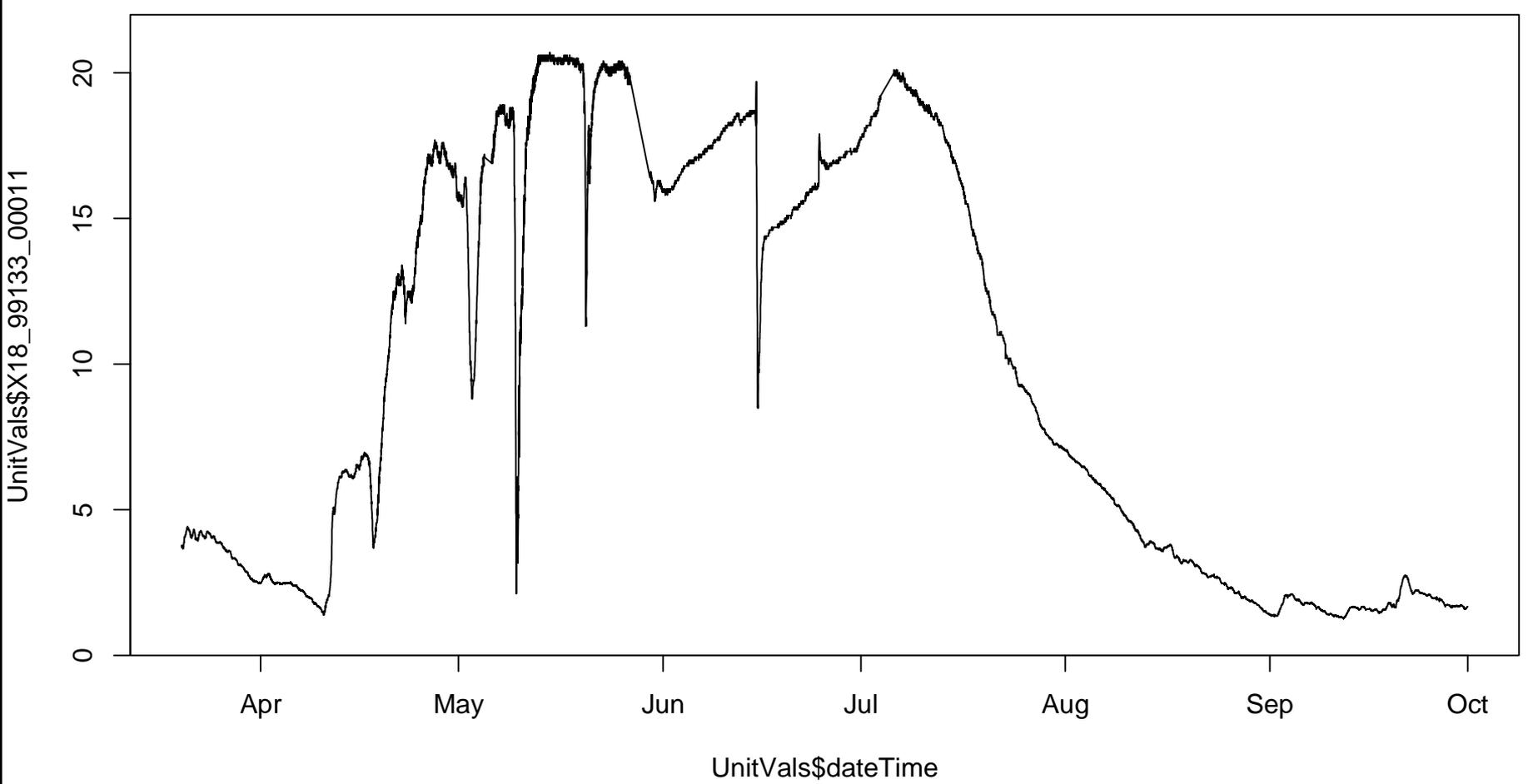


Unit values retrieval (not used by EGRET)

- Raccoon River at Van Metre, IA
 - Nitrate sensor data
 - March – Sept 2013
- ```
> siteID <- "05484500"
> parameterCD <- "99133"
> UnitVals <- retrieveUnitNWISData
 (siteID, parameterCD, "2013-03-01",
 "2013-09-30")
> Summary(UnitVals)
```

```
> summary(UnitVals)
 agency site dateTime tz_cd X18_99133_00011 X18_99133_00011_cd
Length:17720 Length:17720 Min. :2013-03-20 00:00:00 CST:17720 Min. : 1.260 A:17720
Class :character Class :character 1st Qu.:2013-05-08 16:11:15 1st Qu.: 2.540
Mode :character Mode :character Median :2013-06-27 23:52:30 Median : 7.250
 Mean :2013-06-26 23:57:31 Mean : 9.651
 3rd Qu.:2013-08-15 15:33:45 3rd Qu.:16.900
 Max. :2013-09-30 23:45:00 Max. :20.700
```

```
> plot(UnitVals$dateTime,UnitVals$X18_99133_00011,type="l",ylim=c(0,22),yaxs="i")
```



## **Back to our main EGRET example, metadata is next**

- **The getMetaData function is used to retrieve, input, and save metadata about the current analysis**
- **It defines what data you have and where they came from**
- **Inputs are used for labels on figures & tables**
- **Inputs are used to name your saved workspaces, using abbreviations**

**> INFO<-getMetaData(siteID,parameter\_cd)**

**Your site for streamflow data is 01491000 .**

**Your site name is CHOPTANK RIVER NEAR GREENSBORO, MD ,but you can modify this to a short name in a style you prefer.**

**This name will be used to label graphs and tables.**

**If you want the program to use the name given above, just do a carriage return, otherwise enter the preferred short name(no quotes):**

**<cr>**

**The latitude and longitude of the site are: 38.99719 , -75.78581 (degrees north and west).**

**The drainage area at this site is 113 square miles which is being stored as 292.6687 square kilometers.**

**It is helpful to set up a station abbreviation when doing multi-site studies, enter a unique id (three or four characters should work).**

**It is case sensitive. Even if you don't feel you need an abbreviation for your site you need to enter something (no quotes):**

**Chop**

**Your water quality data are for parameter number 00631 which has the name: ' Nitrate plus nitrite, water, filtered, milligrams per liter as nitrogen '.**

**Typically you will want a shorter name to be used in graphs and tables. The suggested short name is: ' Nitrate-nitrite '.**

**If you would like to change the short name, enter it here, otherwise just hit enter (no quotes):**

**Nitrate, filtered, as N**

**The units for the water quality data are: mg/l as N .**

**It is helpful to set up a constituent abbreviation when doing multi-constituent studies, enter a unique id (three or four characters should work something like tn or tp or NO3).**

**It is case sensitive. Even if you don't feel you need an abbreviation you need to enter something (no quotes):**

**no3**

**If you are using supplied data, you still must run the getMetaData command:**

```
> INFO <- getMetaData()
```

**The program will then prompt you to enter metadata about your site and study.**

**All metadata is voluntary except the following required fields:**

- A site name
- A parameter name
- A site abbreviation
- A parameter abbreviation

# Two more commands before we can start our analysis of the data

```
> Sample<-mergeReport()
```

Discharge Record is 11718 days long, which is 32 years

First day of the discharge record is 1979-09-01 and last day is 2011-09-30

The water quality record has 654 samples

The first sample is from 1979-09-25 and the last sample is from 2011-09-29

Discharge: Minimum, mean and maximum 0.00991 4.08 246

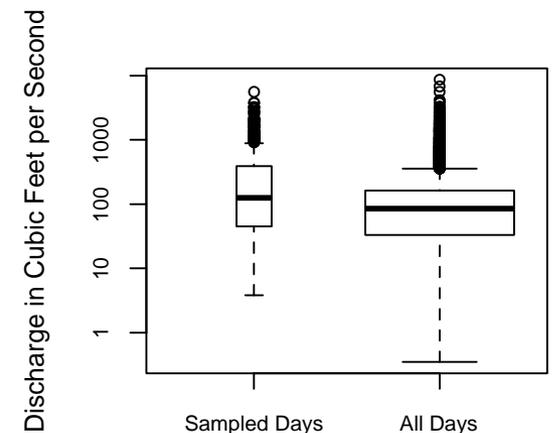
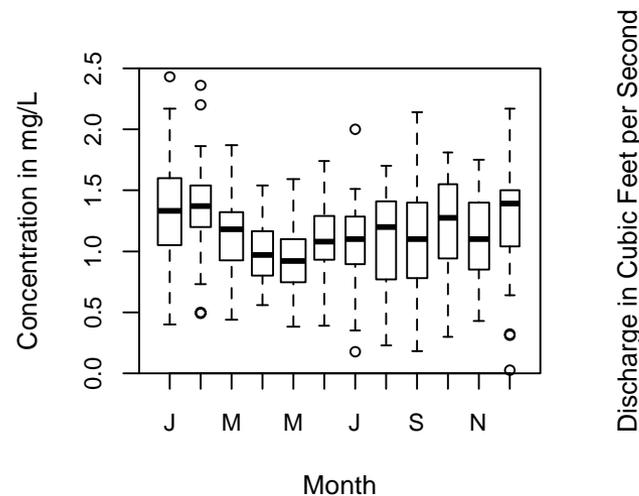
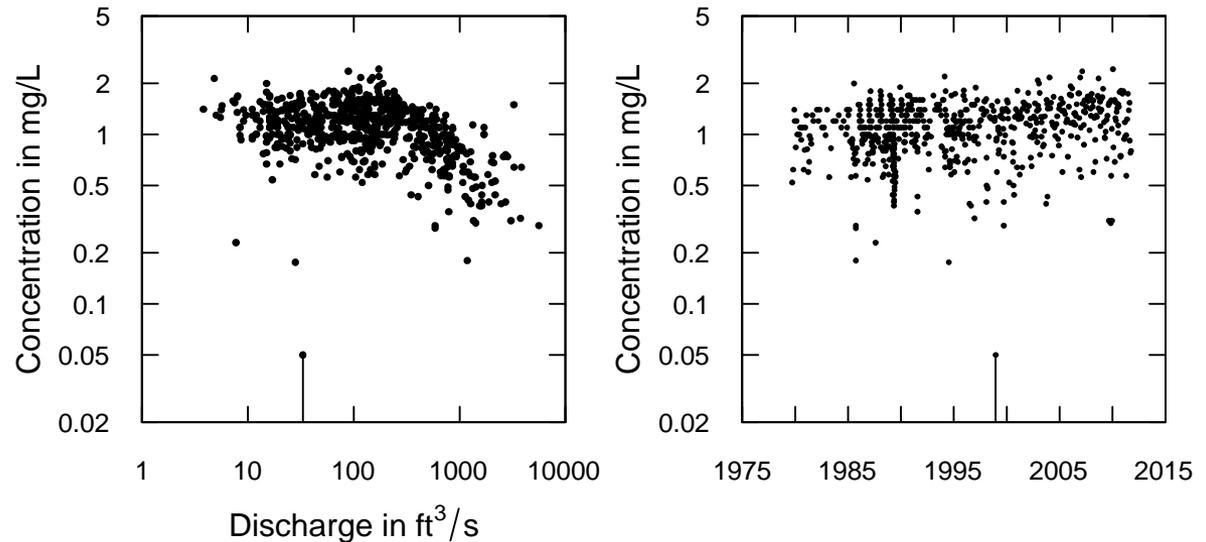
Concentration: Minimum, mean and maximum 0.05 1.1 2.4

Percentage of the sample values that are censored is 0.15 %

# > multiPlotDataOverview(qUnit=1)

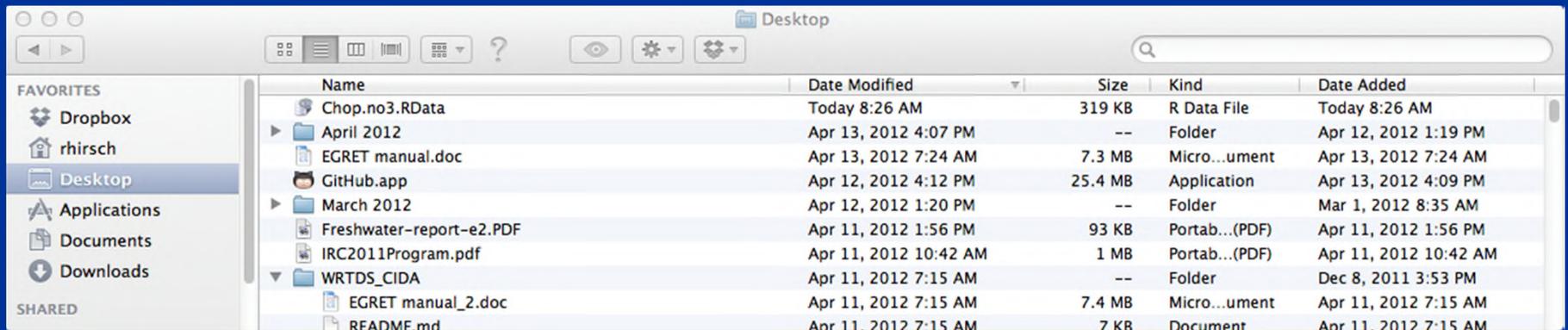
Let's look at the data before we proceed, the function is:

Choptank River near Greensboro, MD  
Nitrate, filtered, as N



# We've gone to all this effort, let's save our work

```
> savePath<-"~/Users/rhirsch/Desktop/"
> saveResults(savePath)
```



Chop.no3.RData

Save it over and over as  
you proceed and add  
results

# We now have 3 data frames

- Sample (654 rows, 14 columns)
- Daily (11,718 rows, 12 columns)
- INFO (1 row, 42 columns)

## > **modelEstimation()**

- Runs the model in cross-validation mode
- Estimates the “surface” for concentration as a function of time and discharge
- Uses the surface to compute daily values of
  - Concentration
  - Flux
  - Flow-normalized concentration
  - Flow-normalized flux
- Adds those to the Daily data frame

**User has choices about some of the parameters of the WRTDS model**

# Now what is in Daily?

## It is a data frame that has dimension (11718, 19)

```
> summary(Daily)
```

| Date               | Q                 | Julian        | Month          | Day           | DecYear      | MonthSeq     |
|--------------------|-------------------|---------------|----------------|---------------|--------------|--------------|
| Min. :1979-09-01   | Min. :9.911e-03   | Min. :47359   | Min. : 1.000   | Min. : 1.0    | Min. :1980   | Min. :1557   |
| 1st Qu.:1987-09-08 | 1st Qu.:9.345e-01 | 1st Qu.:50288 | 1st Qu.: 4.000 | 1st Qu.: 92.0 | 1st Qu.:1988 | 1st Qu.:1653 |
| Median :1995-09-15 | Median :2.407e+00 | Median :53218 | Median : 7.000 | Median :184.0 | Median :1996 | Median :1749 |
| Mean :1995-09-15   | Mean :4.082e+00   | Mean :53218   | Mean : 6.529   | Mean :183.3   | Mean :1996   | Mean :1749   |
| 3rd Qu.:2003-09-22 | 3rd Qu.:4.616e+00 | 3rd Qu.:56147 | 3rd Qu.:10.000 | 3rd Qu.:274.0 | 3rd Qu.:2004 | 3rd Qu.:1845 |
| Max. :2011-09-30   | Max. :2.464e+02   | Max. :59076   | Max. :12.000   | Max. :366.0   | Max. :2012   | Max. :1941   |

| Qualifier        | i             | LogQ              | Q7               | Q30              | Leap          |
|------------------|---------------|-------------------|------------------|------------------|---------------|
| Length:11718     | Min. : 1      | Min. :-4.61412    | Min. : 0.01808   | Min. : 0.09606   | Min. : 1.0    |
| Class :character | 1st Qu.: 2930 | 1st Qu.: -0.06779 | 1st Qu.: 0.99109 | 1st Qu.: 1.17609 | 1st Qu.: 92.0 |
| Mode :character  | Median : 5860 | Median : 0.87835  | Median : 2.55661 | Median : 2.87133 | Median :184.0 |
|                  | Mean : 5860   | Mean : 0.76602    | Mean : 4.08154   | Mean : 4.08059   | Mean :183.3   |
|                  | 3rd Qu.: 8789 | 3rd Qu.: 1.52945  | 3rd Qu.: 4.91095 | 3rd Qu.: 5.68036 | 3rd Qu.:274.0 |
|                  | Max. :11718   | Max. : 5.50678    | Max. :84.00395   | Max. :25.47478   | Max. :365.0   |
|                  |               |                   | NA's : 6.00000   | NA's :29.00000   |               |

| <u>yHat</u>        | <u>SE</u>      | <u>ConcDay</u> | <u>FluxDay</u>   | <u>FNConc</u>  | <u>FNFlux</u> |
|--------------------|----------------|----------------|------------------|----------------|---------------|
| Min. :-1.534999    | Min. :0.1347   | Min. :0.230    | Min. : 1.633     | Min. :0.8208   | Min. : 77.3   |
| 1st Qu.: -0.006091 | 1st Qu.:0.2186 | 1st Qu.:1.033  | 1st Qu.: 98.053  | 1st Qu.:1.0524 | 1st Qu.:168.3 |
| Median : 0.130494  | Median :0.2504 | Median :1.195  | Median : 248.578 | Median :1.2042 | Median :317.3 |
| Mean : 0.117362    | Mean :0.2678   | Mean :1.194    | Mean : 365.030   | Mean :1.1975   | Mean :361.5   |
| 3rd Qu.: 0.258278  | 3rd Qu.:0.3002 | 3rd Qu.:1.353  | 3rd Qu.: 482.075 | 3rd Qu.:1.3286 | 3rd Qu.:536.0 |
| Max. : 0.659426    | Max. :0.6129   | Max. :1.962    | Max. :5705.826   | Max. :1.7017   | Max. :928.3   |

# “Period of Analysis” concept in EGRET.

- Could be water year
- Could be calendar year
- Could be April-May-June
- Could be Dec-Jan-Feb-Mar
- Could be only May...

**paStart** = calendar month that starts Period

**paLong** = length of Period, in months

# Period of analysis set up

Say we want calendar year

```
INFO <- setPA(paStart = 1, paLong=12)
```

Say we want April, May, June

```
INFO <- setPA(paStart = 4, paLong = 3)
```

Default is water year

# Units in EGRET

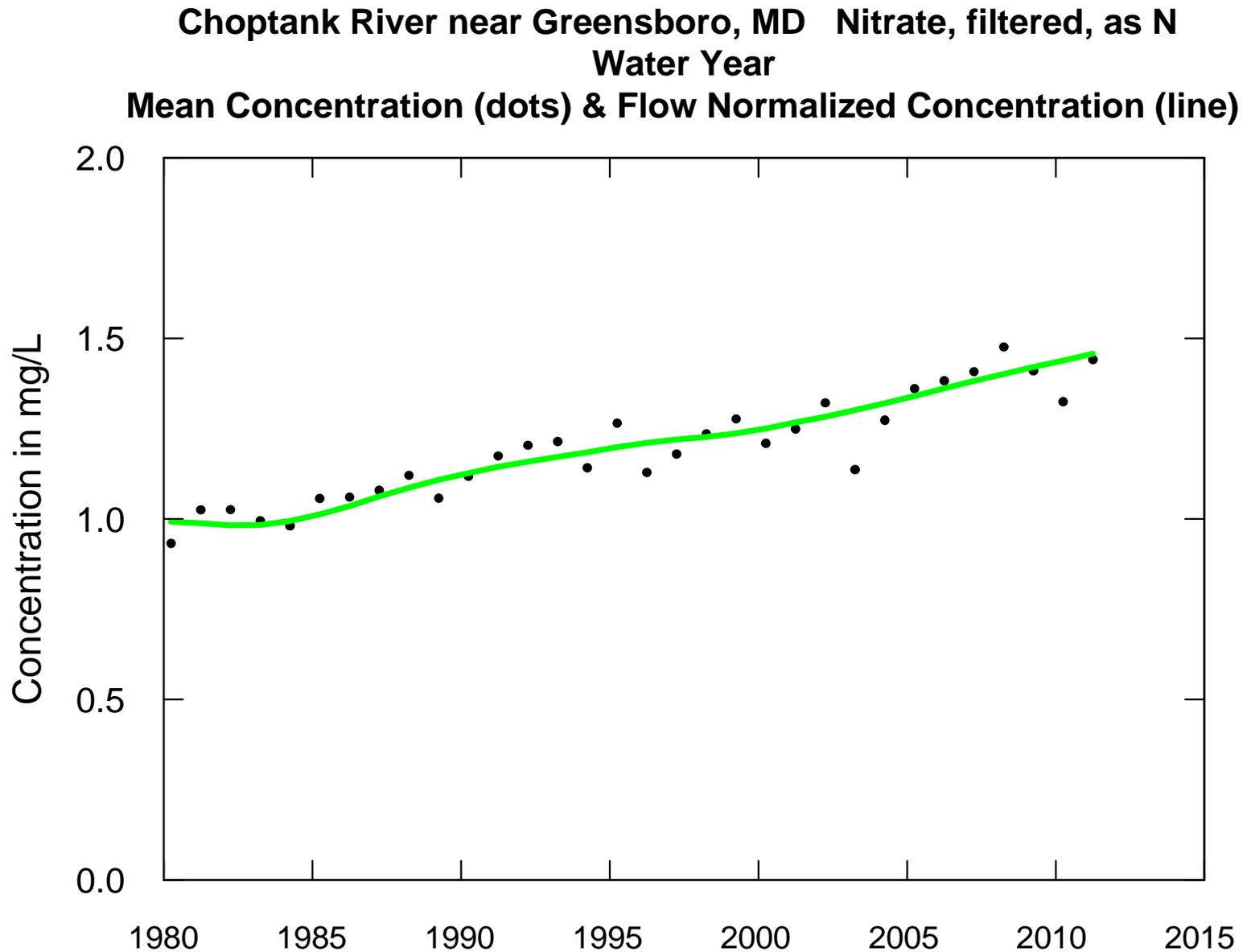
Everything stored as:

$\text{m}^3/\text{s}$ ,  $\text{kg}/\text{day}$ , or  $\text{mg}/\text{L}$

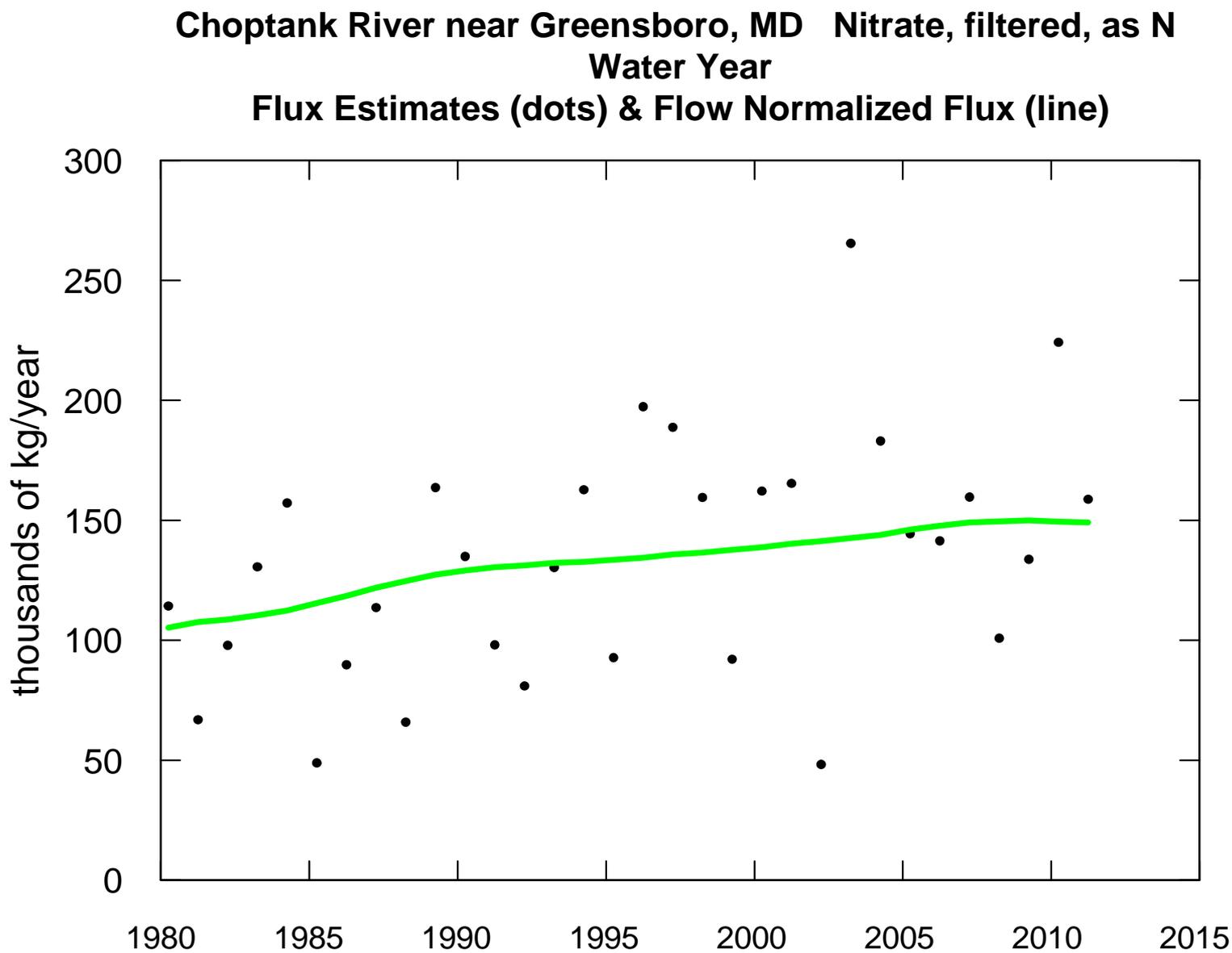
But each graphic or table has a wide choice of units (English and SI) that the user can select

**Now lets see some trend results**

# > plotConcHist(1980,2012)



```
> plotFluxHist(1980,2012,fluxUnit=8)
```



> tableResults ( $\alpha$ Unit=1, fluxUnit=5)

Choptank River near Greensboro, MD  
Nitrate, filtered, as N  
Water Year

| <u>Year</u> | <u>Discharge</u><br>cfs | <u>Conc</u> | <u>FN Conc</u><br>mg/L | <u>Flux</u><br>tons/yr | <u>FN Flux</u> |
|-------------|-------------------------|-------------|------------------------|------------------------|----------------|
| 1980        | 150.2                   | 0.932       | 0.992                  | 126.0                  | 116            |
| 1981        | 78.3                    | 1.025       | 0.988                  | 73.7                   | 119            |
| 1982        | 107.6                   | 1.025       | 0.982                  | 107.9                  | 120            |
| 1983        | 176.1                   | 0.995       | 0.983                  | 143.9                  | 122            |
| 1984        | 201.9                   | 0.981       | 0.994                  | 173.3                  | 124            |
| 1985        | 53.6                    | 1.056       | 1.012                  | 53.8                   | 127            |
| 1986        | 92.8                    | 1.060       | 1.036                  | 99.0                   | 131            |
| 1987        | 119.1                   | 1.079       | 1.062                  | 125.2                  | 134            |
| 1988        | 66.0                    | 1.120       | 1.086                  | 72.6                   | 137            |
| 1989        | 198.2                   | 1.057       | 1.108                  | 180.4                  | 140            |
| 1990        | 141.5                   | 1.118       | 1.126                  | 148.7                  | 142            |
| 1991        | 97.0                    | 1.174       | 1.144                  | 108.1                  | 144            |
| 1992        | 77.2                    | 1.204       | 1.158                  | 89.2                   | 145            |
| .           |                         |             |                        |                        |                |
| .           |                         |             |                        |                        |                |
| .           |                         |             |                        |                        |                |
| .           |                         |             |                        |                        |                |
| 2007        | 151.2                   | 1.408       | 1.382                  | 176.0                  | 164            |
| 2008        | 90.5                    | 1.476       | 1.401                  | 111.1                  | 165            |
| 2009        | 130.0                   | 1.410       | 1.420                  | 147.4                  | 165            |
| 2010        | 254.0                   | 1.324       | 1.438                  | 247.1                  | 165            |
| 2011        | 185.2                   | 1.441       | 1.458                  | 175.0                  | 164            |

# How to see trends as numbers

```
yearPoints = c(1980,1995,2011)
```

```
tableChange(fluxUnit=5,yearPoints)
```

```
> tableChange(fluxUnit=5, yearPoints=c(1980, 1995, 2011))
```

Choptank River near Greensboro, MD

Nitrate, filtered, as N

Water Year

### Concentration trends

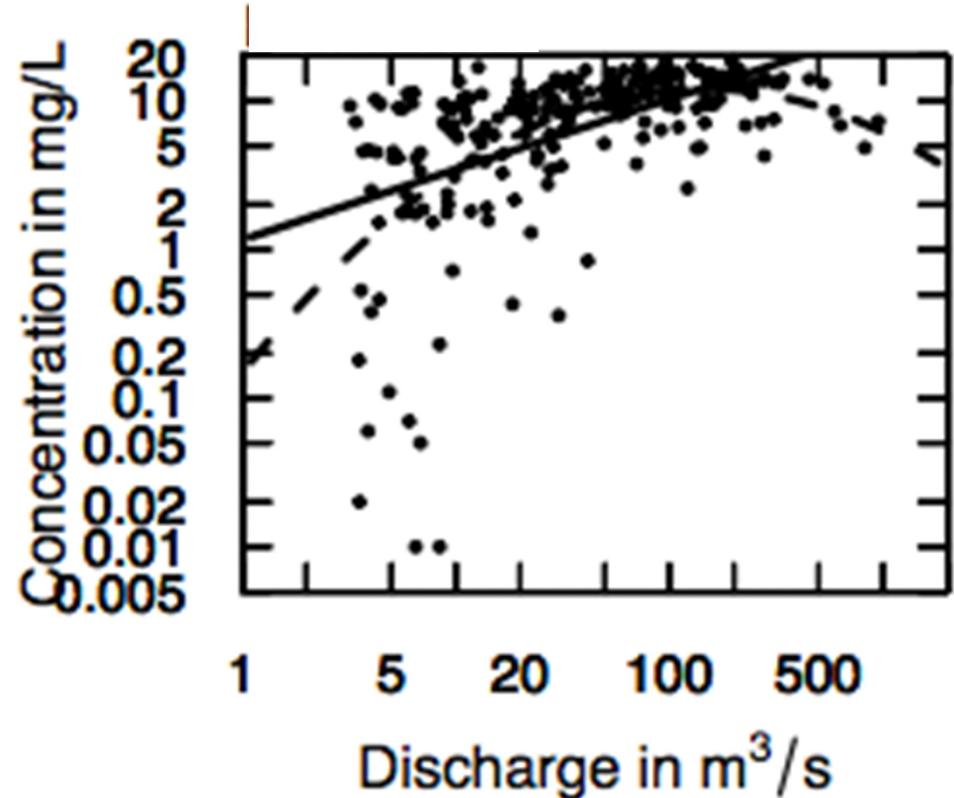
| time span |    |      | change | slope   | change | slope |
|-----------|----|------|--------|---------|--------|-------|
|           |    |      | mg/L   | mg/L/yr | %      | %/yr  |
| 1980      | to | 1995 | 0.21   | 0.014   | 21     | 1.4   |
| 1980      | to | 2011 | 0.47   | 0.015   | 47     | 1.5   |
| 1995      | to | 2011 | 0.26   | 0.016   | 22     | 1.4   |

### Flux Trends

| time span |    |      | change  | slope      | change | slope |
|-----------|----|------|---------|------------|--------|-------|
|           |    |      | tons/yr | tons/yr/yr | %      | %/yr  |
| 1980      | to | 1995 | 31      | 2.1        | 27     | 1.8   |
| 1980      | to | 2011 | 48      | 1.6        | 42     | 1.3   |
| 1995      | to | 2011 | 17      | 1.1        | 12     | 0.73  |

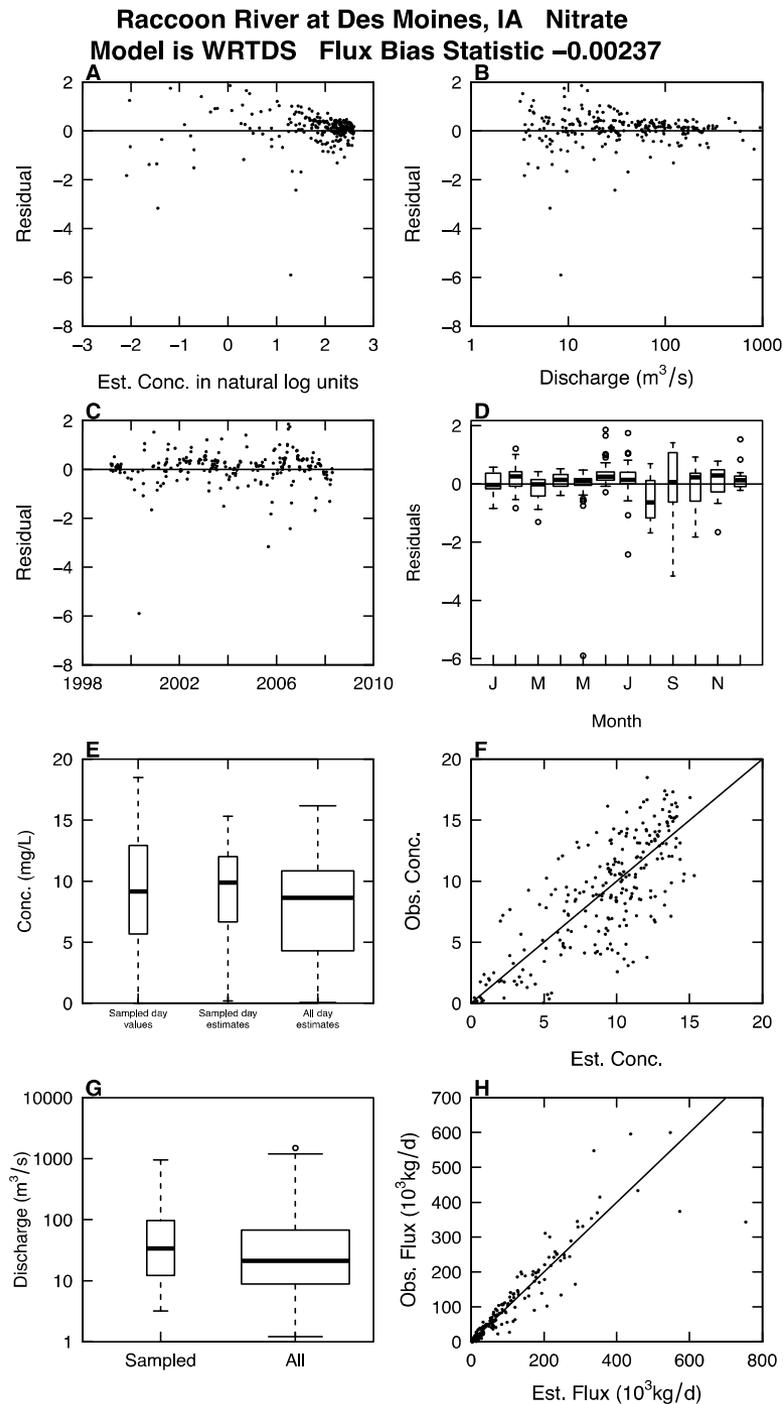


# I'm going to switch data sets to Nitrate for the Raccoon River at Des Moines Iowa



**EGRET**  
produces a  
diagnostic  
plot to help  
spot  
serious  
problems  
with the  
model

`fluxBiasMulti(fluxUnit=4)`

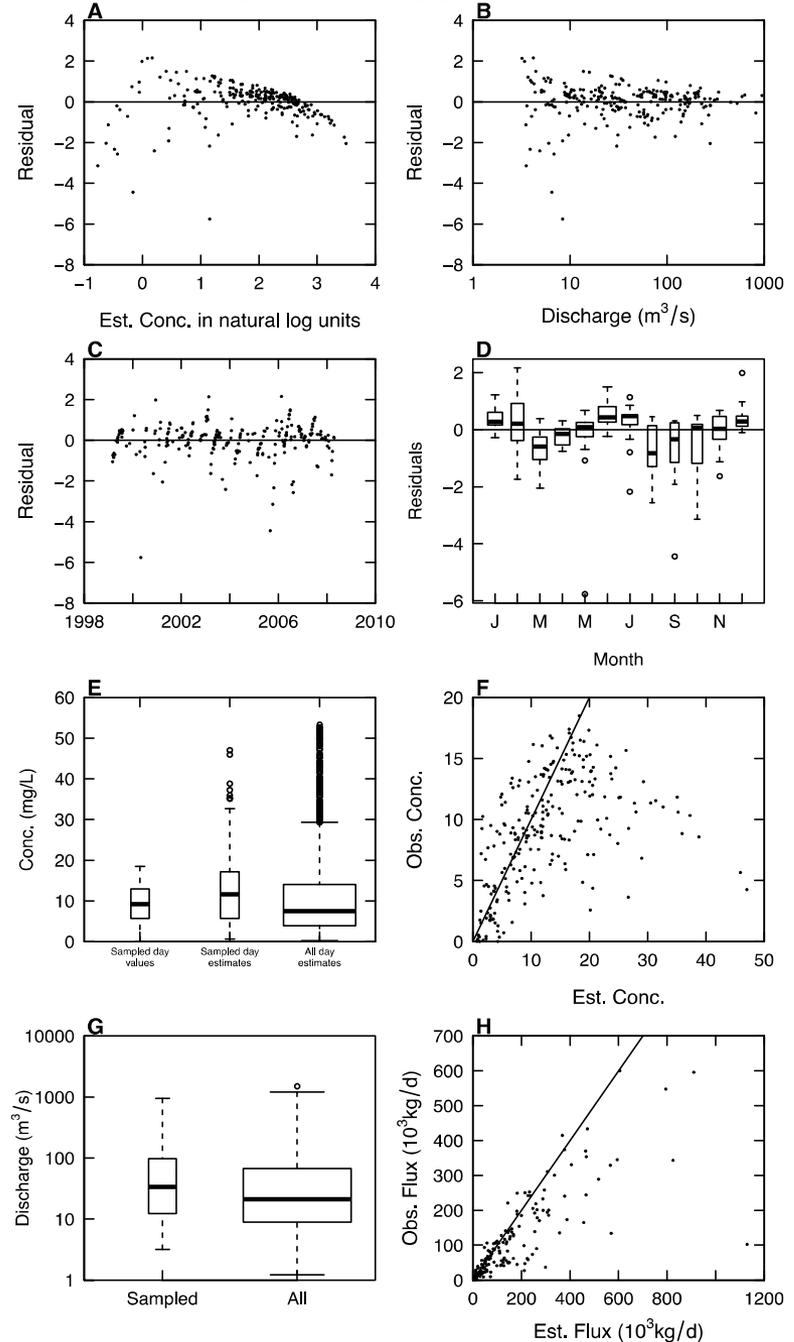


This same type of plot can be used to look at other models, here the **LOADEST7**

fluxBiasMulti(fluxUnit=4)



Raccoon River at Des Moines, IA Nitrate  
Model is L7 Flux Bias Statistic 0.319



**Diagnostics and potential problems with estimating mean flux, see:**

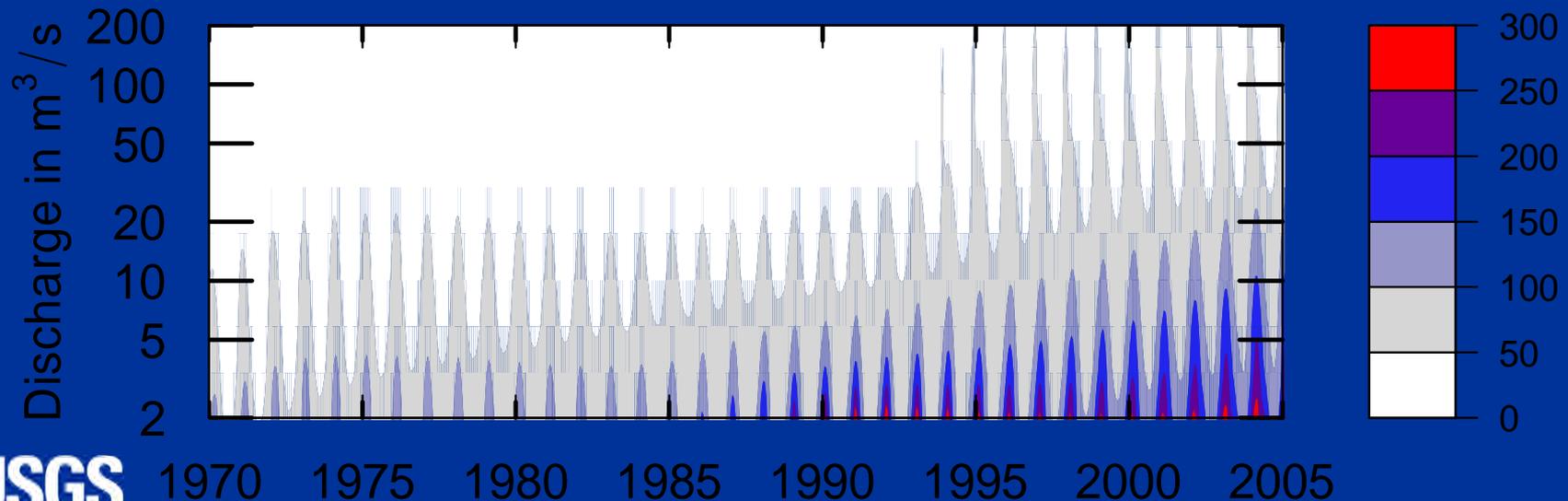
**Hirsch, R.M., 2014, Large biases in regression-based constituent flux estimates: causes and diagnostics. Journal of the American Water Resources Association, in press.**

**Bottom line, look at the fit before you use a statistical model!!!**

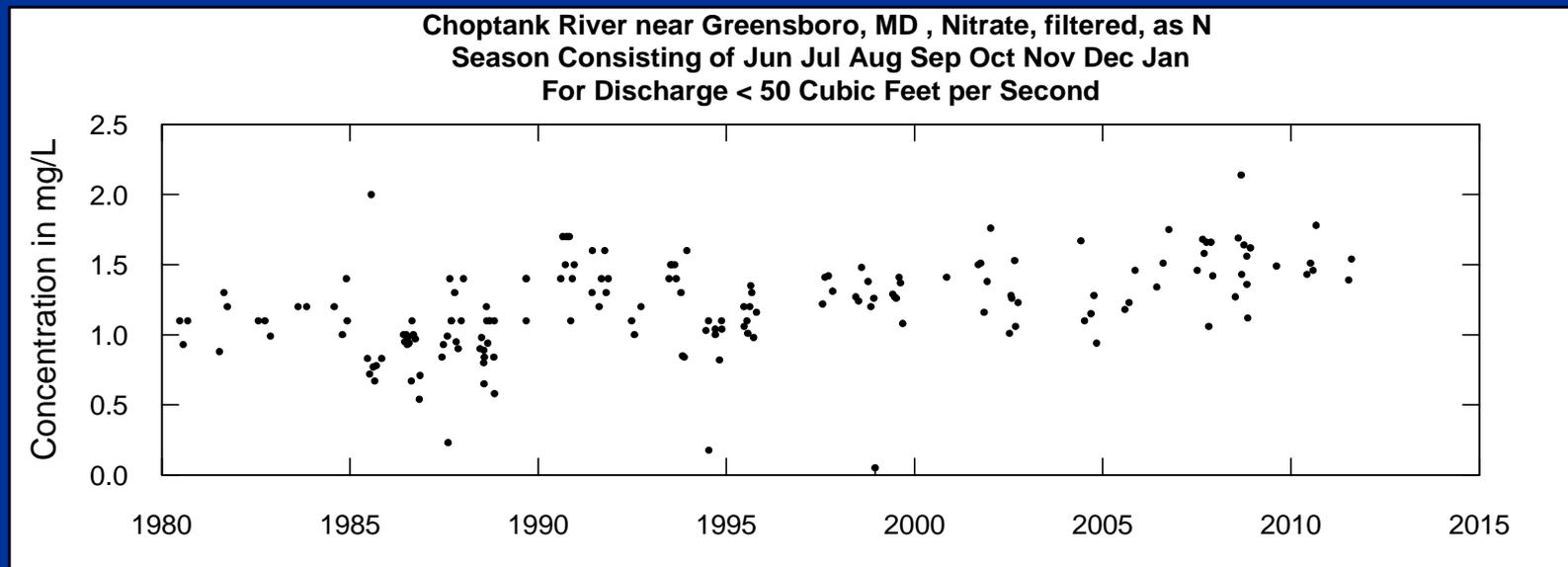
# How difficult is it to make those contour plots?

```
>plotContours(yearStart=1970, yearEnd=2005,
qBottom=2, qTop=200, qUnit=2,
contourLevels=seq(0,300,50))
```

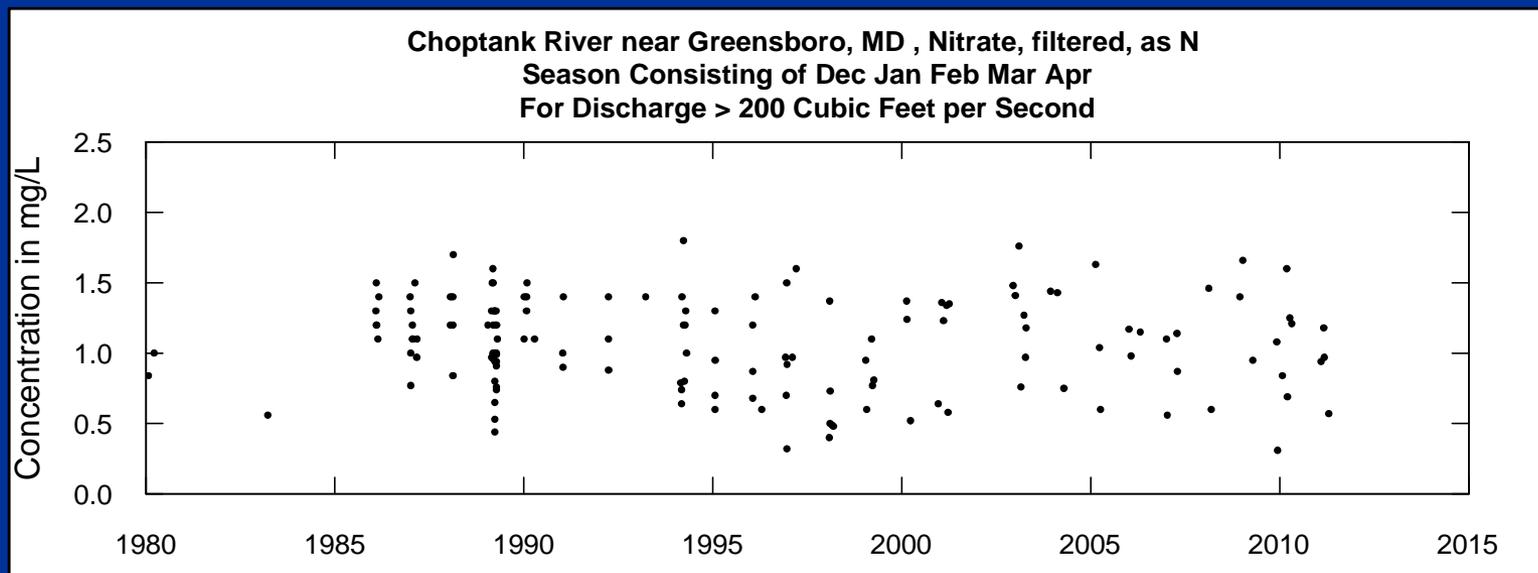
Milwaukee River at Milwaukee, WI Chloride  
Estimated Concentration Surface in Color



> plotConcTime(qUnit=1,qUpper=50,paLong=8,paStart=6,concMax=2.5)



> plotConcTime(qUnit=1,qLower=200,paLong=5,paStart=12,concMax=2.5)



**When all is said and done:**

**The only way to figure out what is happening to our planet is to measure it,**

**and this means tracking changes decade after decade**

**and poring over the records.**



# dataDelivery and EGRET

- Information and software available at: <https://github.com/USGS-R/EGRET/wiki>

