July 23, 2014

Phase 6 Watershed Model Prototype:

building sensitivities into the model …

Gopal Bhatt

[gopal.bhatt@psu.edu]

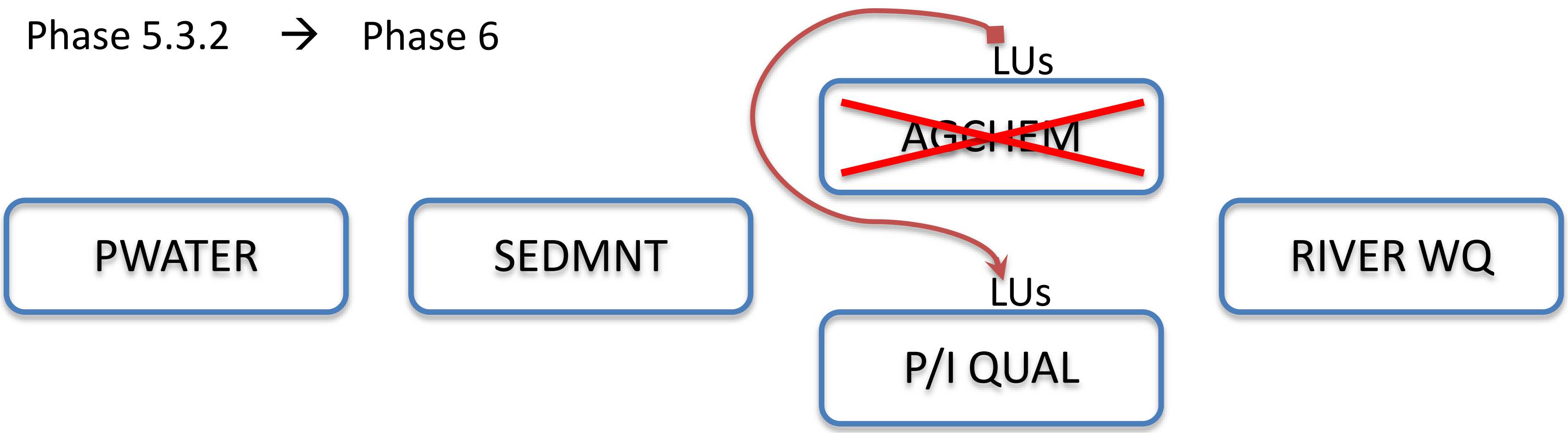
Outline …

- Brief Review of Phase-6 Prototype & Calibration
- Implementation of Sensitivities in the Model
  - Overview of sensitivity
  - HSPF PQUAL sub-model and challenges
  - Strategy to build in sensitivities & prototype
  - Limitations of the strategy
- Overview of an Alternative Approach
  - Refine PQUAL strategy using breakthrough curves

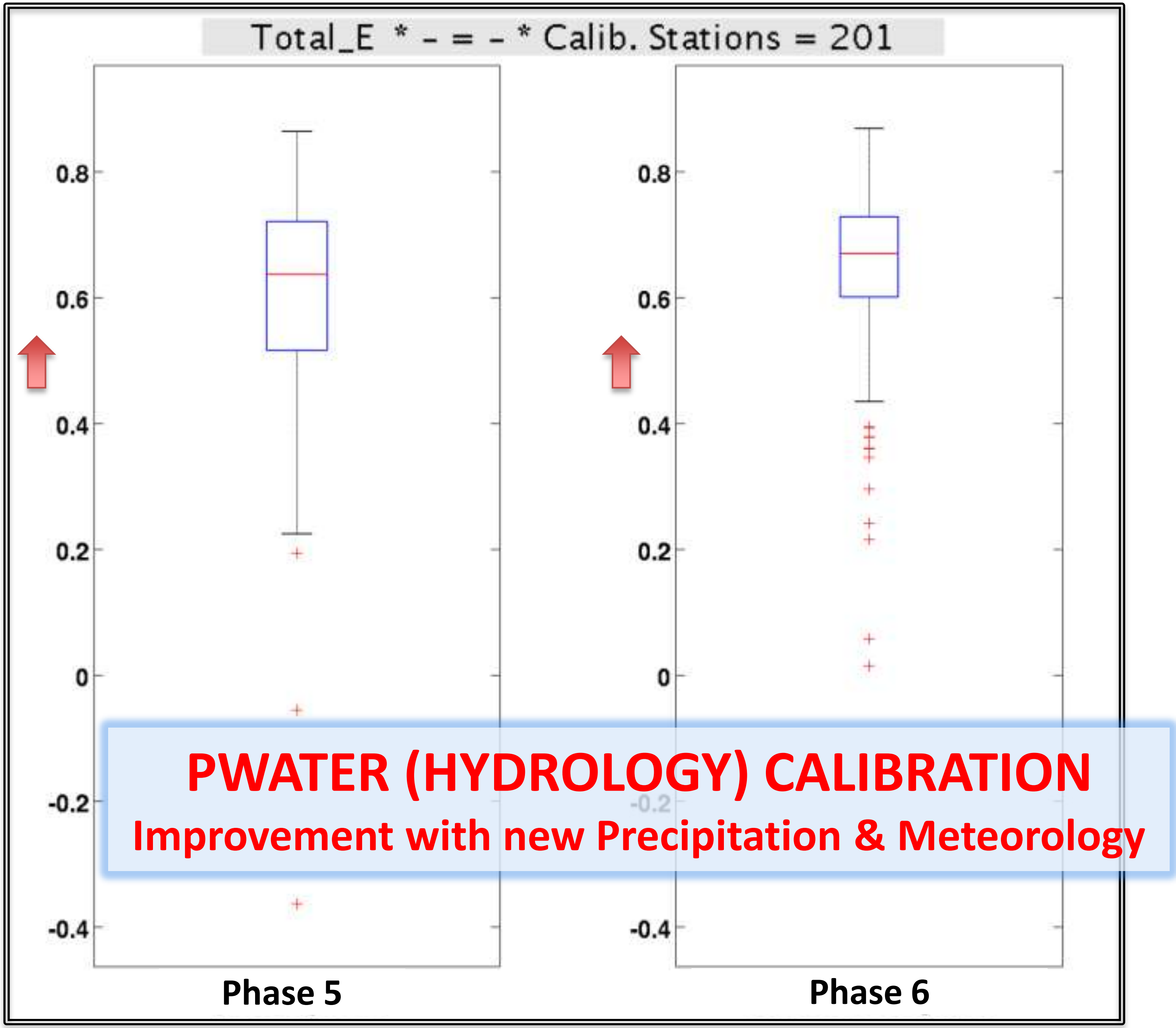
Brief Review of Phase-6 Prototype & Calibration

Phase 6 Watershed Model

Watershed Model Calibration:

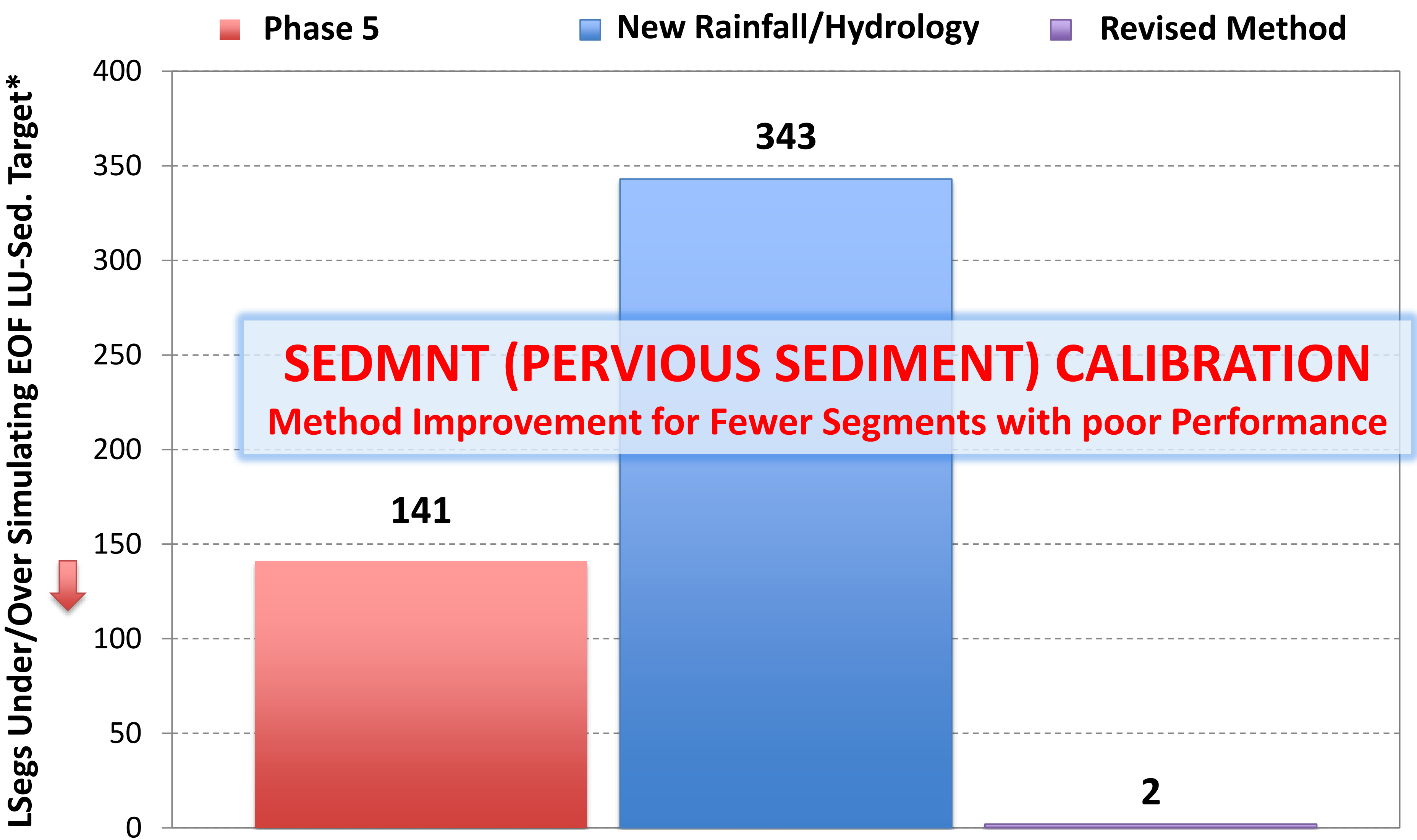


We are able to calibrate watershed model with this new setup with model performance indices as par compared to P532.



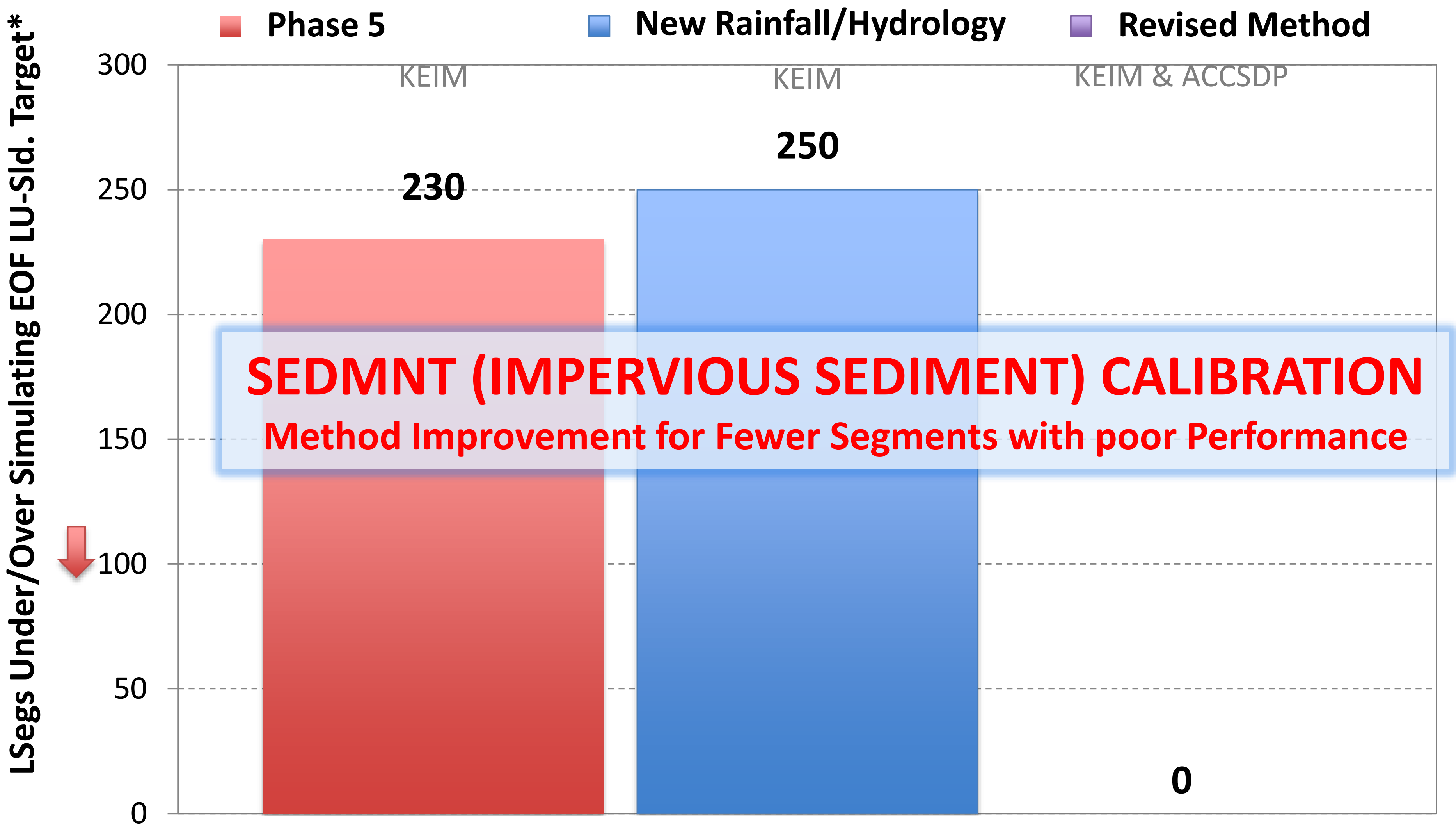
Total_E * - = - * Calib. Stations = 201
0.8
0.6
0.4
0.2
0
-0.2
-0.4
Phase 5
Phase 6
PWATER (HYDROLOGY) CALIBRATION
Improvement with new Precipitation & Meteorology

Improvement in Matching the a-priori *Targets**



*Total Number of Land Segments (367) x Number of **Pervious** Land Uses (25) = 9175

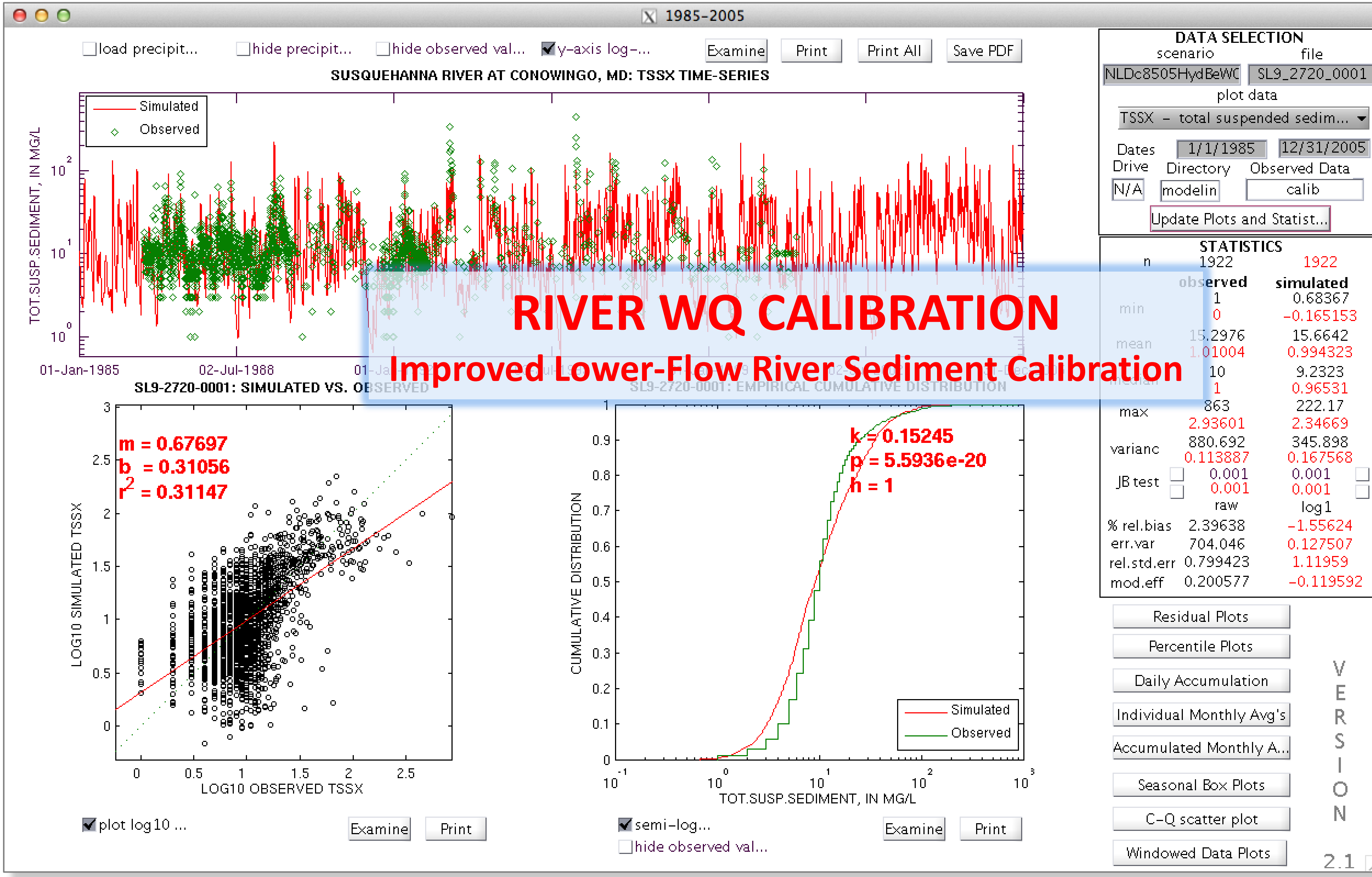
Improvement in Matching the a-priori *Targets**



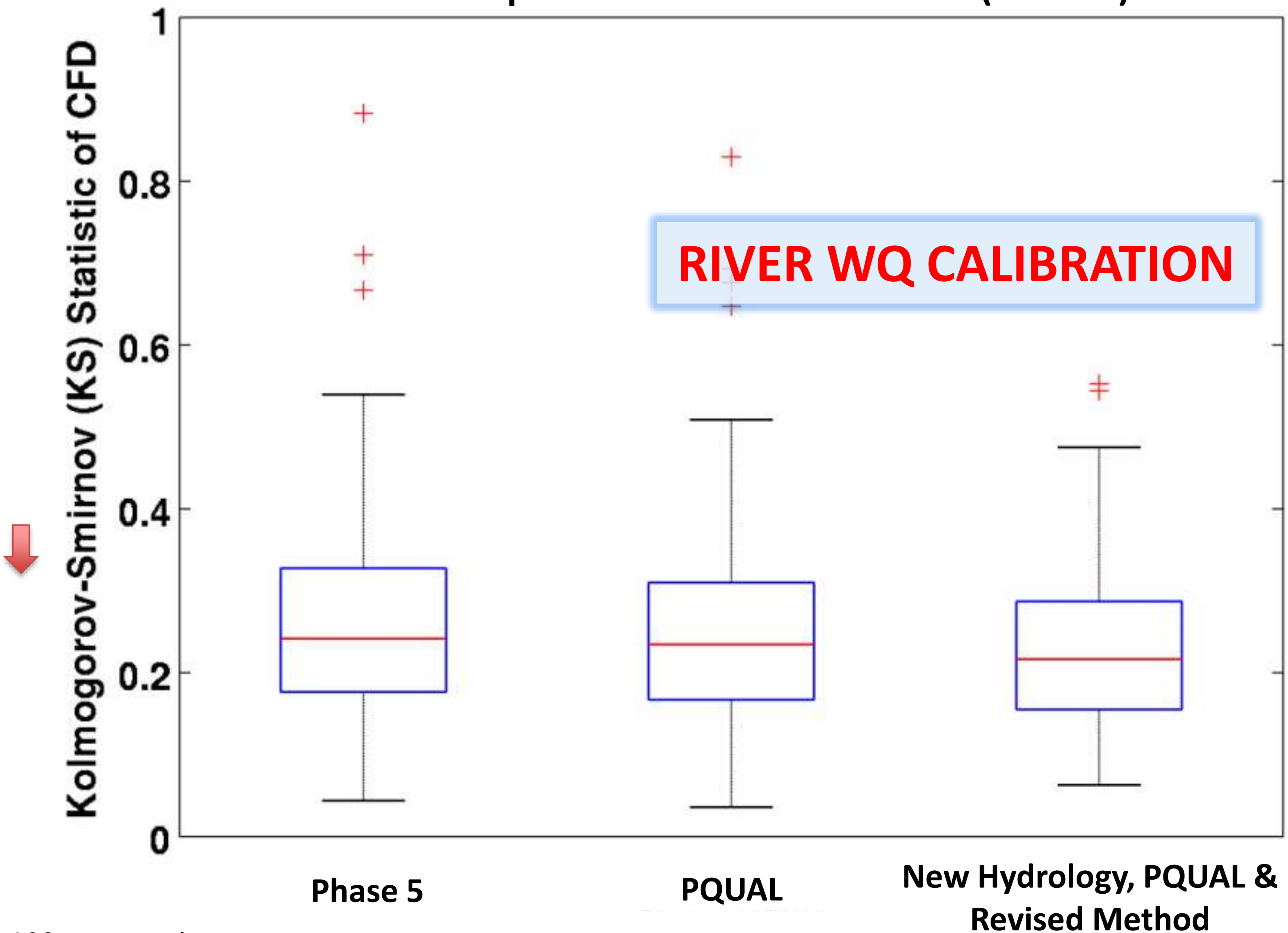
* Total Number of Land Segments (367) x Number of **Impervious** Land Uses (5) = 1835

Prototype Phase 6 – TSSX : : 1985 – 2005

Susquehanna River near Conowingo, MD

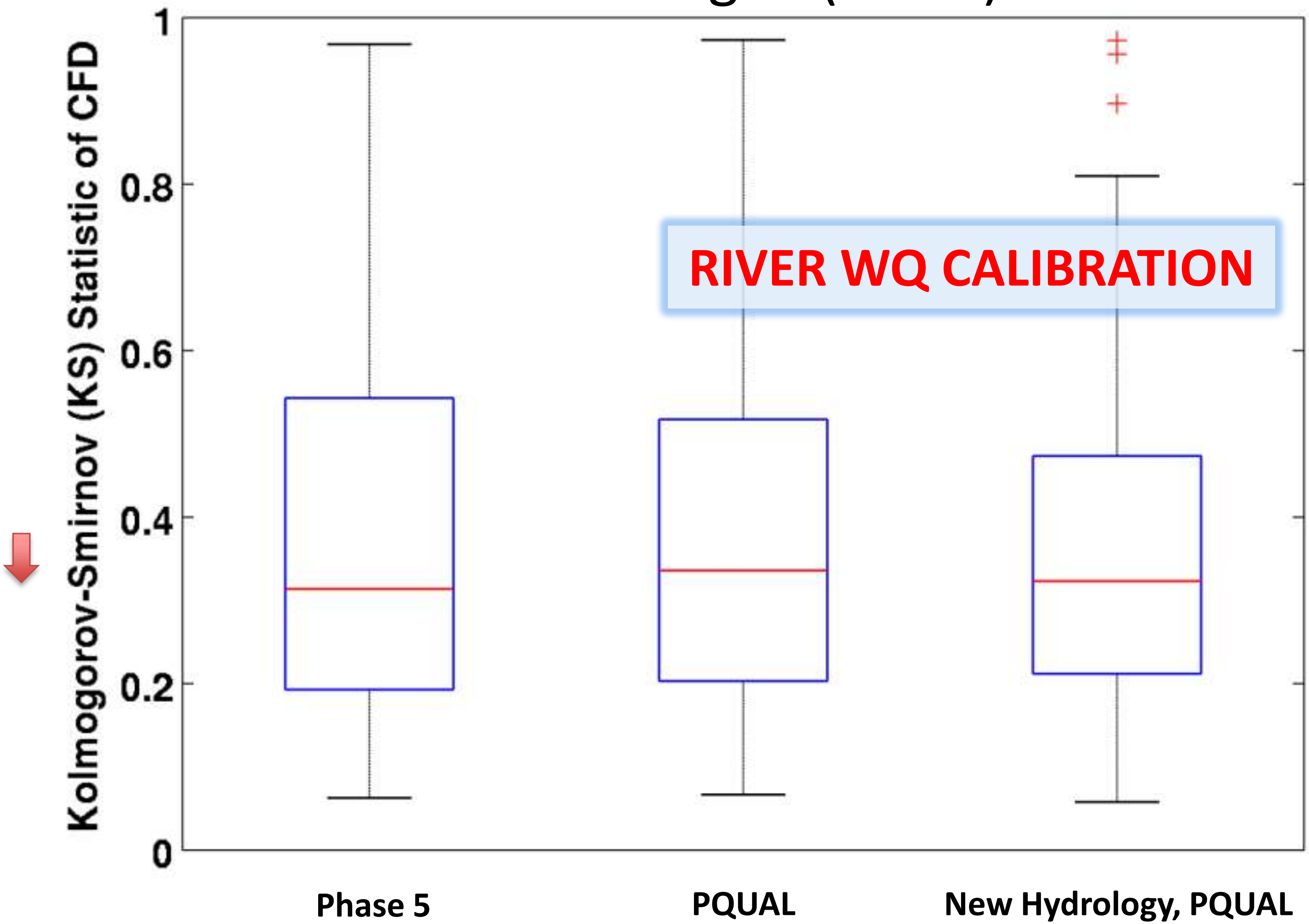


Total Suspended Sediment (TSSX)



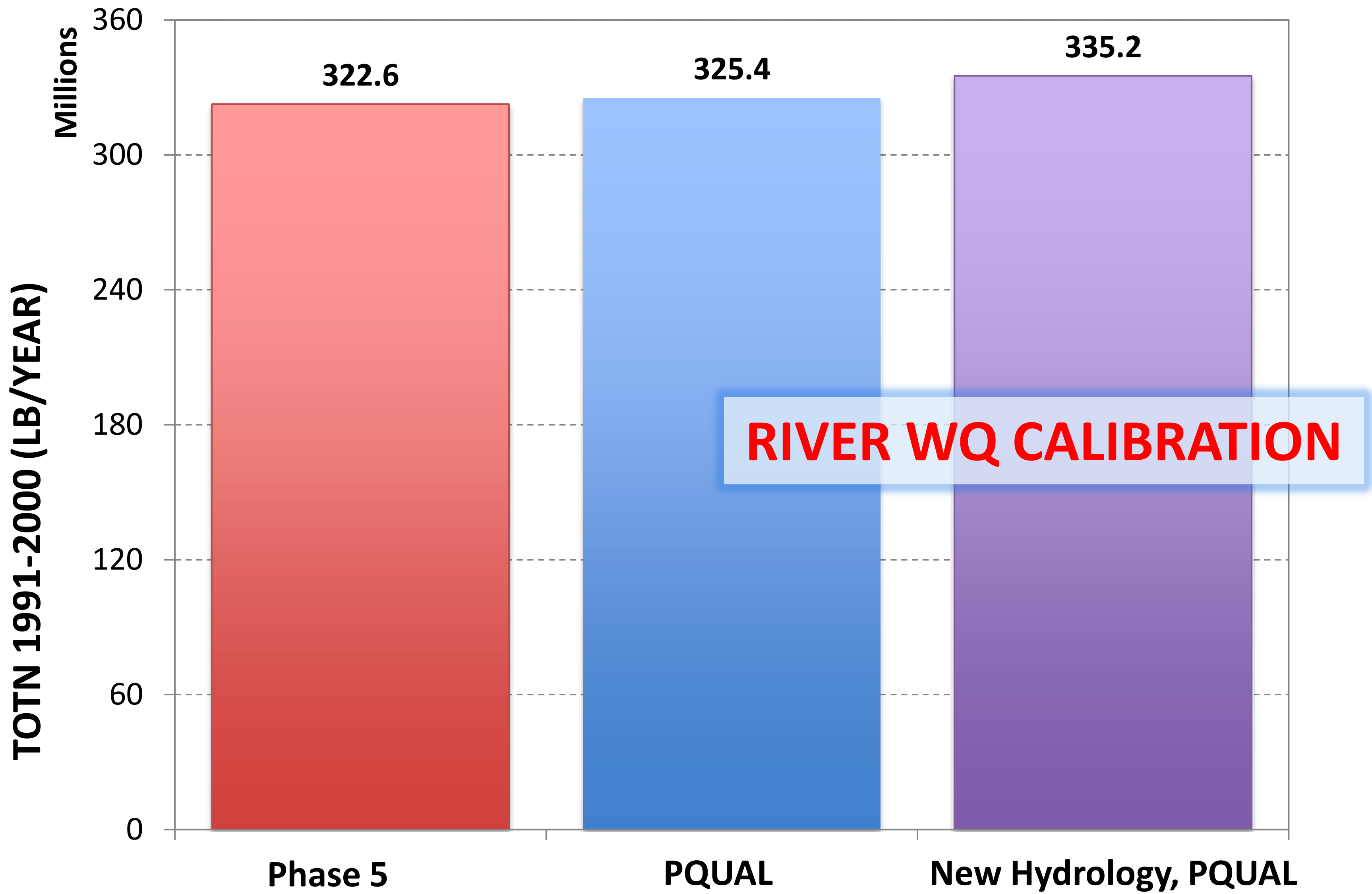
193 gage stations

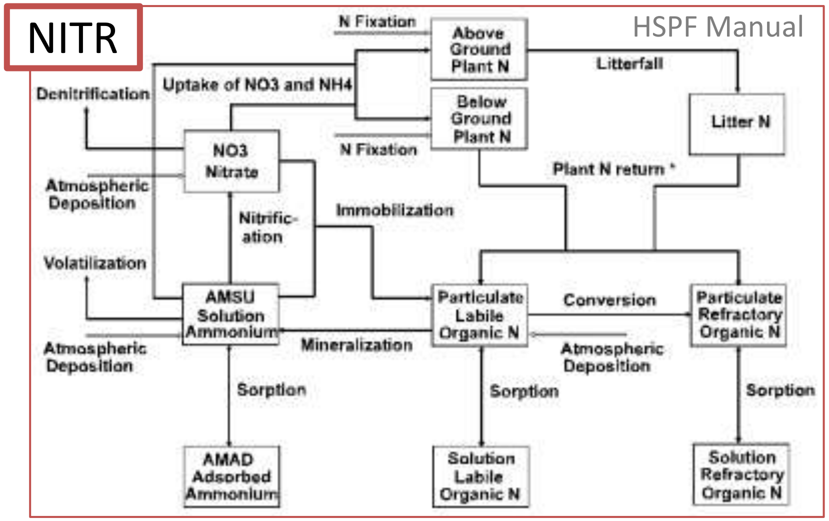
Total Nitrogen (TOTN)

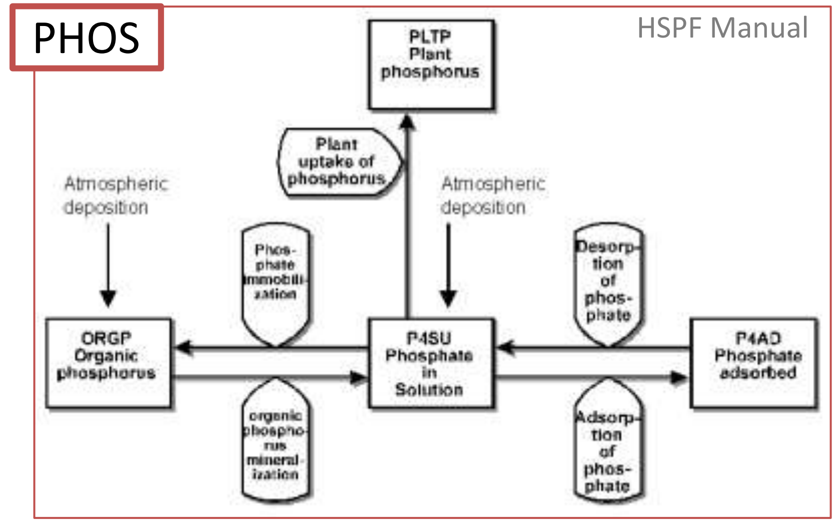


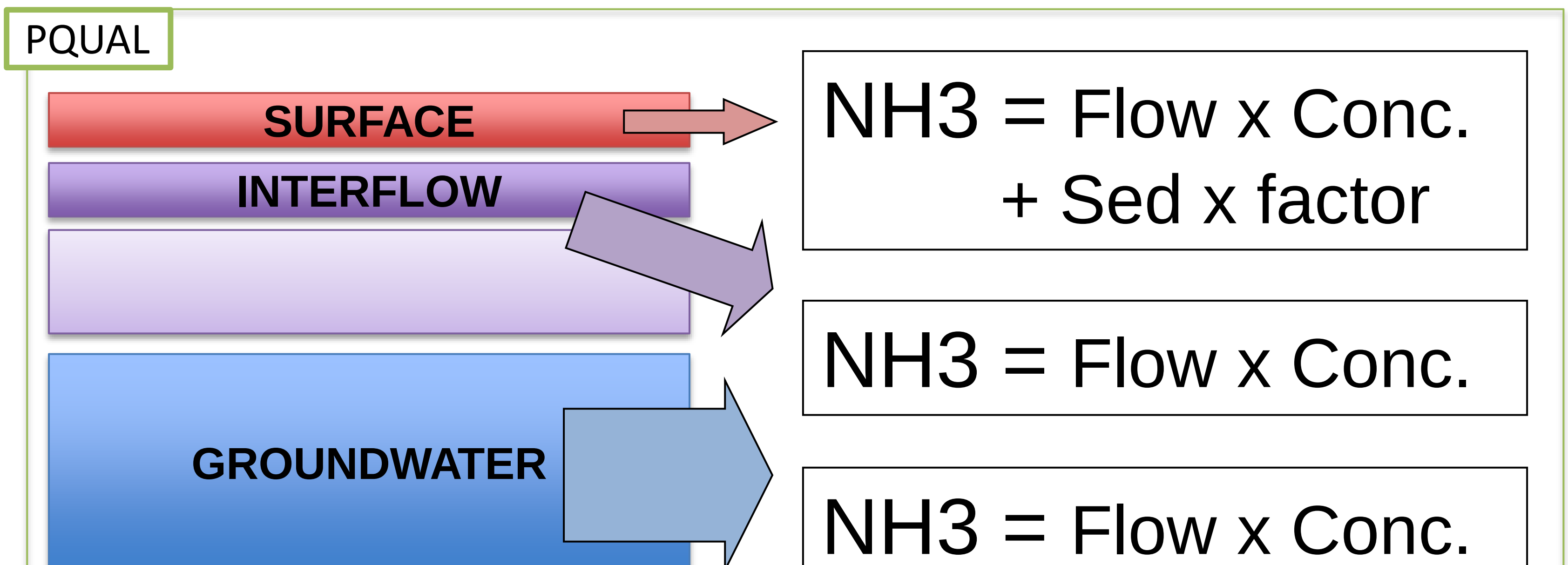
149 gage stations

Total Nitrogen Delivered to the Bay







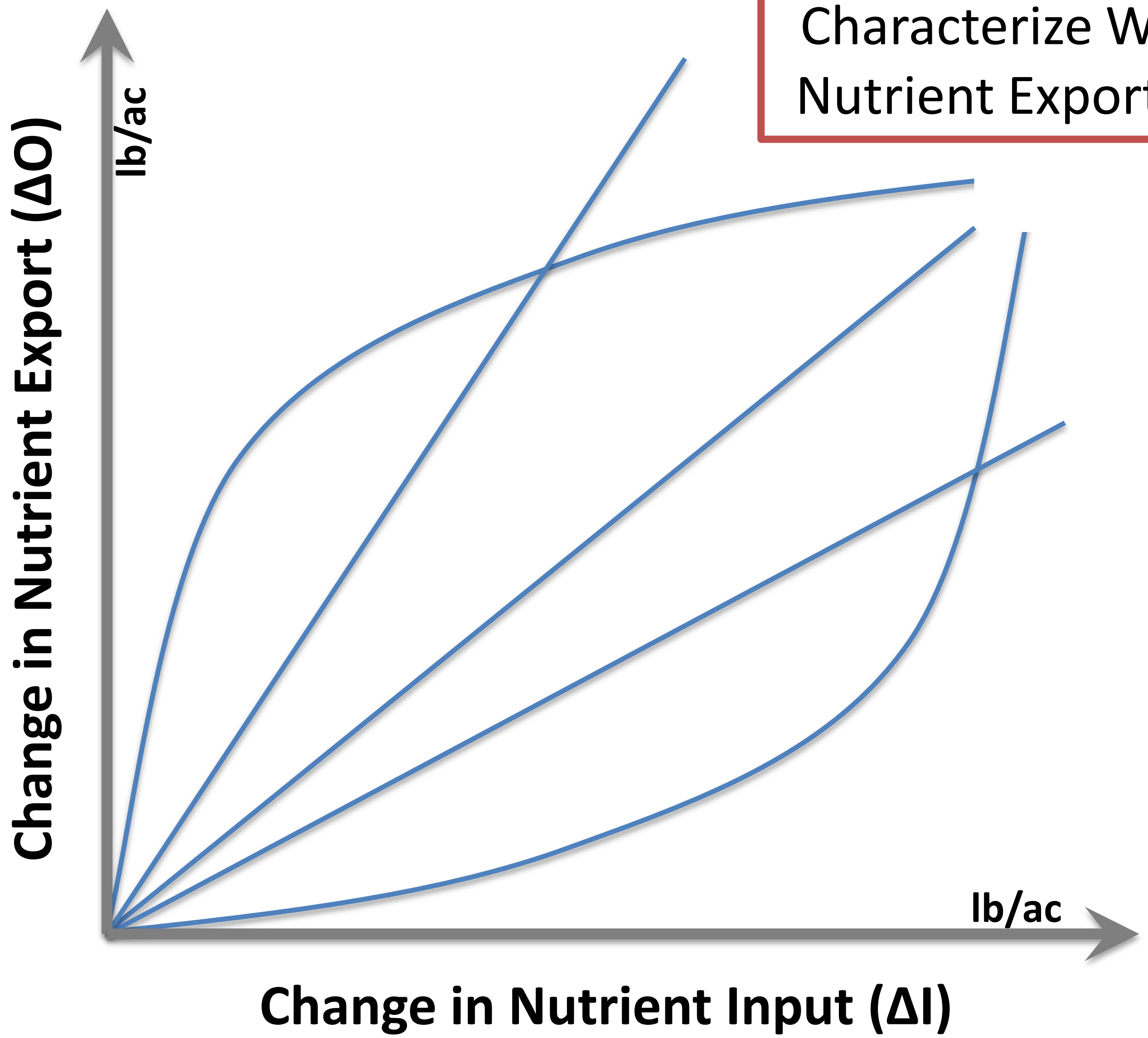


Adapted from Shenk, 2009

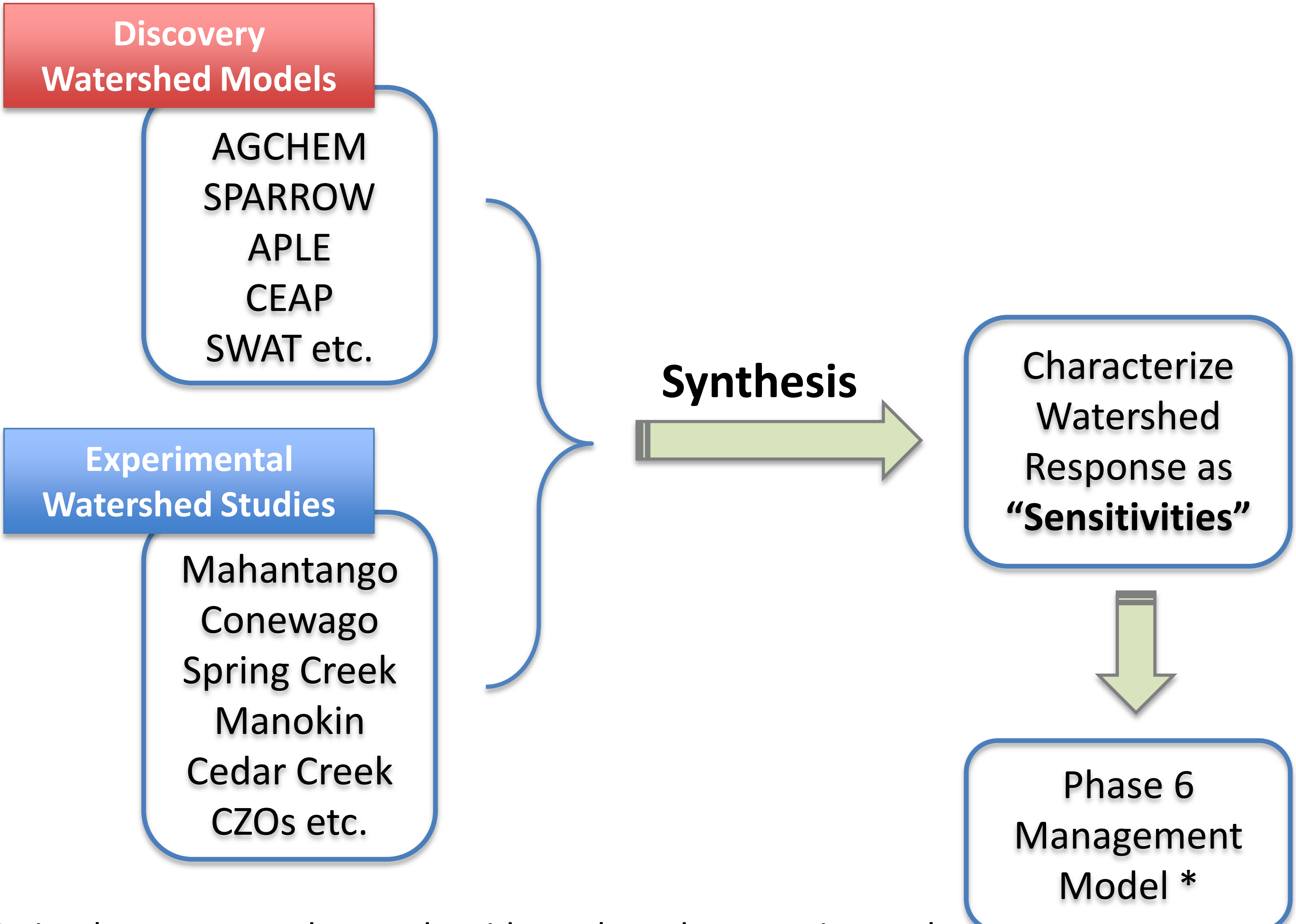
Implementation of Sensitivities in the Model

Watershed Model Nutrient Export "Sensitivity"

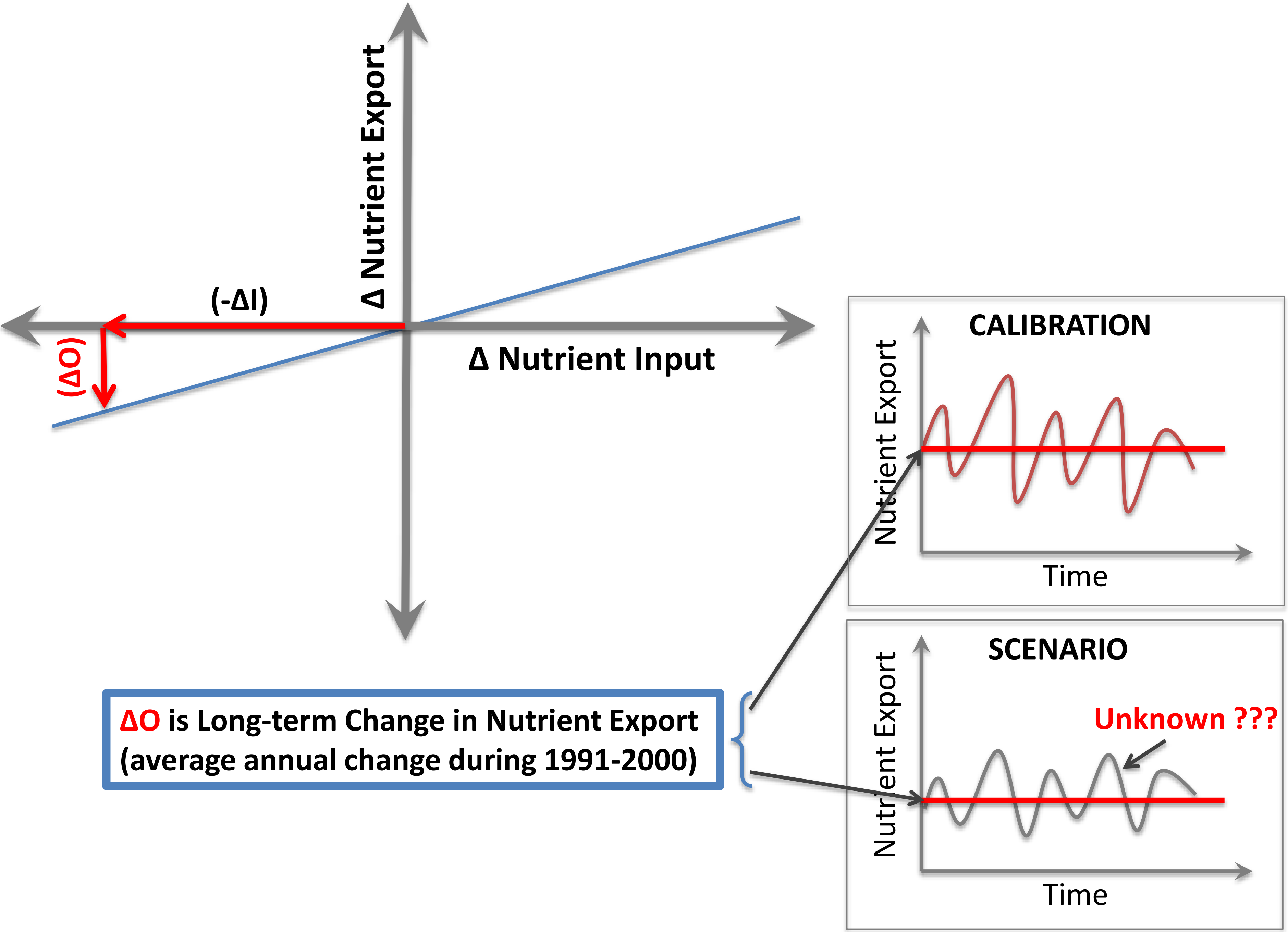
Characterize Watershed's Nutrient Export Response

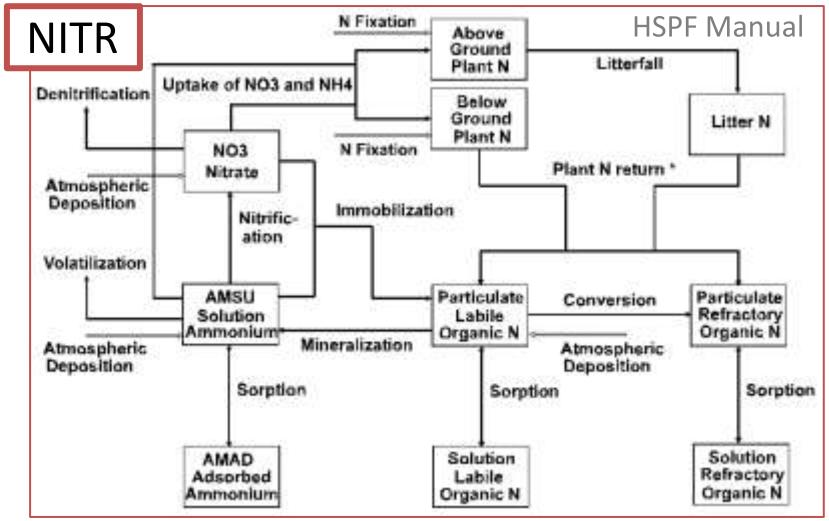


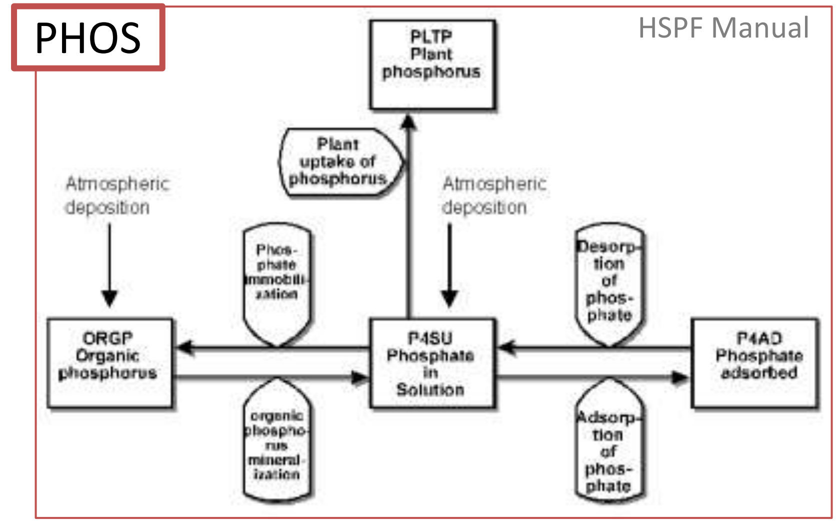
Watershed Model Nutrient Export Sensitivity

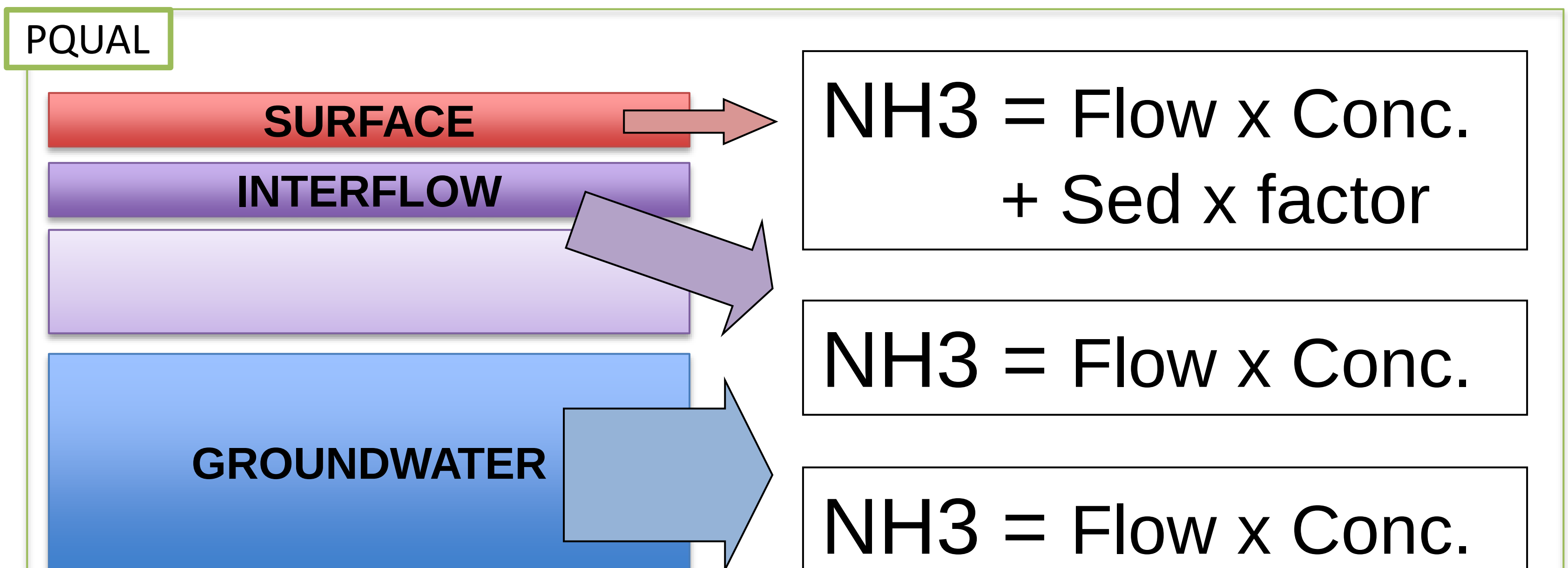


* A simple, easy to understand, evidence based accounting tool.


Δ Nutrient Export
(-ΔI)
(ΔO)
Δ Nutrient Input
CALIBRATION
Nutrient Export
Time
SCENARIO
Nutrient Export
Unknown ???
Time
ΔO is Long-term Change in Nutrient Export
(average annual change during 1991-2000)

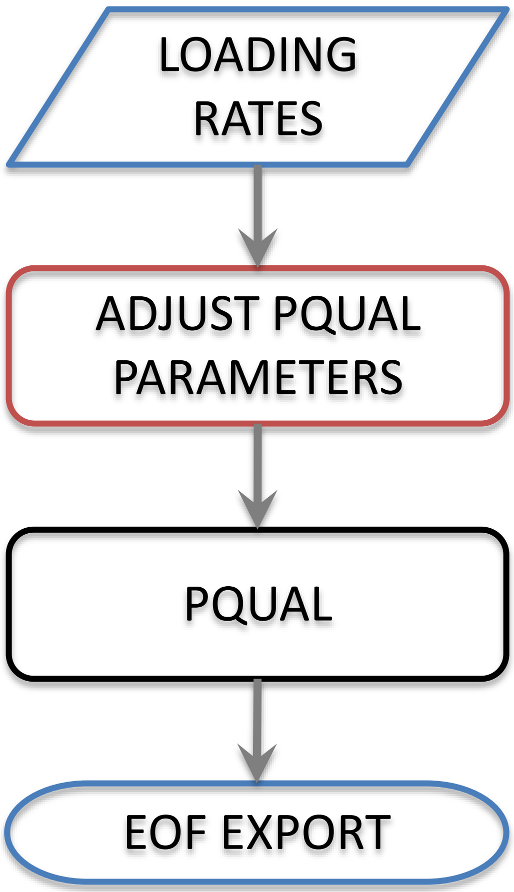






Adapted from Shenk, 2009

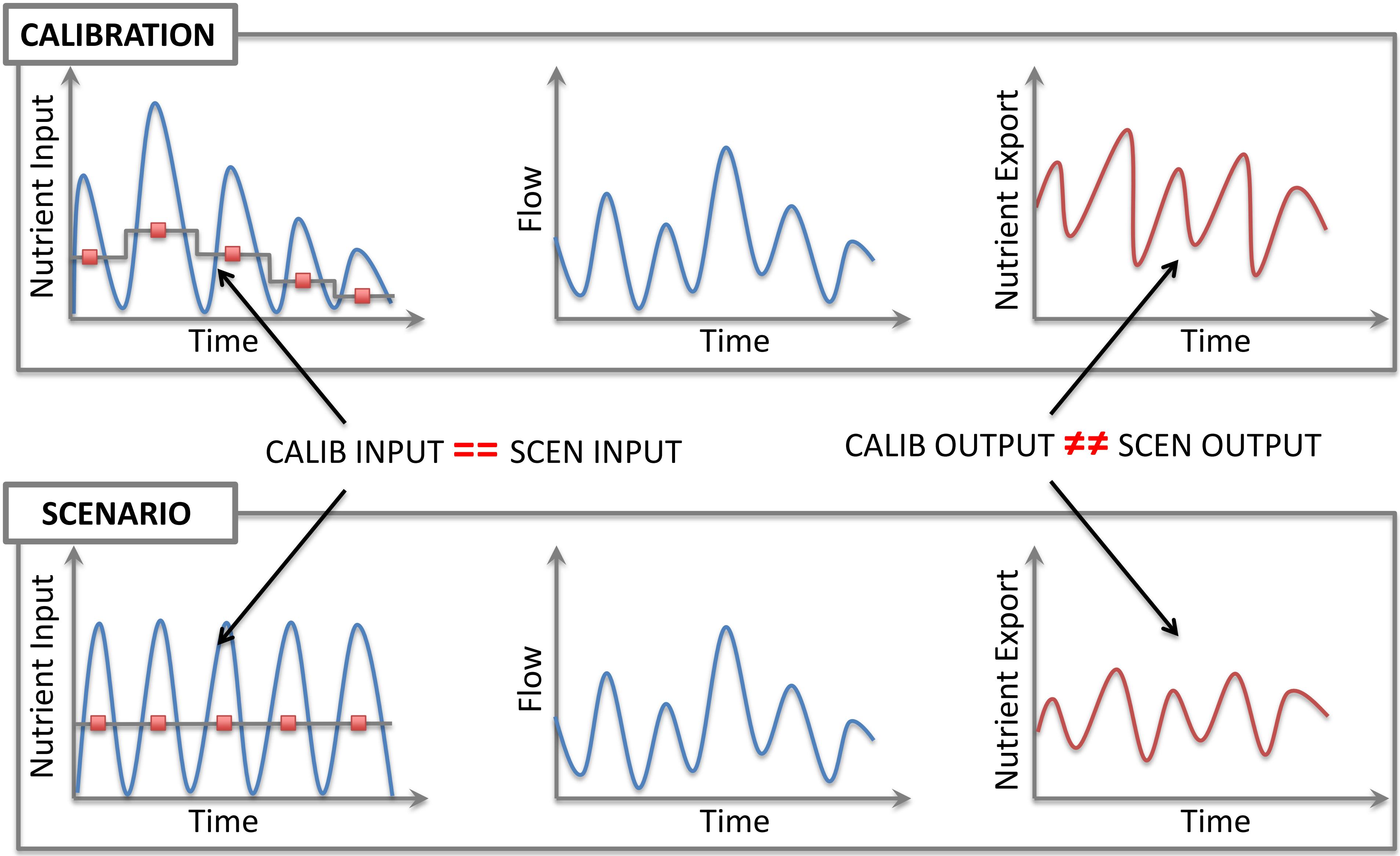
PQUAL Calibration



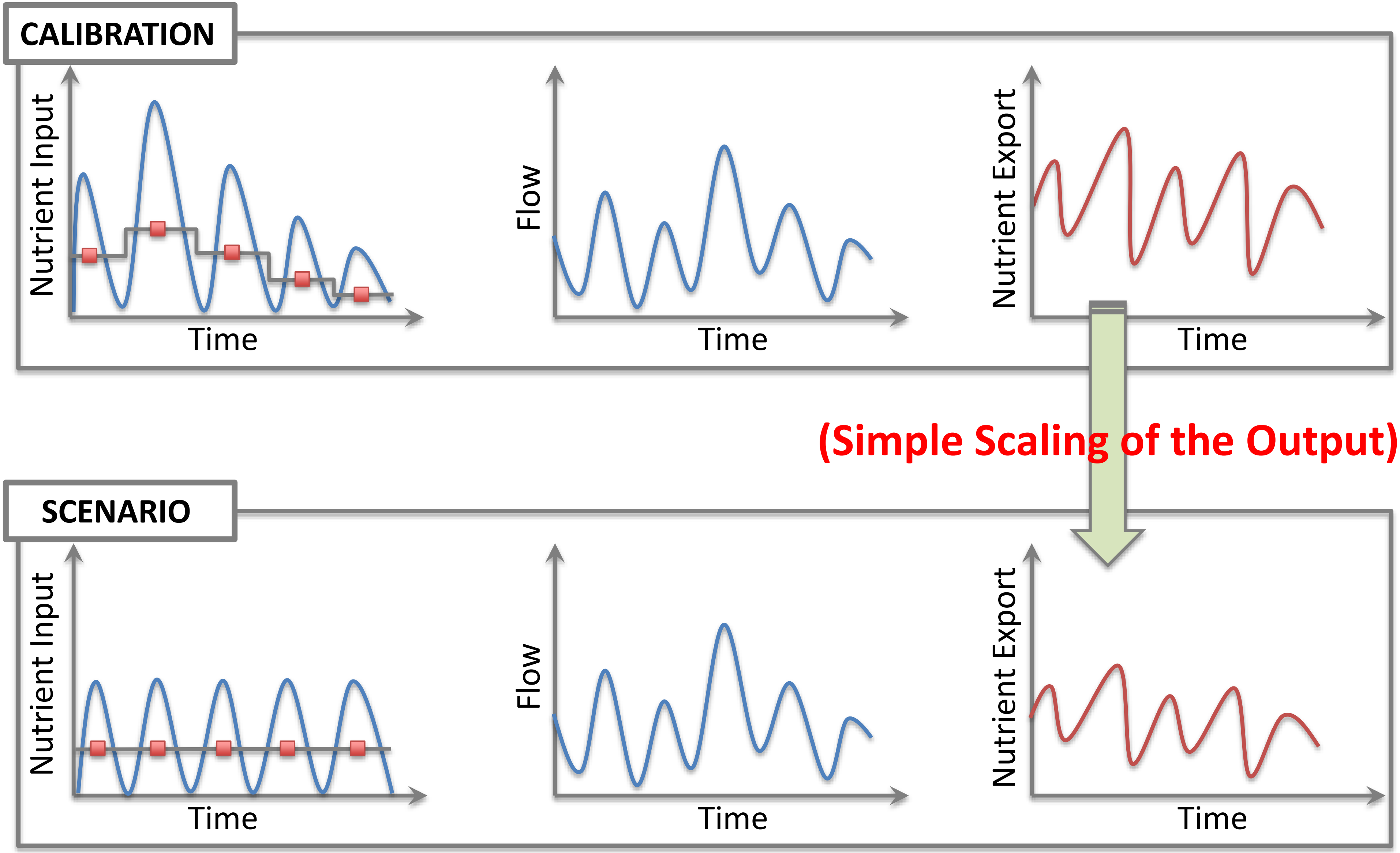
During calibration average PQUAL parameters are adjusted annually based on annual input loads.

This acts as a mechanism to translate inter annual variability in inputs (e.g. atmospheric deposition, fertilizer, manure) to model output (EOF Export).

Challenges: Complexity in creating a simple model…



Scenarios should be evaluated outside PQUAL for consistency!


CALIBRATION
Nutrient Input
Time
Flow
Time
Nutrient Export
Time
(Simple Scaling of the Output)
SCENARIO
Nutrient Input
Time
Flow
Time
Nutrient Export
Time

Phase 6 Watershed Model

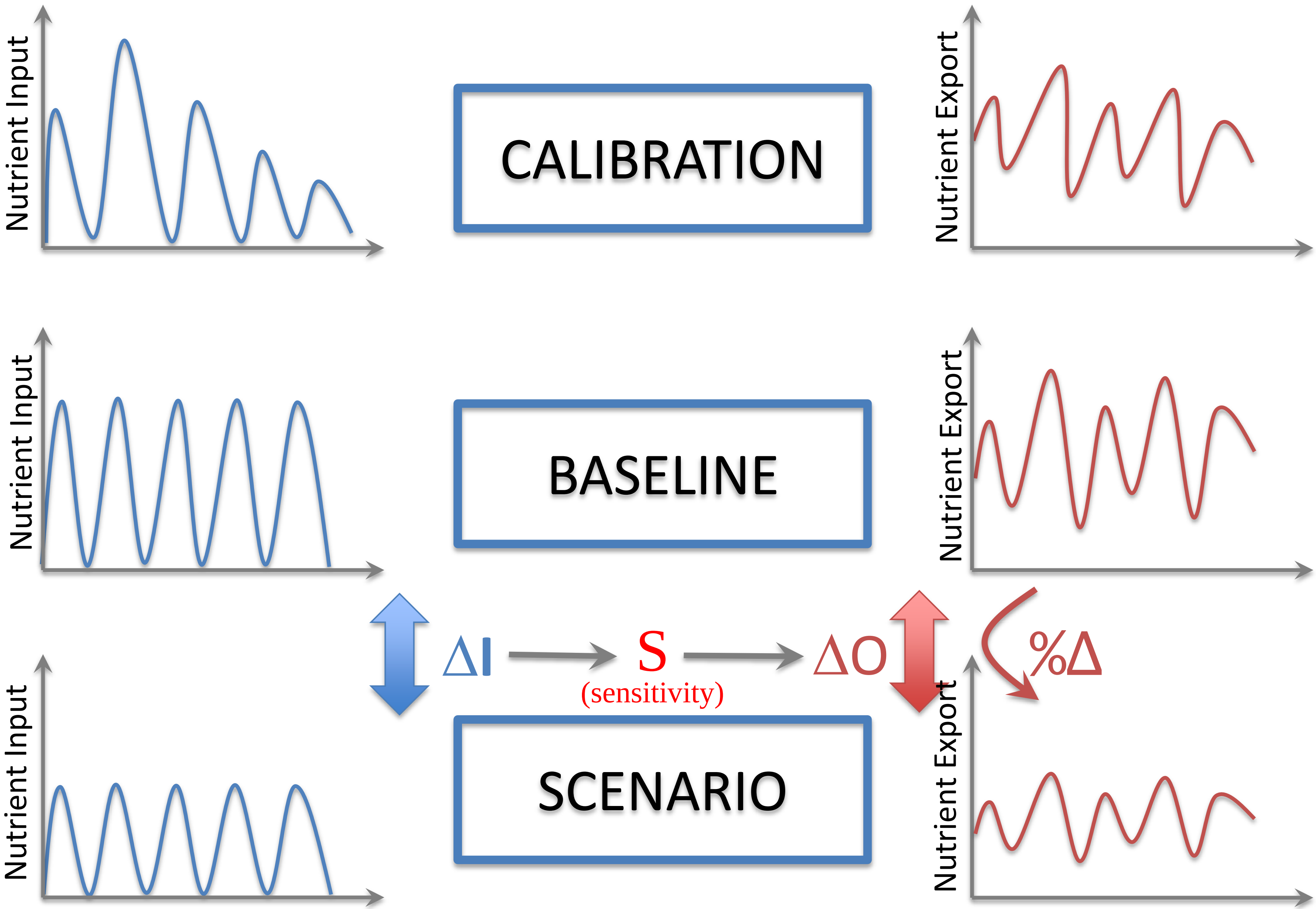
building sensitivities into the model

Strategy: For a given land use and land segment, adjust EOF nutrient export time-series based on changes in application rates and corresponding ***sensitivities***.

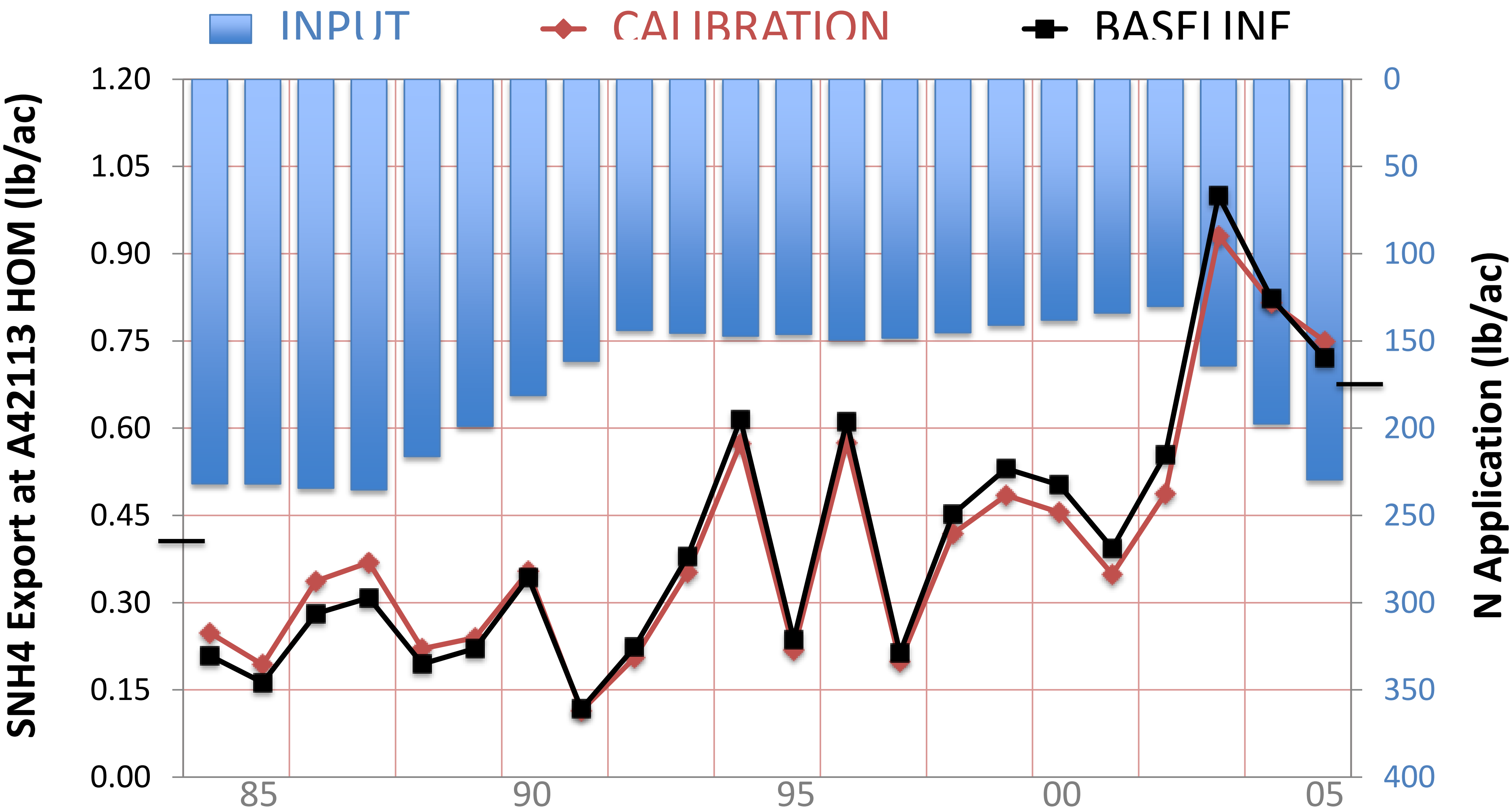
Step 1: Remove background loading signals from *calibration* EOF time-series to create *baseline*. Note, management scenarios have repeated annual application rates.

Step 2: Develop a tool to grab *sensitivities* to application sources; combine with *changes in nutrient inputs*; and apply changes in nutrient export to the *baseline*.

Sensitivity: Conceptual Details

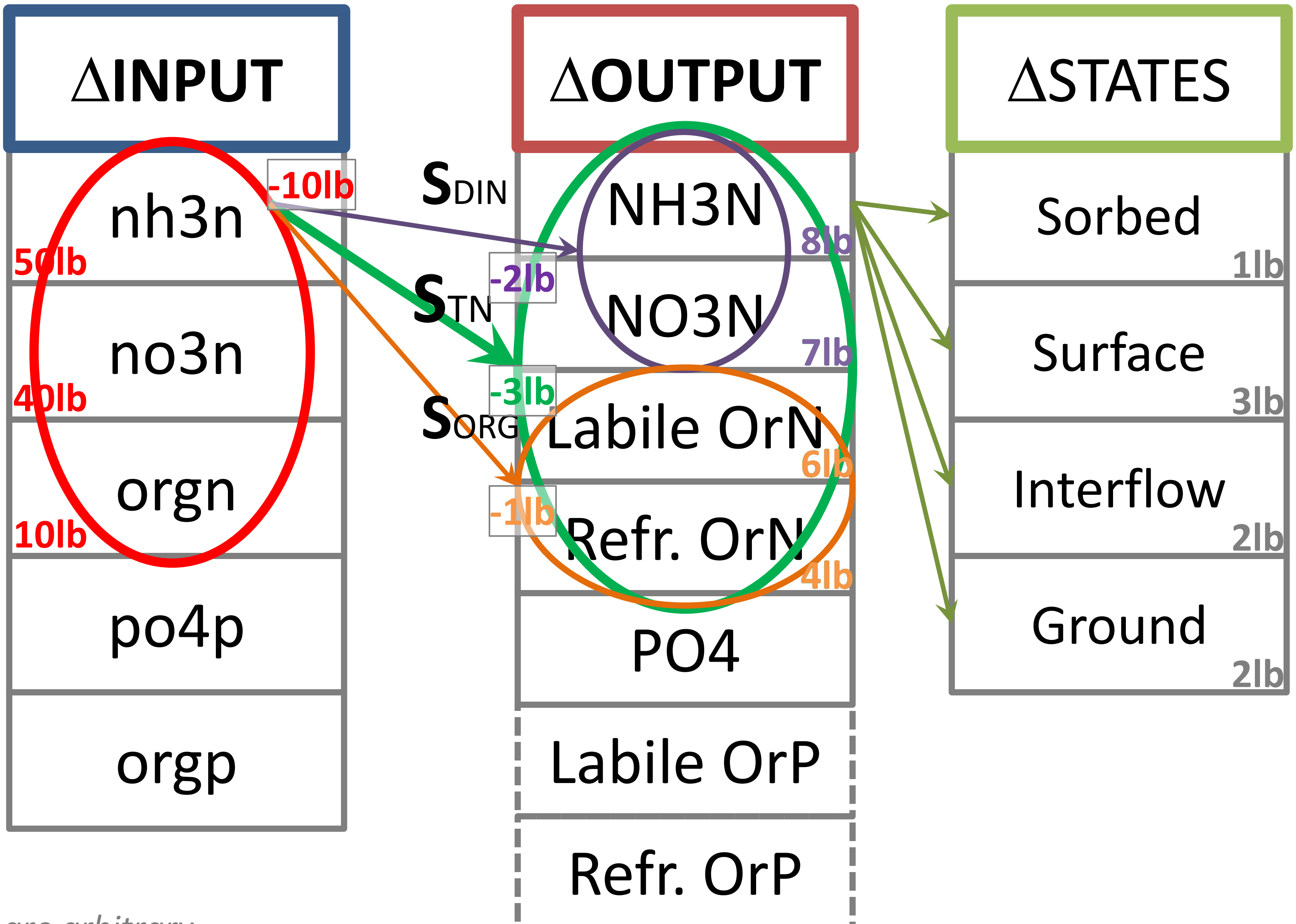


Steps 1: EOF SNH3 Export – *Calibration* vs. *Baseline*



* Here, flow is driving inter-annual differences in baseline export.
* The differences in annual loads between the two scenario are due to adjustments to the PQUAL parameters.

Step 2: Apply Sensitivities to *Baseline*



loads are arbitrary

Generalized Sensitivity Formulation

$$SENSITIVITY = S_{SRC,CON}$$

$$where,$$

$$SRC : SOURCE\left(AtDep, Manure, Fertilizer, Legume, Uptake, ...\right)$$

$$CON : CONSTITUENTS\left(NH3, NO3, LON, RON, PO4, LOP, ROP\right)$$

$$OUT_{CON}^{SCEN} - OUT_{CON}^{CALIB} = \sum_{J}^{SRC} f\left(S_{J,CON}, IN_{J,CON}^{SCEN}, IN_{J,CON}^{CALIB}, OUT_{CON}^{CALIB}, Others\right)$$

A Subroutine for Simple Sensitivity *

$$OUT_{CON}^{SCEN} - OUT_{CON}^{CALIB} = \sum_{J}^{SRC} \left[S_{J,CON} \times \left(IN_{J,CON}^{SCEN} - IN_{J,CON}^{CALIB} \right) \right]$$

SENSITIVITES

ATDEP	lsegmt	NO3	NH3	LON	RON	PO4	mNH3	mNO3	mLON	mRON	mPO4
	A10001	1x0.43	1x0.43	2x0.012	2x0.012	3x0.1	D1	D1	D1	D1	D1
FERTILIZER	lsegmt	NO3	NH3	LON	RON	PO4	mNH3	mNO3	mLON	mRON	mPO4
	A10001	1x0.23	1x0.23	2x0.005	2x0.005	3x0.1	D1	D1	D1	D1	D1
LEGUME	lsegmt	NO3	NH3	LON	RON	PO4	mNH3	mNO3	mLON	mRON	mPO4
	A10001	1x0.41	1x0.41	2x0.009	2x0.009	3x0.1	D1	D1	D1	D1	D1
UPTAKE	lsegmt	NO3	NH3	LON	RON	PO4	mNH3	mNO3	mLON	mRON	mPO4
	A10001	1x-0.05	1x-0.05	2x0.006	2x0.006	3x0.1	D1	D1	D1	D1	D1

∆INPUT (SCENARIO – CALIBRATION)

apptyp	no3n	nh3n	orgn	po4p	orgp
atdep	-2.16E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
coverc	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
plow	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
fert	-3.27E+01	-9.82E+01	0.00E+00	1.23E+00	0.00E+00
manure	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
legume	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
uptake	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
muptak	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
reforg	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

HAND CALCULATION		TOTAL_N	TOTAL_P
	ATDEP	-9.55E-01	0.00E+00
	FERTILIZER	-3.08E+01	1.23E-01
	TOTAL	**-31.72**	**0.12**

TOTAL N	**-31.72**
TOTAL P	**0.12**

OUTPUT

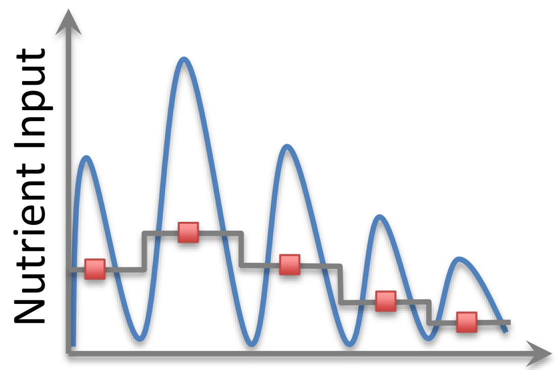
qual1	state1	out_calib	2.87E+00	delta_out	-2.46E-01	pcent_delta	-0.0855
qual1	state2	out_calib	1.93E+00	delta_out	-1.65E-01	pcent_delta	-0.0855
qual1	state3	out_calib	1.19E+01	delta_out	-1.02E+00	pcent_delta	-0.0855
qual1	state4	out_calib	1.19E+01	delta_out	-1.02E+00	pcent_delta	-0.0855
qual2	state2	out_calib	6.42E+00	delta_out	-5.49E-01	pcent_delta	-0.0855
qual2	state3	out_calib	7.87E+01	delta_out	-6.73E+00	pcent_delta	-0.0855
qual2	state4	out_calib	2.49E+02	delta_out	-2.13E+01	pcent_delta	-0.0855
qual3	state1	out_calib	6.26E-01	delta_out	-5.95E-03	pcent_delta	-0.0095
qual3	state2	out_calib	2.06E-02	delta_out	-1.95E-04	pcent_delta	-0.0095
qual3	state3	out_calib	2.64E+00	delta_out	-2.50E-02	pcent_delta	-0.0095
qual3	state4	out_calib	3.25E+00	delta_out	-3.09E-02	pcent_delta	-0.0095
qual4	state1	out_calib	5.95E+00	delta_out	-5.65E-02	pcent_delta	-0.0095
qual4	state2	out_calib	1.95E+00	delta_out	-1.85E-02	pcent_delta	-0.0095
qual4	state3	out_calib	2.47E+01	delta_out	-2.35E-01	pcent_delta	-0.0095
qual4	state4	out_calib	3.25E+01	delta_out	-3.09E-01	pcent_delta	-0.0095
qual5	state1	out_calib	3.86E+00	delta_out	2.29E-02	pcent_delta	0.0059
qual5	state2	out_calib	7.99E-01	delta_out	4.74E-03	pcent_delta	0.0059
qual5	state3	out_calib	1.60E+01	delta_out	9.47E-02	pcent_delta	0.0059
qual5	state4	out_calib	2.01E-01	delta_out	1.19E-03	pcent_delta	0.0059

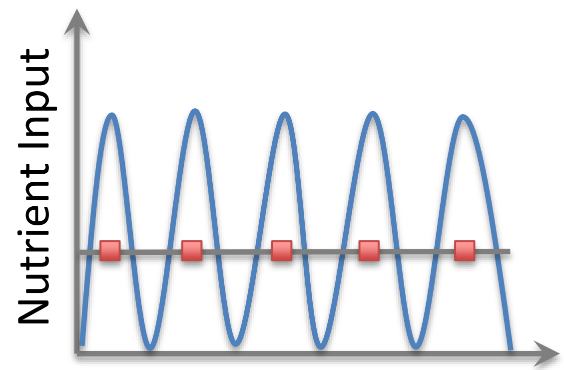
Conclusions: Sensitivity Prototype

- Calibration run was de-trended to create a baseline scenario to be used for running management scenarios.
- Sensitivity based accounting of nutrient export was implemented.
- Sensitivity algorithm was developed to offer maximum flexibility.
- Sensitivity code was verified.
- Code offers ability to incorporate appropriate sensitivity functions.

Limitations of the Framework …

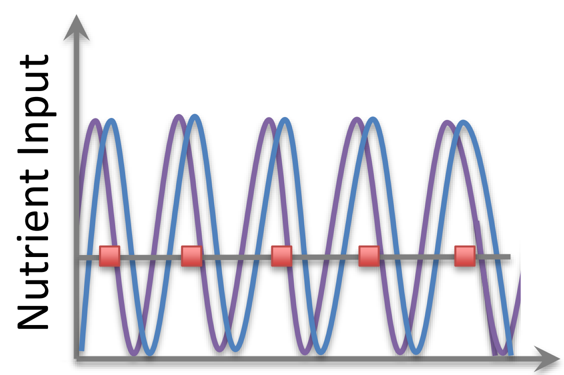
- Currently PQUAL calibration does not account for seasonality of input (+/-)





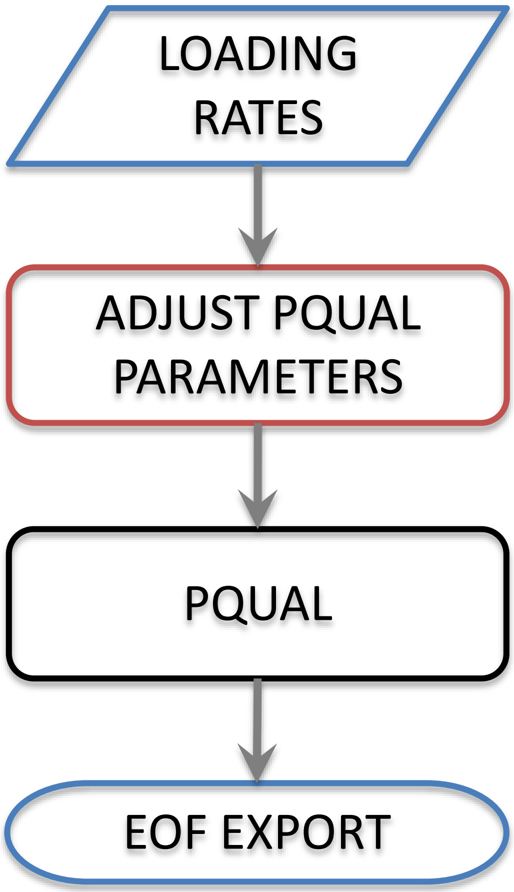
- Export estimated from 'sensitivities' using this method would <u>not</u> be able to account for changes in input pattern, if any.

E.g., Fertilizer application in April vs. June



Overview of an Alternative Approach

PQUAL Calibration

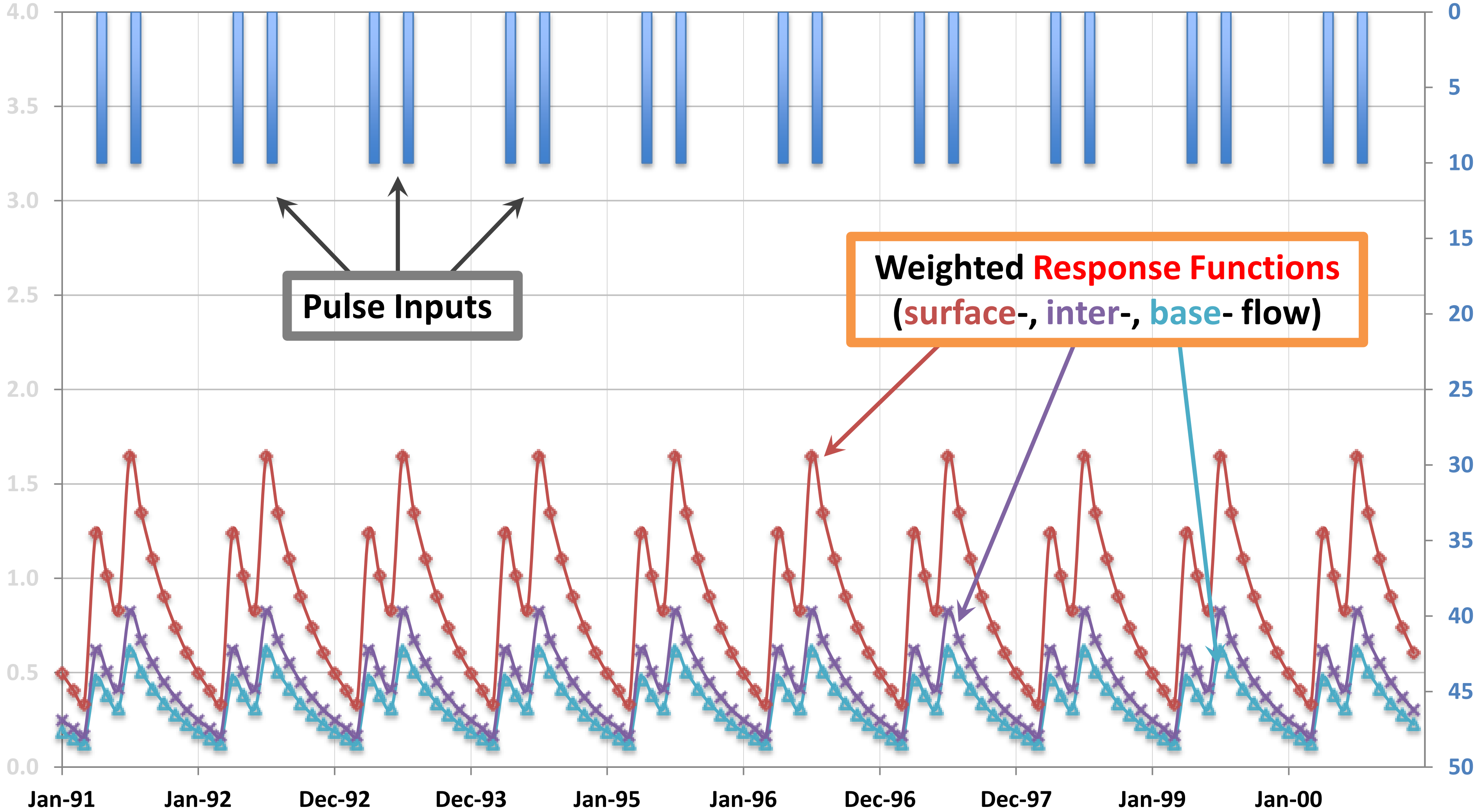


Currently PQUAL parameters are adjusted based on annual loads. Therefore simulated response do not see any intra-annual variability in input.

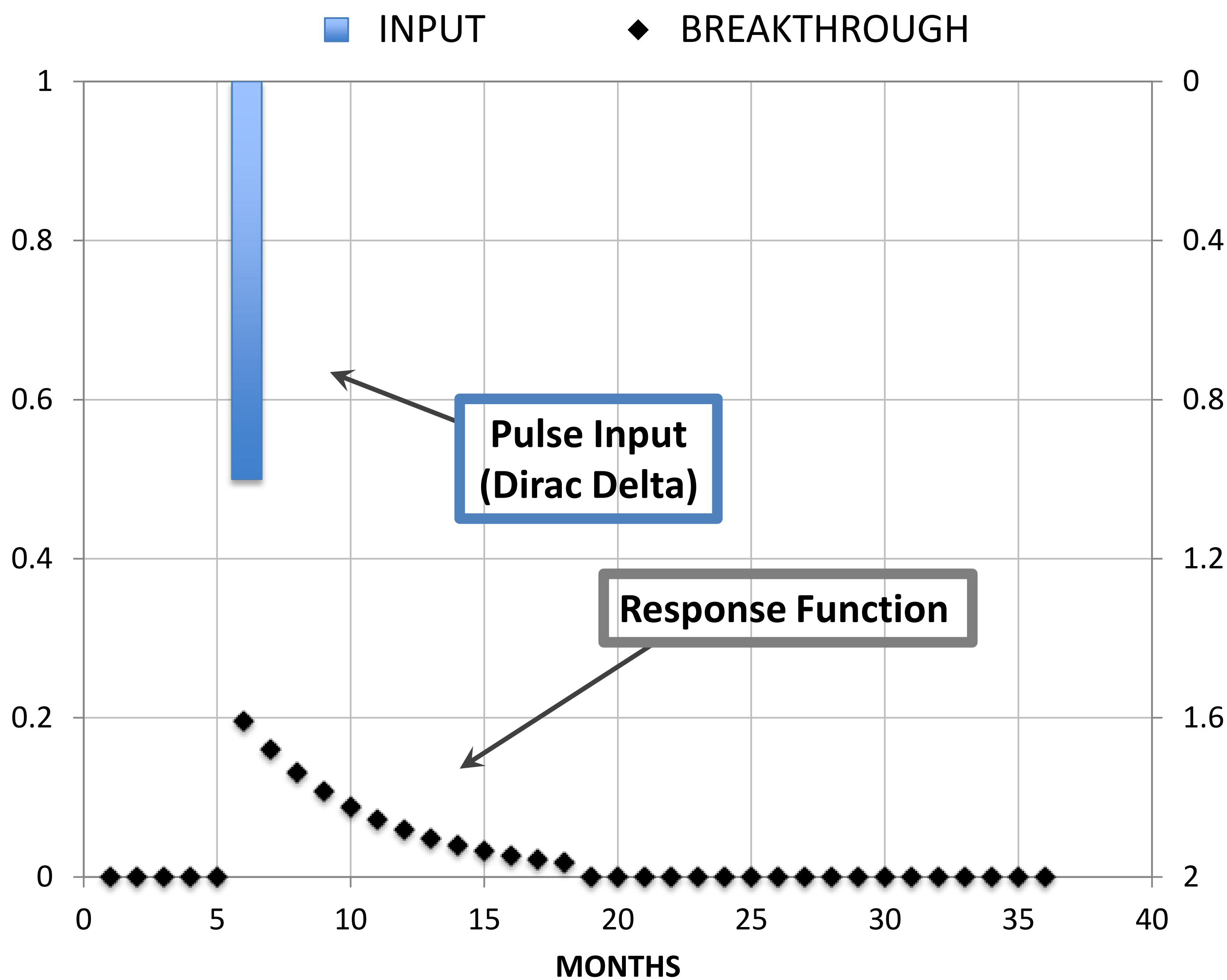
Shortening the time-scale (e.g., month) would help but we would not be able to account for memory of the system due to the lack of storage term.

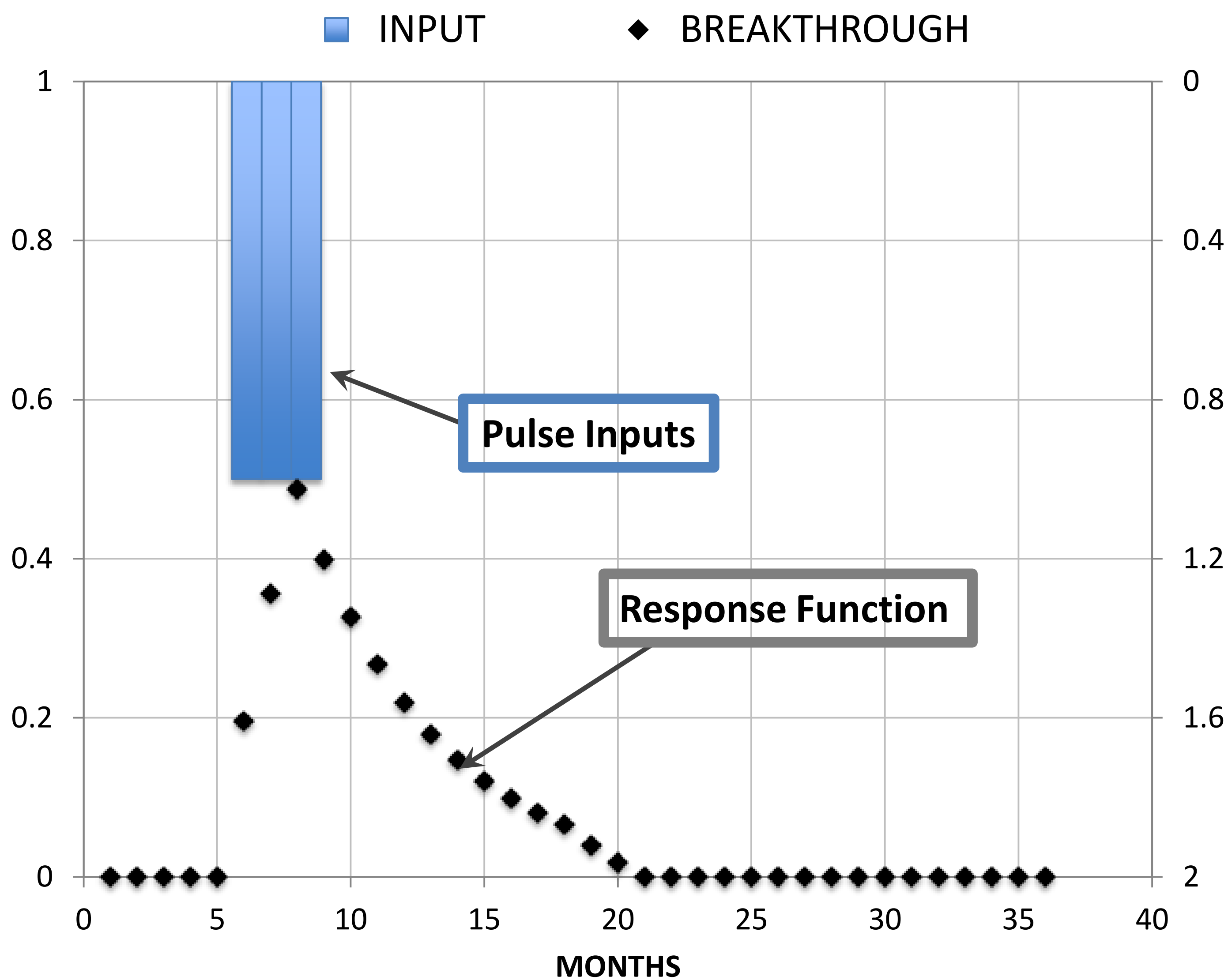
We need a new strategy!

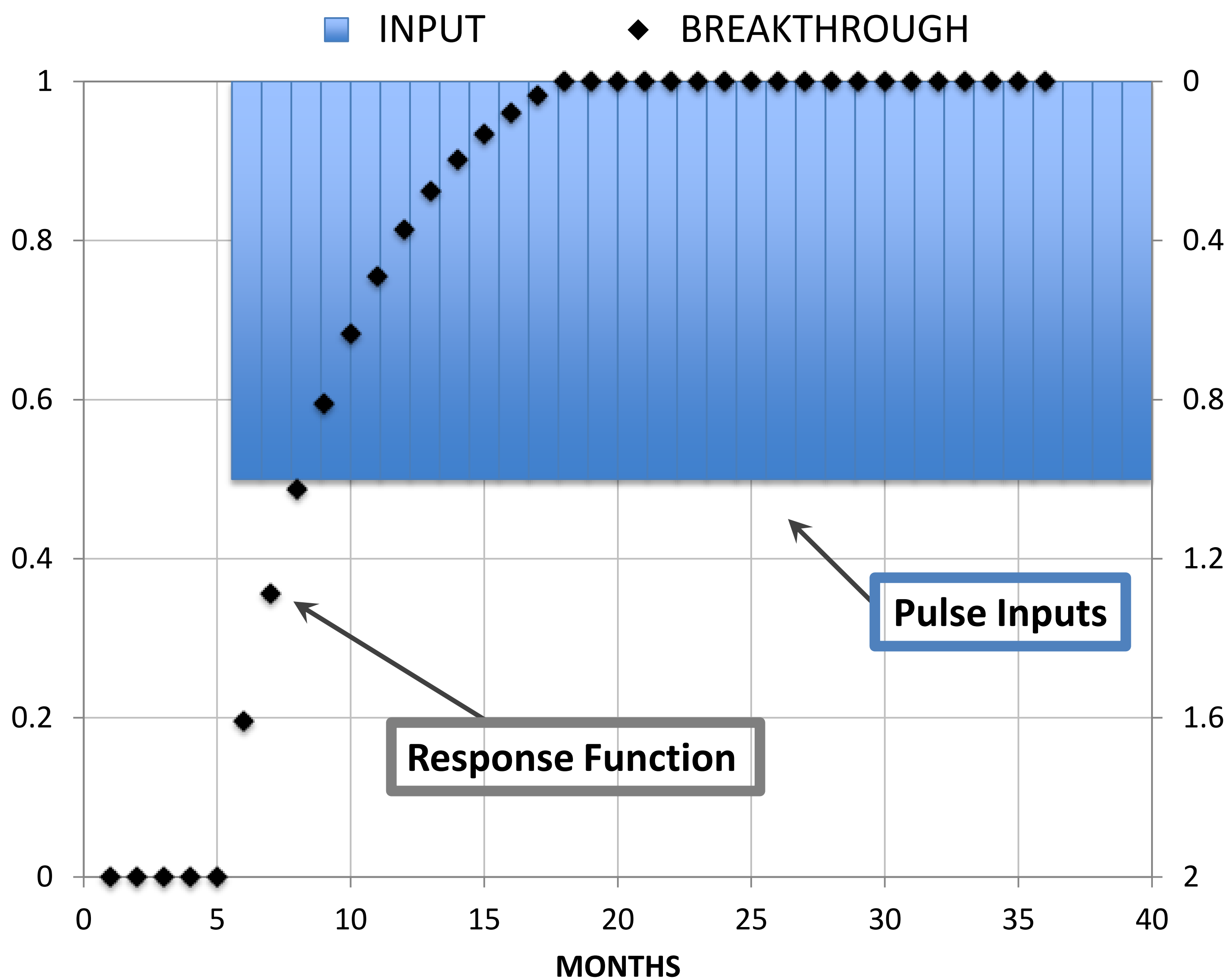
A Simple Spreadsheet based Example …

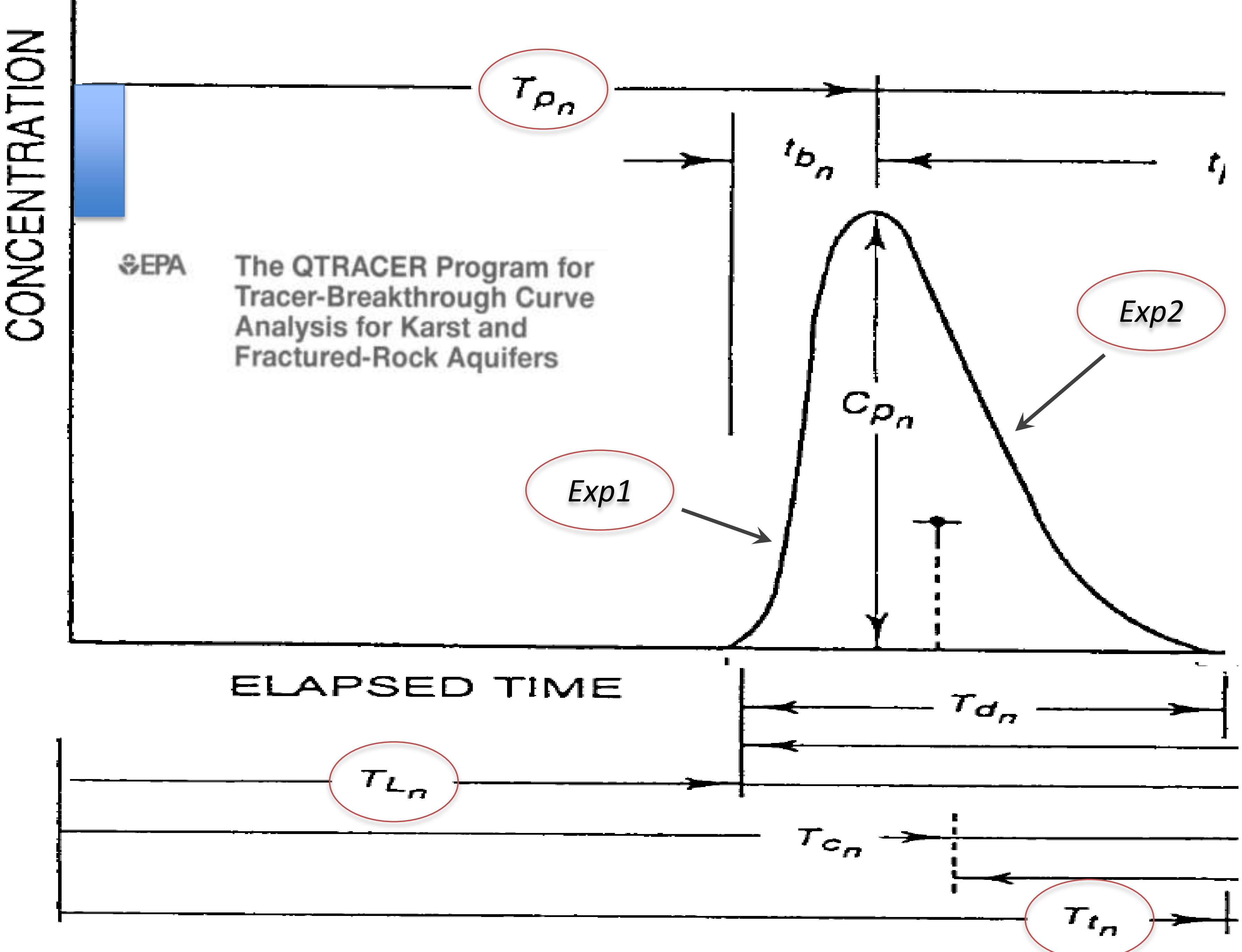


Development & Testing of a Subroutine …

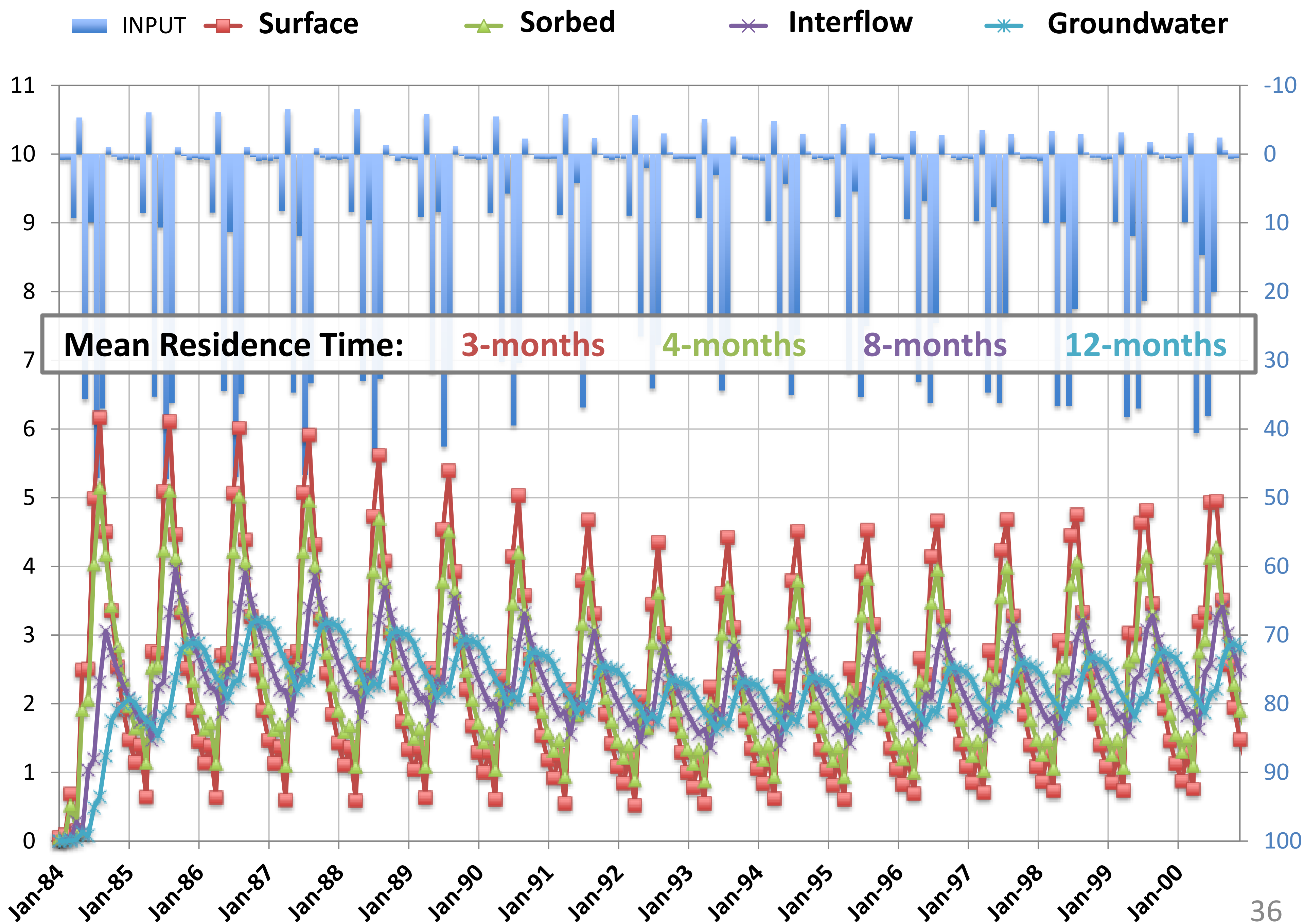



INPUT
BREAKTHROUGH
Pulse Inputs
Response Function
MONTHS
1
0.8
0.6
0.4
0.2
0
0.4
0.8
1.2
1.6
2
0
5
10
15
20
25
30
35
40


INPUT
BREAKTHROUGH
1
0.8
0.6
0.4
0.2
0
0
0.4
0.8
1.2
1.6
2
0
5
10
15
20
25
30
35
40
MONTHS
Pulse Inputs
Response Function



http://www.epa.gov/ncea/pdfs/qtracer/qtracerch03.pdf

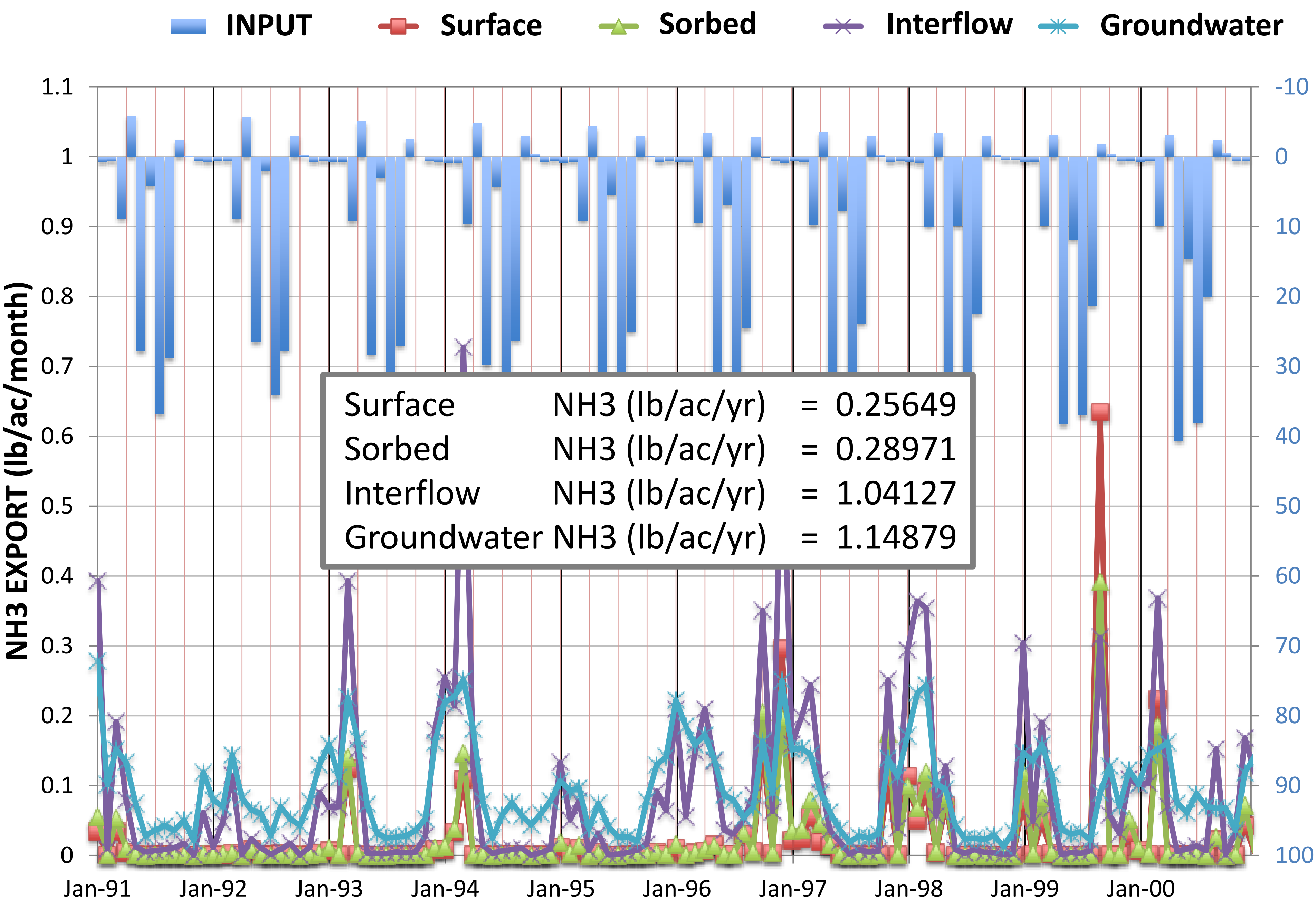

INPUT
Surface
Sorbed
Interflow
Groundwater
Mean Residence Time: 3-months 4-months 8-months 12-months
0
1
2
3
4
5
6
7
8
9
10
11
-10
0
10
20
30
40
50
60
70
80
90
100
Jan-84
Jan-85
Jan-86
Jan-87
Jan-88
Jan-89
Jan-90
Jan-91
Jan-92
Jan-93
Jan-94
Jan-95
Jan-96
Jan-97
Jan-98
Jan-99
Jan-00

Calibration : : A10001 HOM

high till w/**o** **m**anure

- EOF Export Targets:
  - **Stormflow** **NH_3** (lb/ac/yr) = 1.58748
  - **Baseflow** **NH_3** (lb/ac/yr) = 1.14879

- Flow (PWATER):
  - SURO (in/ac/yr) = 1.07687974
  - WSSD (tn/ac/yr) = 3.18039107
  - IFWO (in/ac/yr) = 3.50402546
  - AGWO (in/ac/yr) = 9.32850075


INPUT
Surface
Sorbed
Interflow
Groundwater
NH3 EXPORT (lb/ac/month)
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-10
0
10
20
30
40
50
60
70
80
90
100
Surface NH3 (lb/ac/yr) = 0.25649
Sorbed NH3 (lb/ac/yr) = 0.28971
Interflow NH3 (lb/ac/yr) = 1.04127
Groundwater NH3 (lb/ac/yr) = 1.14879
Jan-91
Jan-92
Jan-93
Jan-94
Jan-95
Jan-96
Jan-97
Jan-98
Jan-99
Jan-00

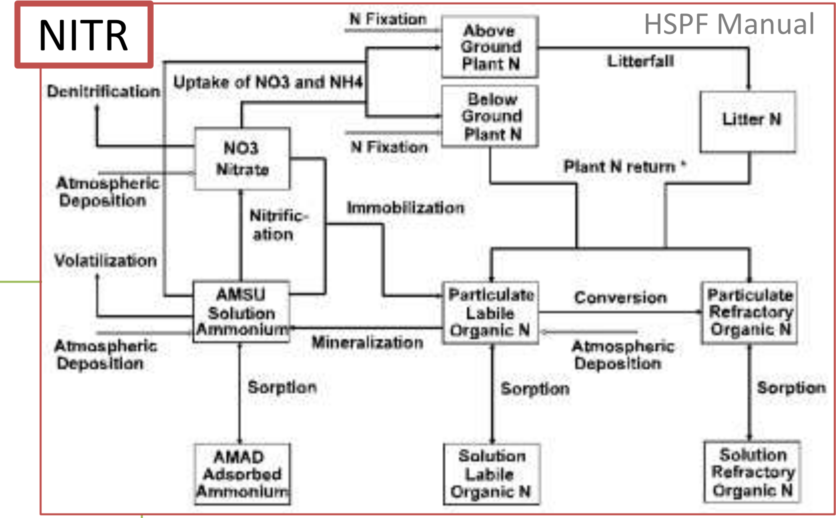
Advantages …

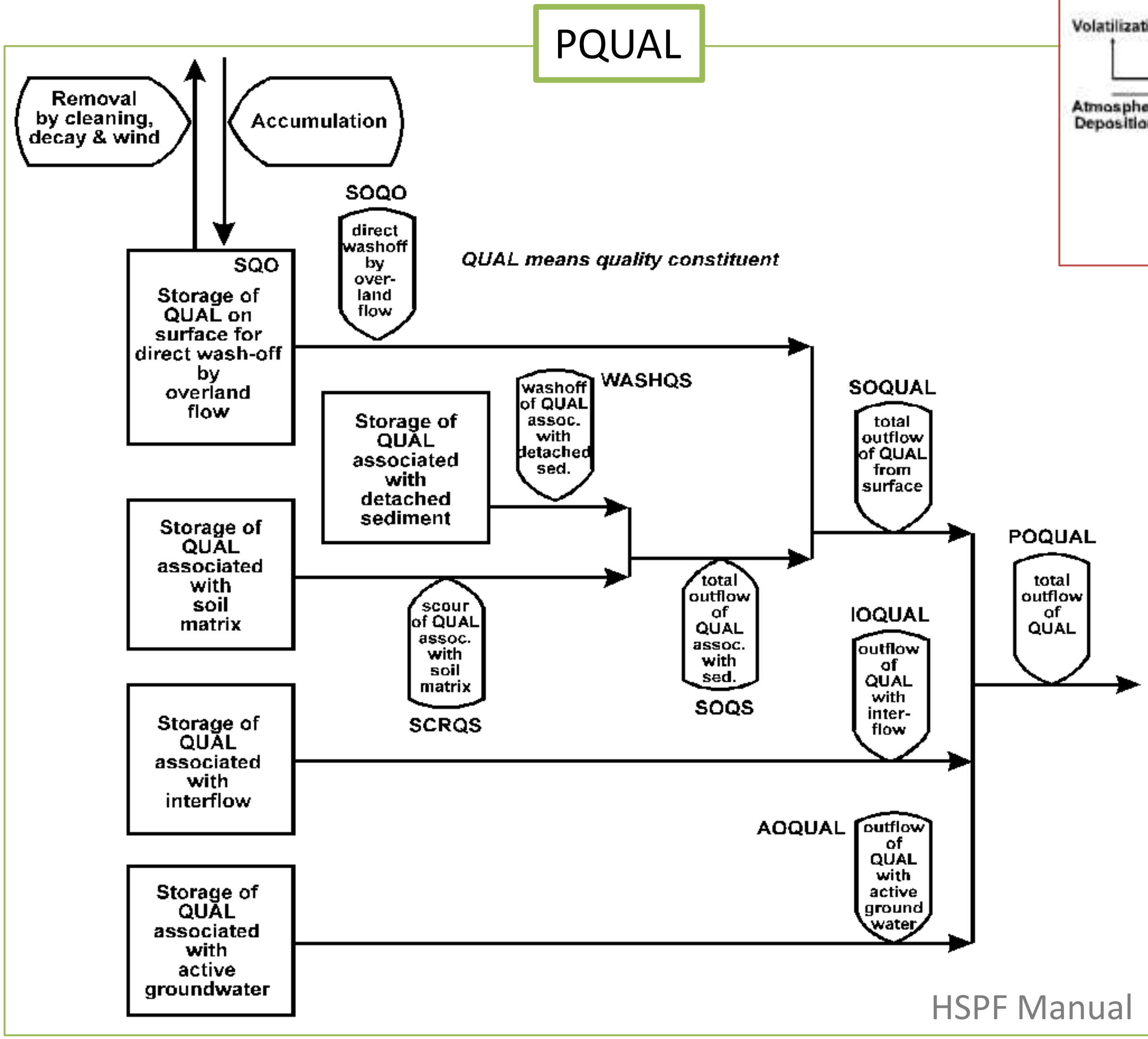
- Proposed framework is simple, easy to understand; and offers accounting of management scenarios.
- Offers ability to incorporate evidence based understanding of the watershed response.
  - E.g., Sensitivity, Residence time
- Framework ensures consistency between long-term export estimated from ‘sensitivity’ and export from hourly outputs.
- Framework is directly related to inputs. It provides ability to handle scenarios with not only changes in application rate, but application pattern.

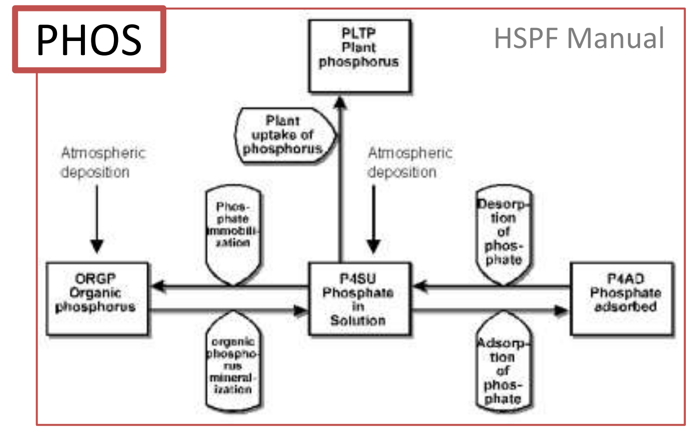
Next Steps …

- Continue with the implementation of Breakthrough Curve (BTC) Approach.
- Combine sensitivities with BTC Approach for running management scenario.

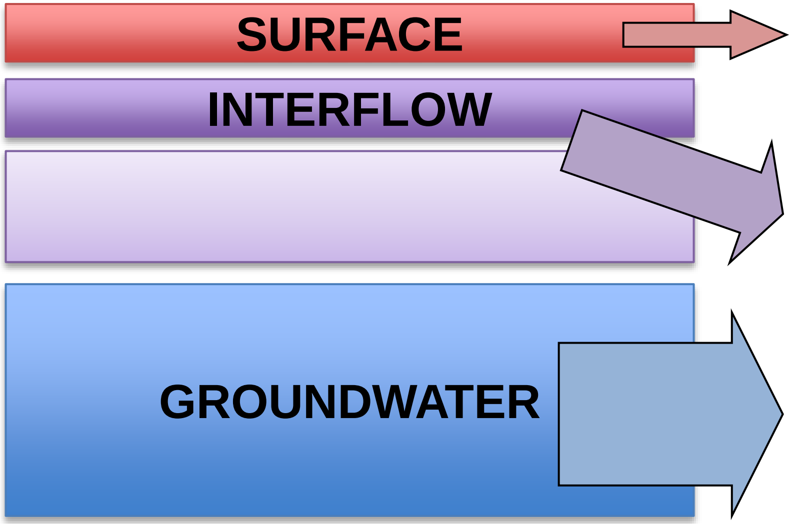
Appendix A







POQUAL = SOQUAL + IOQUAL + AOQUAL



Adapted from Shenk, 2009

NH3 = Flow x Conc. + Sed x factor

NH3 = Flow x Conc.

NH3 = Flow x Conc.

SOQO = SQO x [1.0 – EXP (–SURO x WSFAC)] (susceptibility to washoff)

SQO = ACQOP + SQOS x [1 – REMQOP] (rate of accumulation)

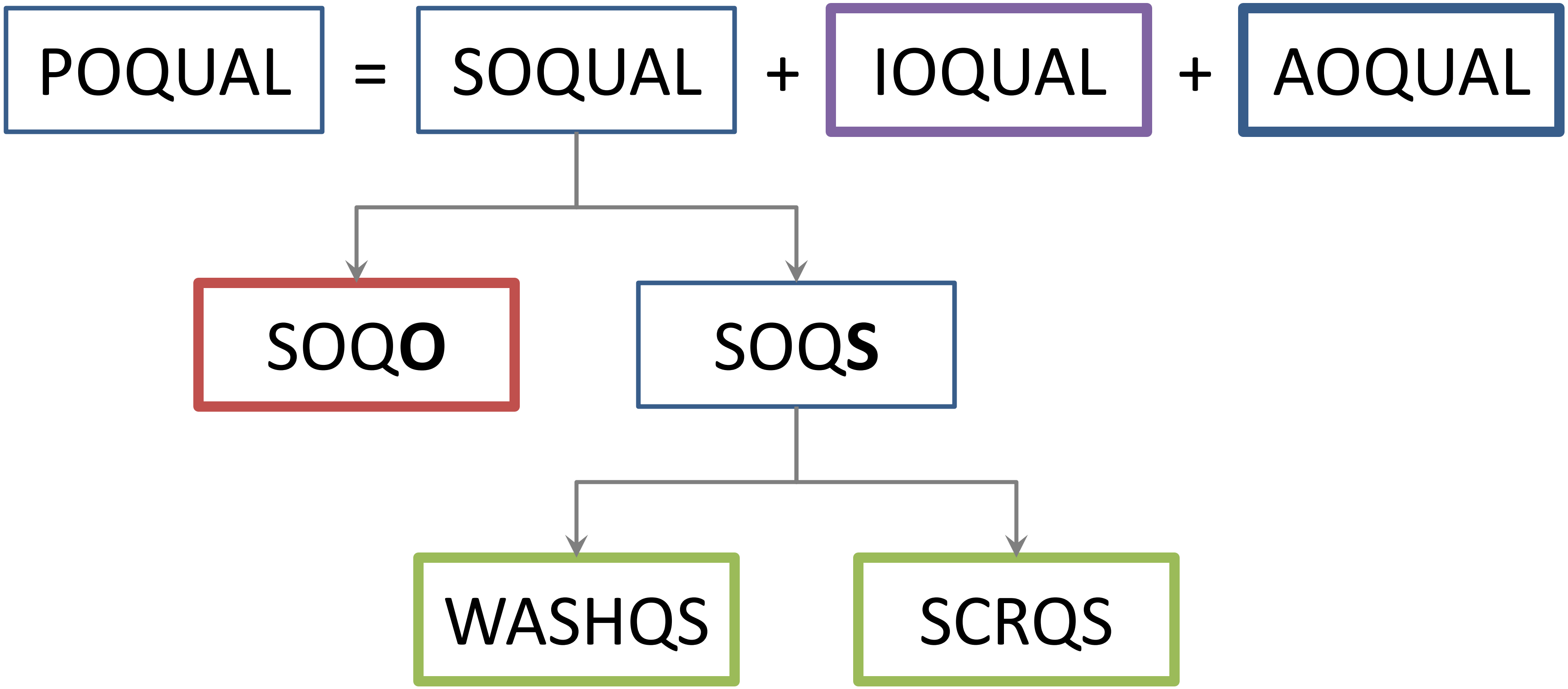
WASHQS = WSSD x POTFW (wash-off potency factor)

SCRQS = SCRSD x POTFS (scour potency factor)

IOQUAL = IFWO x IOQC

AOQUAL = AGWO x AOQC

Total Outflow of Water Quality Constituent (P**O**QUAL)



SOQO = SQO x [1.0 – EXP (–SURO x WSFAC)]

(susceptibility to washoff)

SQO = <u>ACQOP</u> + SQOS x [1 – REMQOP] (rate of accumulation)

SOQS (total sediment associated flux of the constituent) = WASHQS (removal of constituents by detached sediment washoff) + SCRQS (removal of constituents by scouring of soil matrix)

WASHQS = WSSD x <u>POTFW</u> (wash-off potency factor)

SCRQS = SCRSD x POTFS (scour potency factor)

IOQUAL = IFWO x <u>IOQC</u>

AOQUAL = AGWO x <u>AOQC</u>

PQUAL based Scenarios in Phase 5.3.2

Adjust PQUAL Parameters:

1. for changes in Total Application Rate (Input)

$$Scenario\ Avg\ Parameter = \left(\frac{Calibration\ Avg\ Parameter}{2}\right) \cdot \left(1 + \frac{Scenario\ AvgAnn\ Application}{Calibration\ AvgAnn\ Application}\right)$$

2x Application *translates to* **1.5x Nutrient Export**

2. for changes in Annual Application Rate in scenario

$$Scenario\ Parameter\ Y = \left(\frac{Scenario\ Avg\ Parameter}{2}\right) \cdot \left(1 + \frac{Scenario\ Y\ Application}{Scenario\ AvgAnn\ Application}\right)$$

Linear annual scaling of PQUAL parameters

Appendix B: Expanded Formulation …

A →

$$OUT^{SCEN}_{CON} - OUT^{CALIB}_{CON} = \sum_{J}^{SRC} \left[S_{J,CON} \times \left(IN^{SCEN}_{J,CON} - IN^{CALIB}_{J,CON} \right) \right]$$

B →

$$OUT^{SCEN}_{CON} - OUT^{CALIB}_{CON} = \sum_{J}^{SRC} \left[S_{J,CON} \times IN^{SCEN}_{J,CON} \right] - OUT^{CALIB}_{CON}$$

…

C →

SRC (J) ϵ [A,V,P,F,M,L,T,U,R]

- Above methods that are **exclusive** to each other.
- A method switch will be assigned a-priori

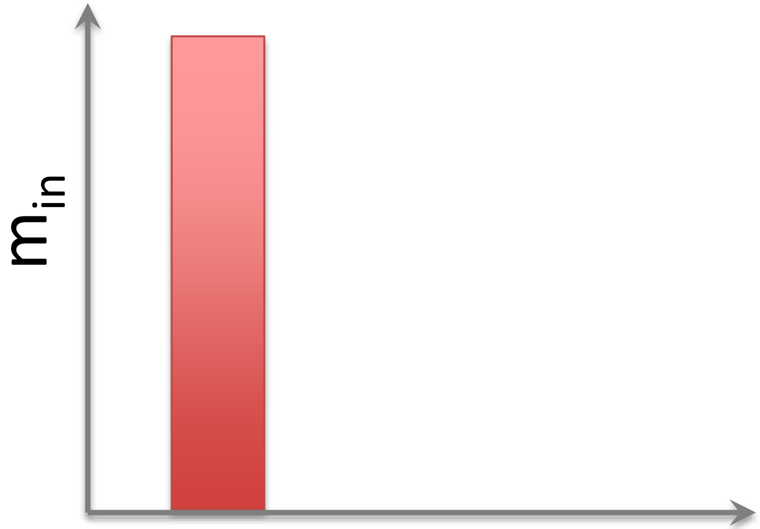
For a constituent compute percentage change in yield.

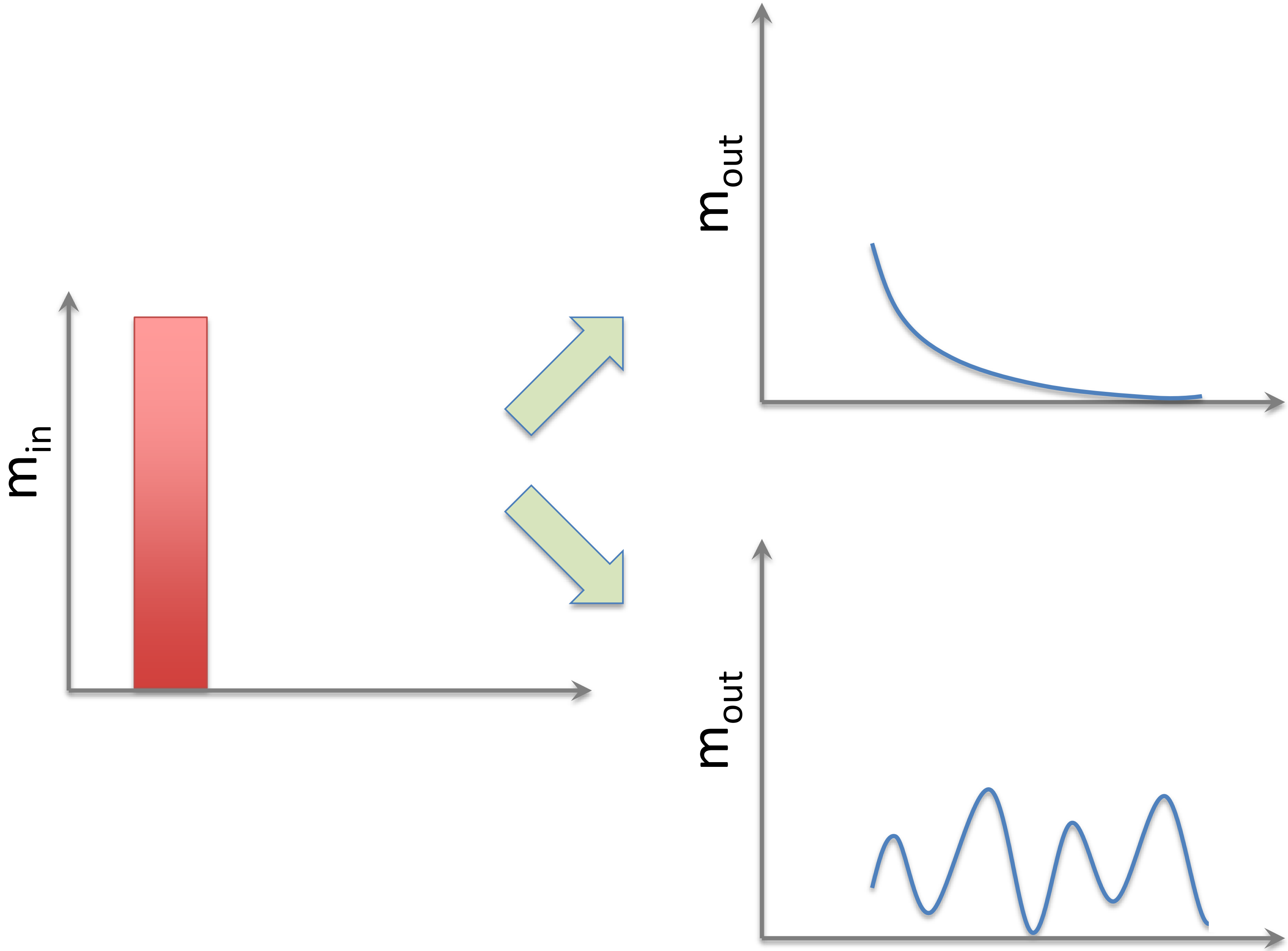
At time = t, apply the percent change to baseline yield.

E.g. **hom_atdep_sensitivity.csv**

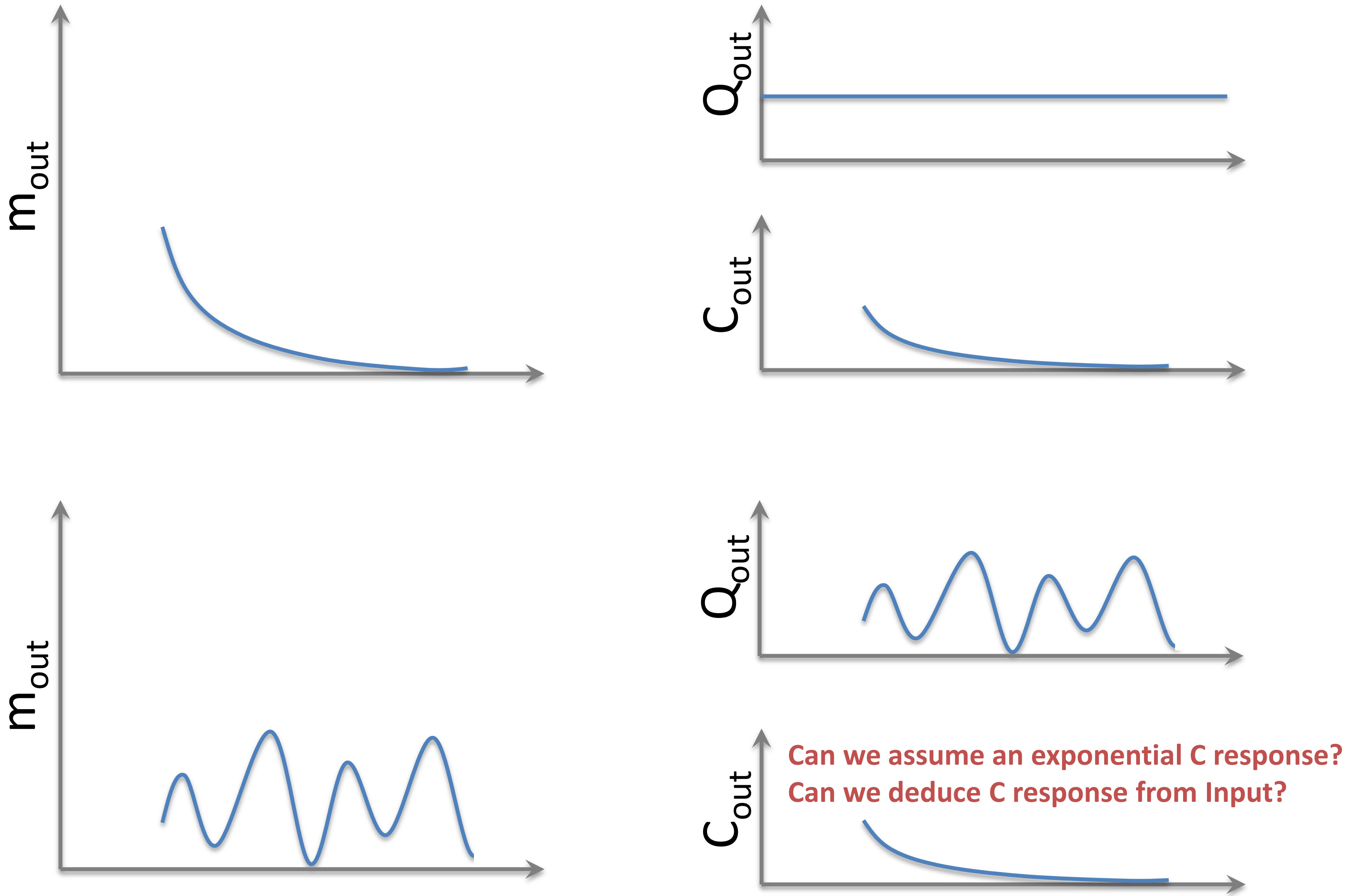
```
lsegmt,NO3,NH3,LON,RON,PO4,mNH3,mNO3,mLON,mRON,mPO4
A10001,1x0.43,1x0.43,2x0.012,2x0.012,3x0.1,D1,D1,D1,D1,D1
A10003,1x0.43,1x0.43,2x0.012,2x0.012,3x0.1,D1,D1,D1,D1,D1
…
```

Appendix C





m_{in}
m_{out}
m_{out}


m_out
Q_out
C_out
m_out
Q_out
C_out
Can we assume an exponential C response?
Can we deduce C response from Input?

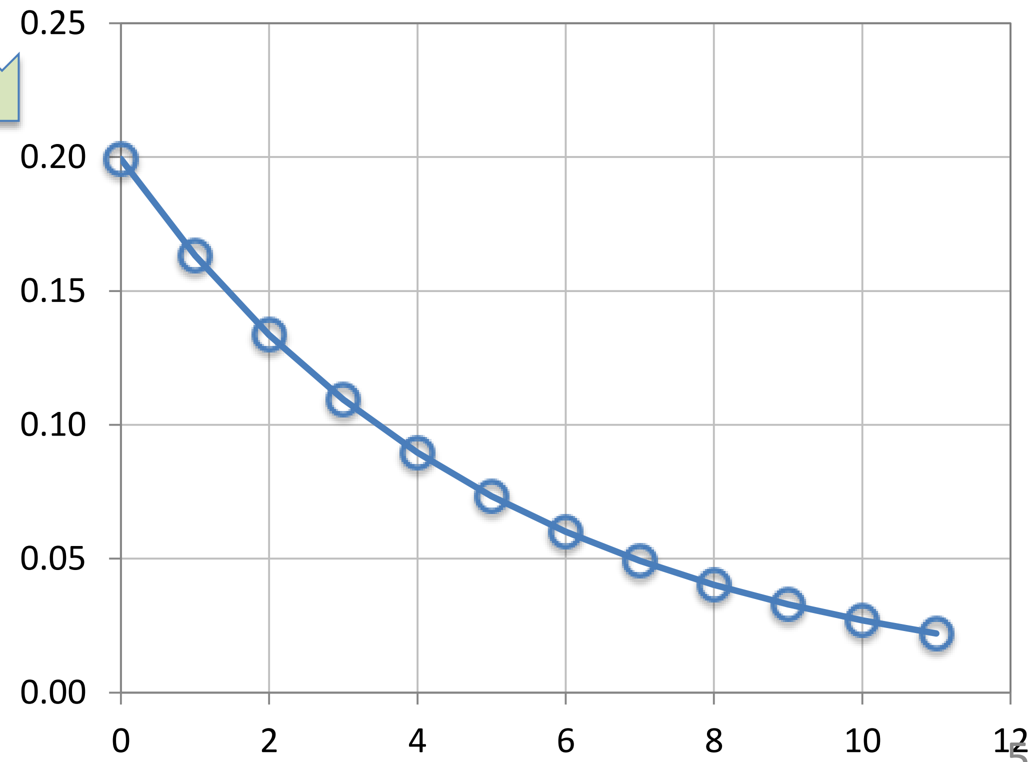
Appendix D: Breakthrough Curve Formulation …

At any given time, $t = T$

$$C_{t=T} = \sum_{t=T}^{t=0} I_t \times \left[K_1 \times EXP\left\{ K_2 \times (t - T) \right\} \right] = K_1 \times f_T$$

where, K_1 and K_2 are LU-based parameter

Memory	Response Fn.	Normalized
0	1.0000	0.1994
1	0.8187	0.1632
2	0.6703	0.1336
3	0.5488	0.1094
4	0.4493	0.0896
5	0.3679	0.0733
6	0.3012	0.0600
7	0.2466	0.0492
8	0.2019	0.0402
9	0.1653	0.0330
10	0.1353	0.0270
11	0.1108	0.0221
		1.0000



$$M_{out} = \sum_{t=0}^{t=H} M_t = \sum_{t=0}^{t=H} Q_t \times C_t$$

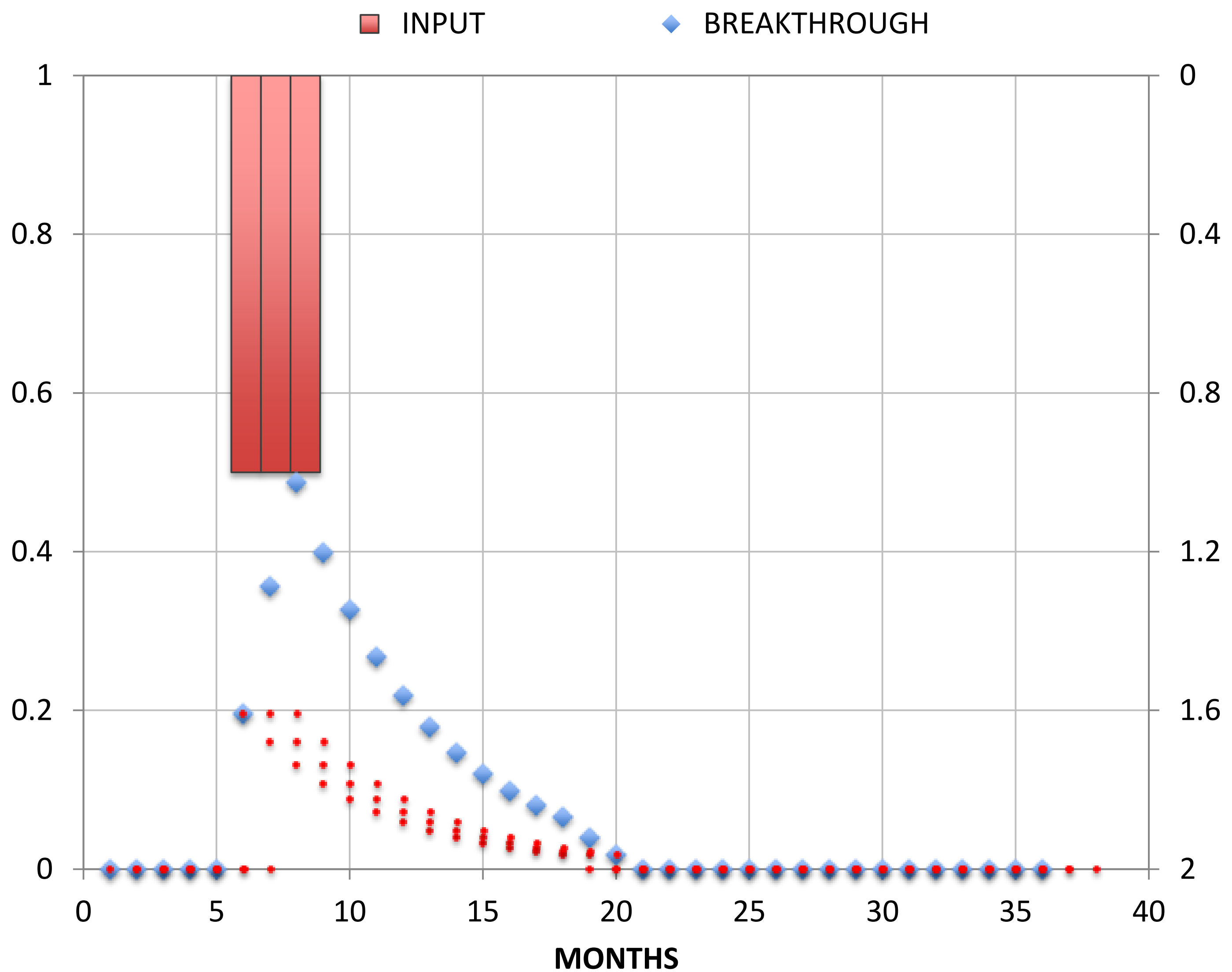
$e.g., t = 01/01/1991\ \ 01{:}00\ to\ 12/31/2000\ \ 24{:}00$

Assuming we know the distribution of C a-priori, based on Inputs

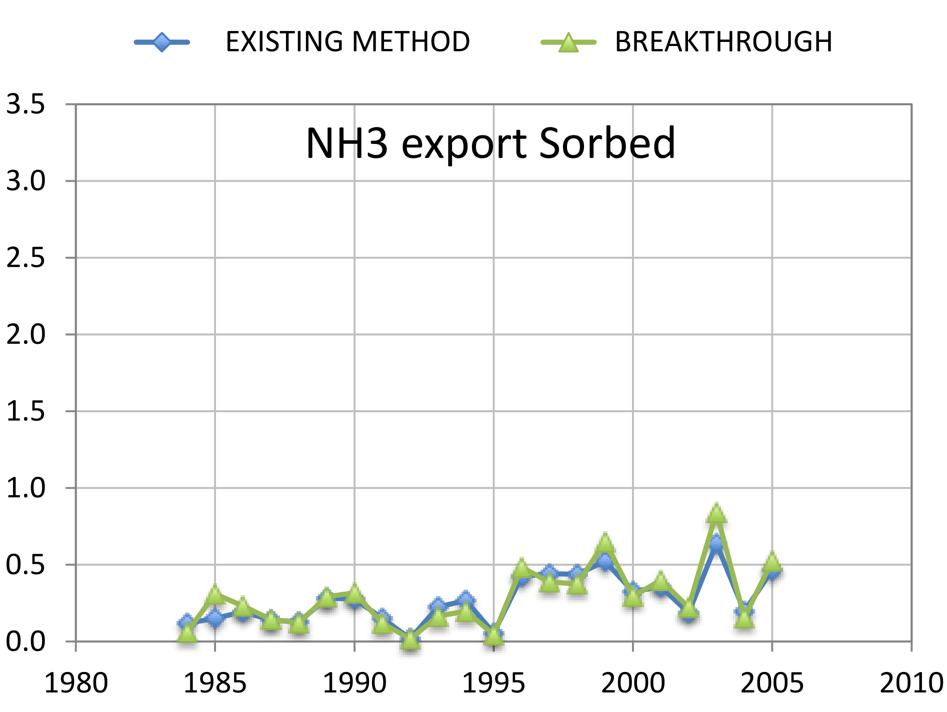
$$M_{out} = \sum_{t=0}^{t=H} Q_t \times K_1 f_t = K_1 \sum_{t=0}^{t=H} Q_t \times f_t$$

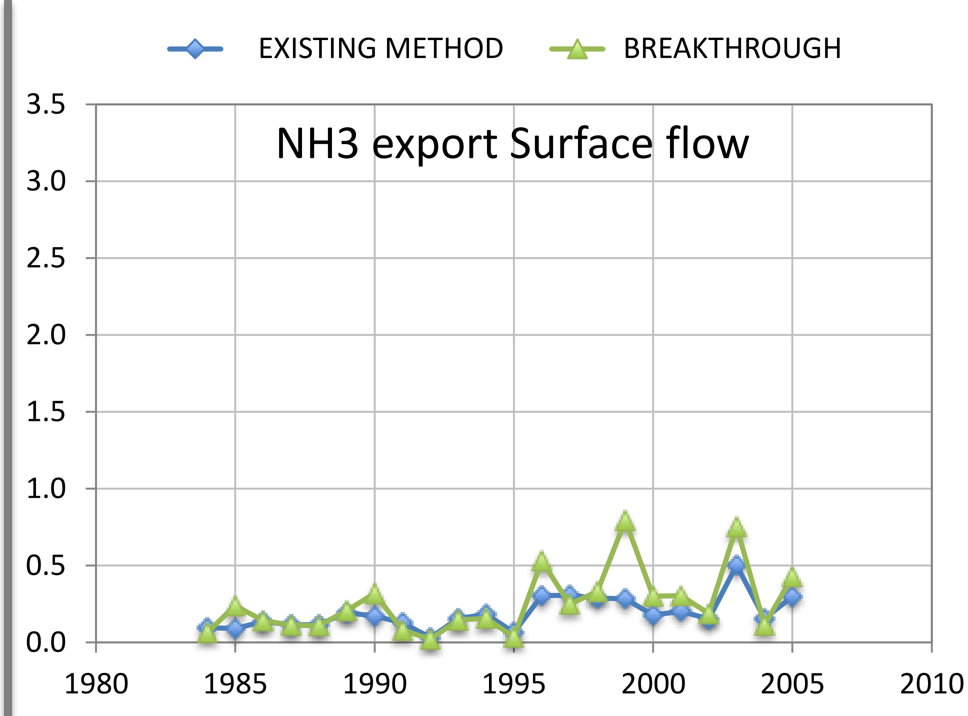
$$K_1 = \frac{M_{out}}{\sum_{t=0}^{t=H} Q_t \times f_t}$$

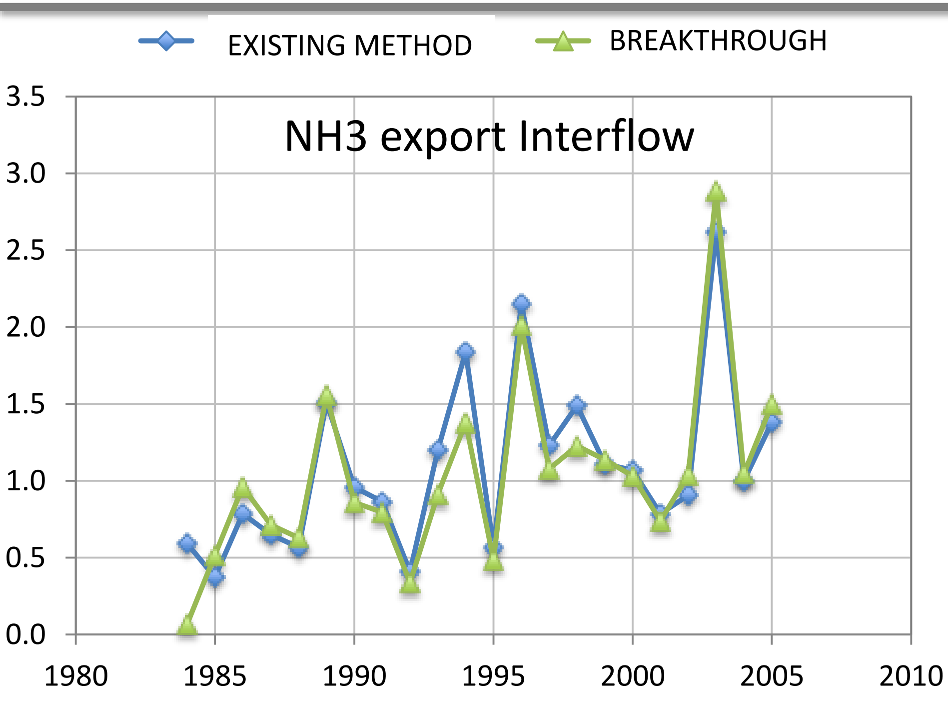
$$K_1 = \frac{\left(EOF\ target,\ lb/ac/yr\right)}{\left(\sum_{t=0}^{t=H} Q_t \times f_t\right) / \left(H/\left(365 \times 24\right)\right)}$$

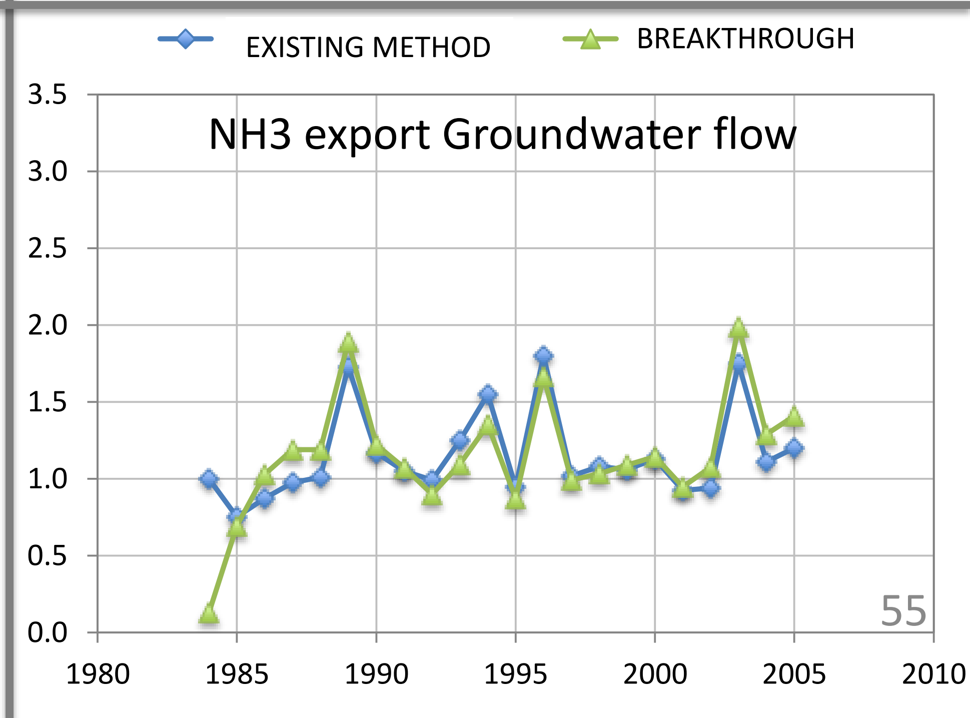

INPUT
BREAKTHROUGH
1
0.8
0.6
0.4
0.2
0
0
0.4
0.8
1.2
1.6
2
0
5
10
15
20
25
30
35
40
MONTHS

Appendix E: PQUAL vs. Breakthrough Curve …


EXISTING METHOD
BREAKTHROUGH
NH3 export Sorbed
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1980
1985
1990
1995
2000
2005
2010


EXISTING METHOD
BREAKTHROUGH
NH3 export Surface flow
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1980
1985
1990
1995
2000
2005
2010


EXISTING METHOD
BREAKTHROUGH
NH3 export Interflow
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1980
1985
1990
1995
2000
2005
2010


EXISTING METHOD
BREAKTHROUGH
NH3 export Groundwater flow
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1980
1985
1990
1995
2000
2005
2010