SWAT-CUP

SWAT- Calibration and Uncertainty analysis Procedures

K. C. Abbaspour

Eawag: Swiss Federal Institute of Aquatic Science and Technology

Content

- Introduction to calibration-uncertainty Analysis

- SWAT-CUP

- Example project

Modeling Components Include:

- Model building,
- Calibration,
- Validation,
- Sensitivity analysis,
- Uncertainty analysis

Calibration

Calibration is adjusting model inputs (parameters, structure, variables, etc.) with the purpose of achieving the best simulation match with observation

Therefore, calibration boils done to the optimization of an objective function

Min: $$g(B) = \sum_{i=1}^{n_1} \left(Q_o - Q_s\right)_i^2$$

Validation

Validation is the process of testing the calibrated parameters with an independent set of data

Without further changes to the parameters

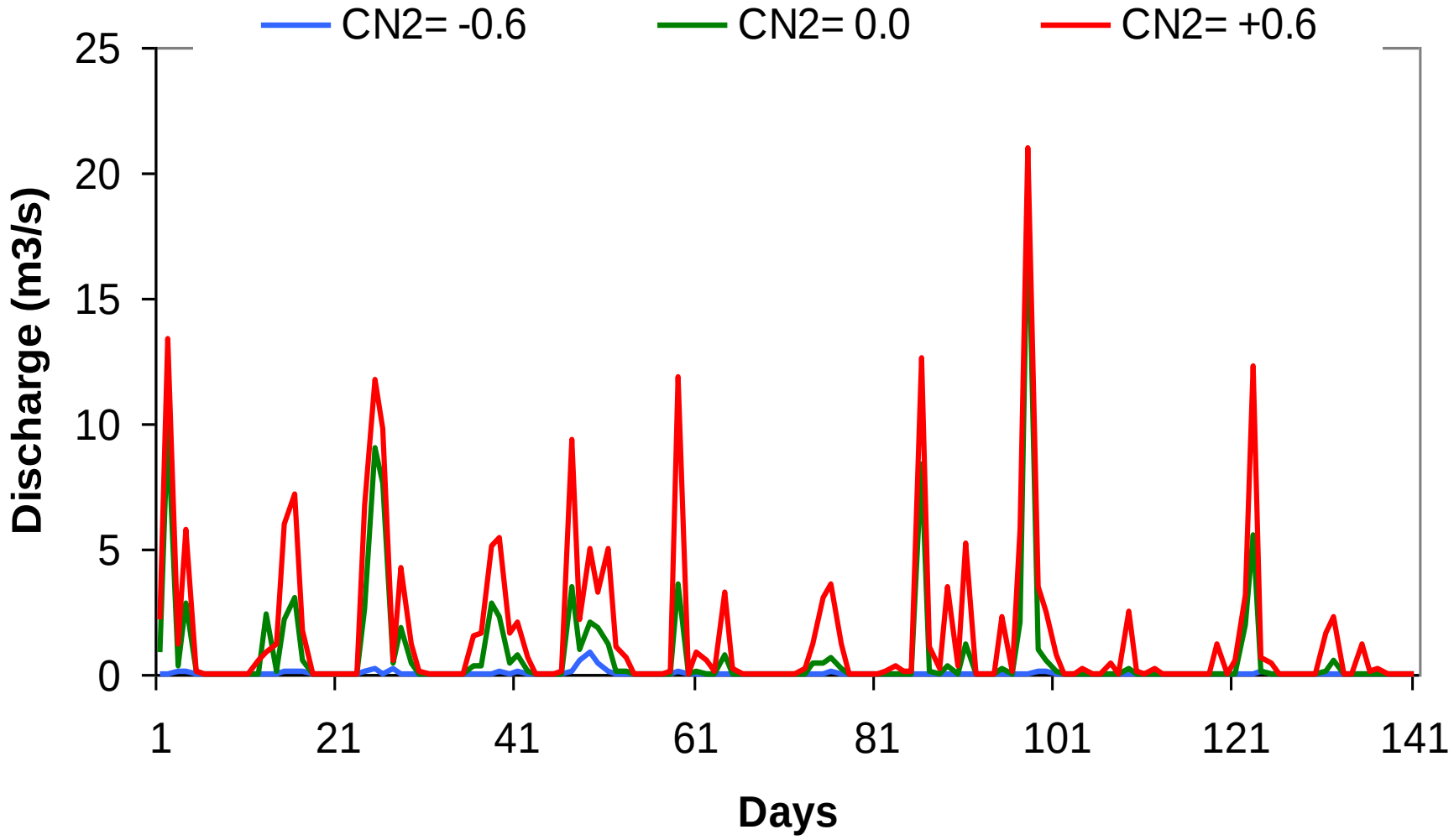
Sensitivity Analysis

Sensitivity analysis is the process of determining the significance of one or a combination of parameters w.r.t the objective function or a model output

(this is important because parameters represent processes)

Example
(CN2)

Sensitivity to CN2



Uncertainty Analysis

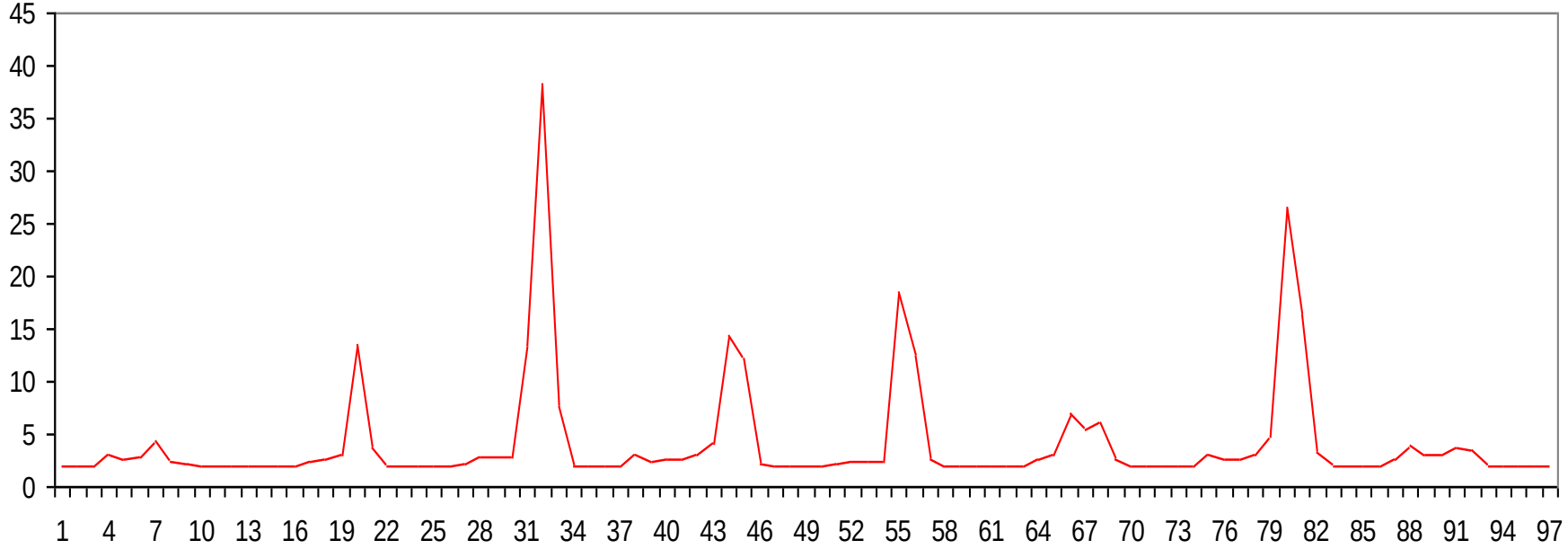
Uncertainty analysis is the process of:

- propagating the uncertainties in the model (inputs, parameters, etc.)
- Quantifying its magnitude
- (needed for risk analysis, etc.)

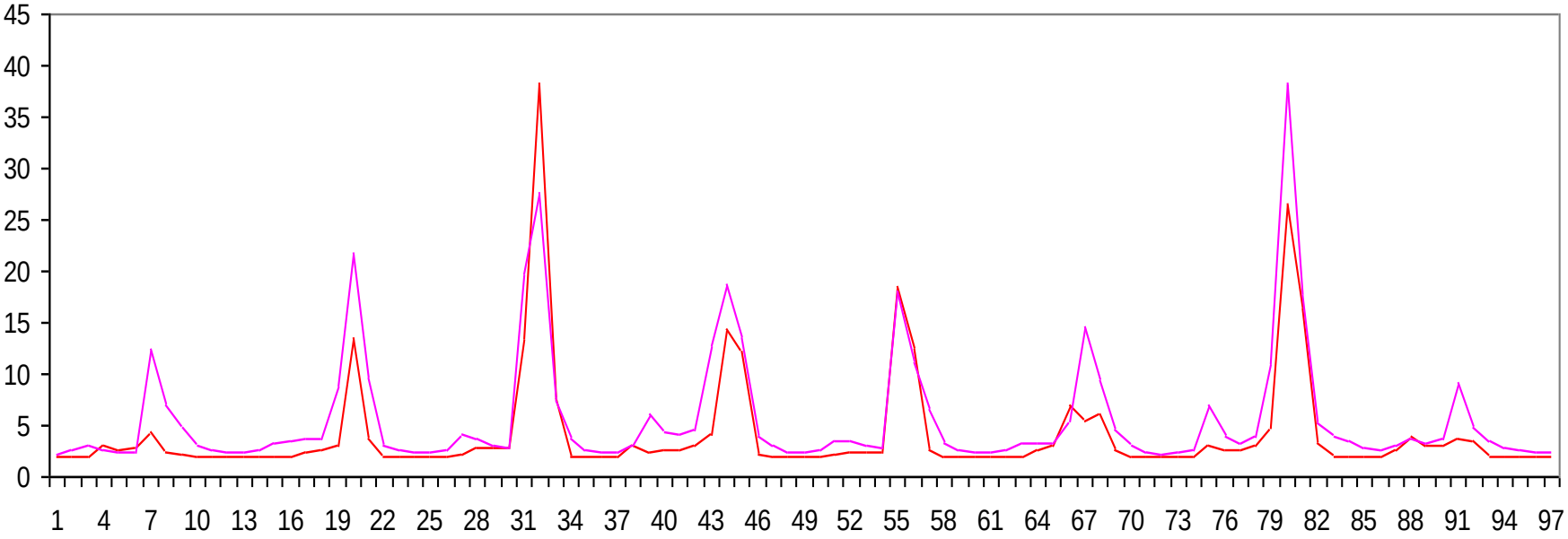
Calibration & Uncertainty analysis

Contrary to the belief that calibration is different from uncertainty analysis, calibration and uncertainty are intimately linked

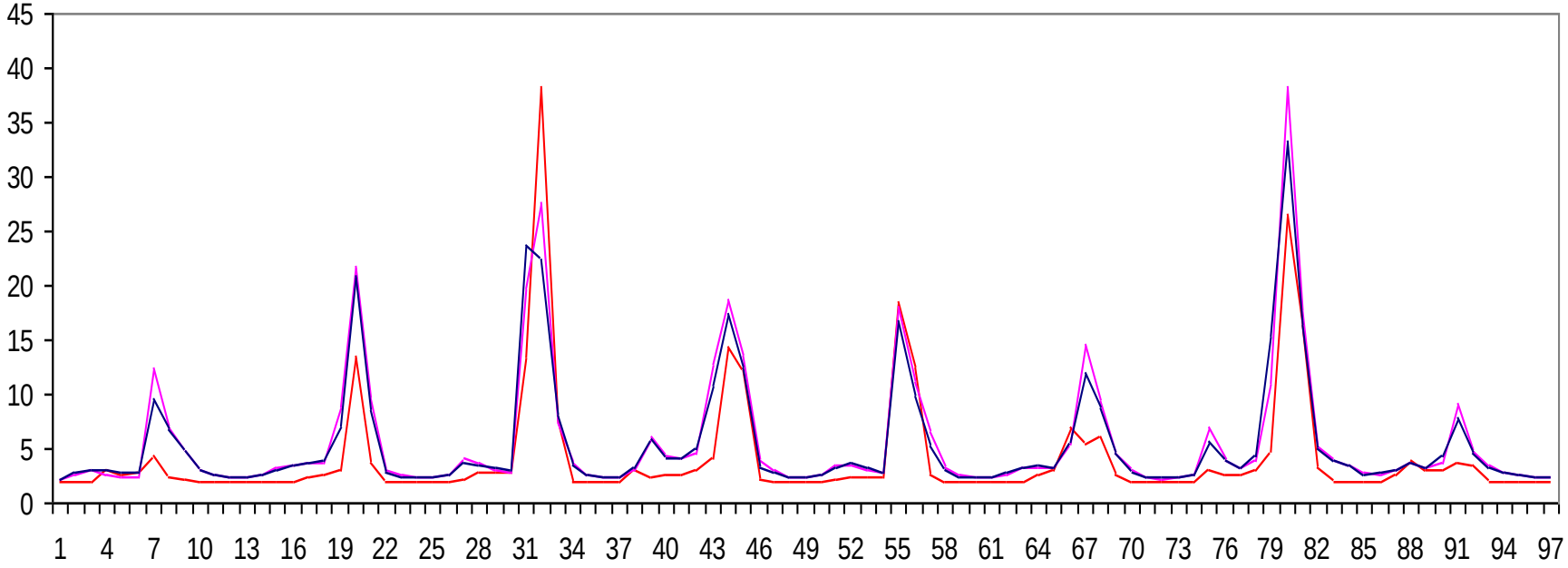
Calibration is subjective ……



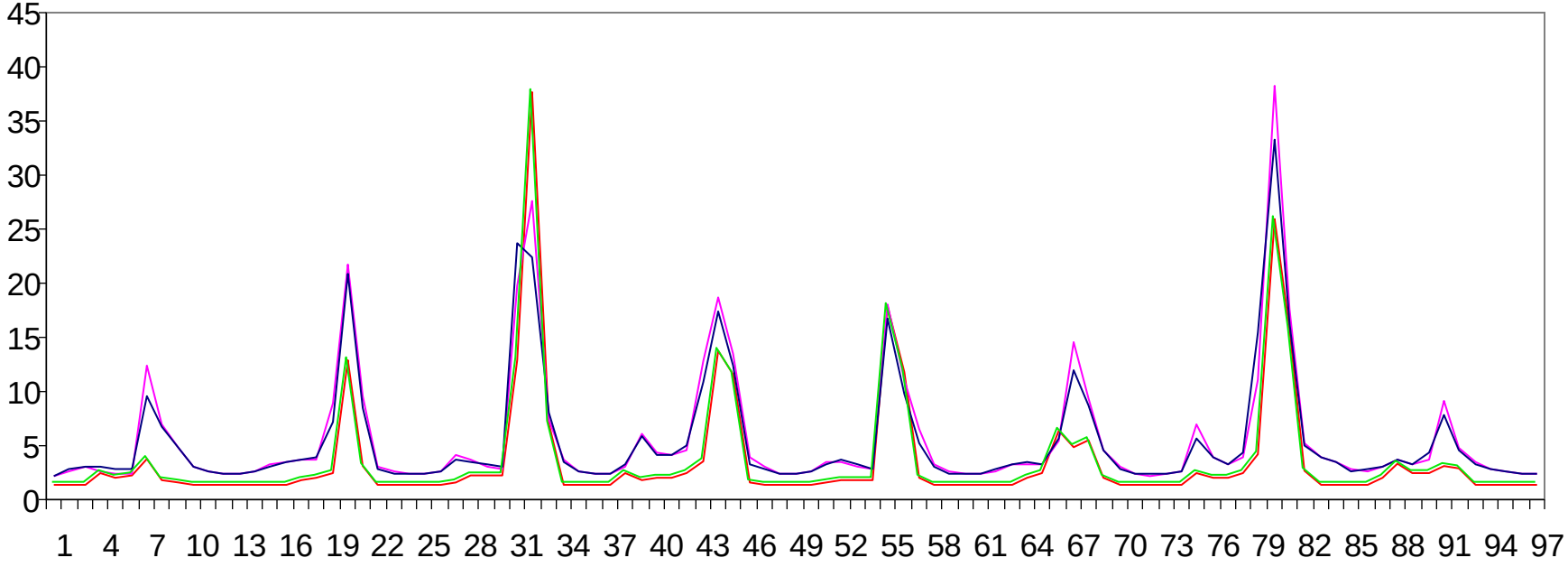
Calibration is subjective ……



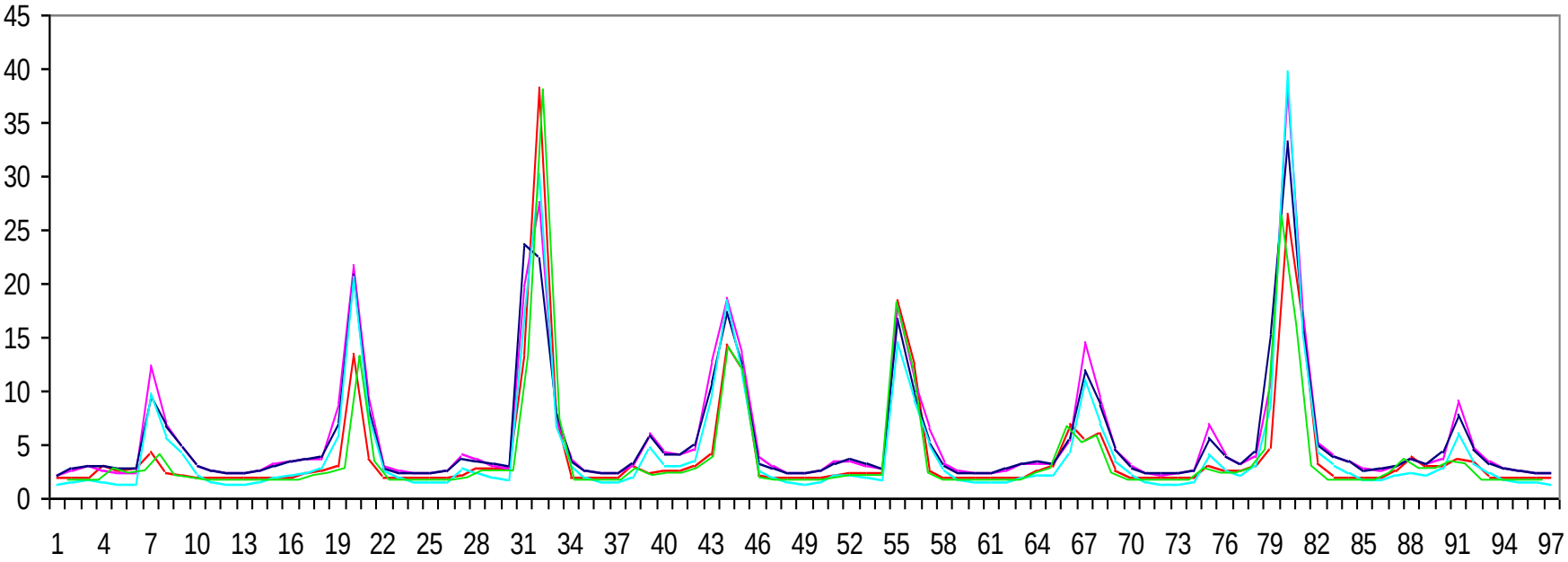
Calibration is subjective ……



Calibration is subjective ……



Calibration is subjective ……



	RMSE	R2	NS	bR2
S1	29.90	0.79	0.67	0.54
S2	29.70	0.90	0.67	0.42
S3	23.50	0.84	0.83	0.58
S4	21.10	0.75	0.80	0.62
S5	23.30	0.84	0.80	0.75

Calibration is subjective ……

	CN2	ALPHA_BF	REVAPMN	GW_REVAP	RCHRG_DP	SOL_AWC	SOL_K	SOL_BD
s1	-0.206	0.25	83.46	0.059	0.095	-0.195	0.572	-0.135
s2	0.110	0.59	66.06	0.056	0.191	-0.256	0.456	-0.191
s3	0.338	0.35	86.14	0.071	0.194	-0.047	0.300	0.086
s4	0.297	0.50	32.87	0.073	0.290	-0.165	0.297	-0.075
s5	0.115	0.40	55.87	0.032	0.101	-0.055	0.355	-0.032

	RMSE	R2	NS	bR2
S1	29.90	0.79	0.67	0.54
S2	29.70	0.90	0.67	0.42
S3	23.50	0.84	0.83	0.58
S4	21.10	0.75	0.80	0.62
S5	23.30	0.84	0.80	0.75

Stochastic vs Deterministic

Deterministic Modelling:

single-valued input parameters → MODEL → single-valued output variables

Stochastic Modelling:

distribution of input parameters → MODEL → distribution of output variables

Issues wrt Calibration of Distributed Watershed Models

- Parameterization

  (most important, difficult, and neglected aspect of calibration)

- Objective function definition

  (most surprising aspect of calibration)

- Non-uniqueness (Uncertainty)

  (most difficult part to quantify and communicate)

- Parameter conditionality

  (most disappointing aspect of calibration)

- Positioning observed outlets in SWAT

  (causes the biggest headache in calibration)

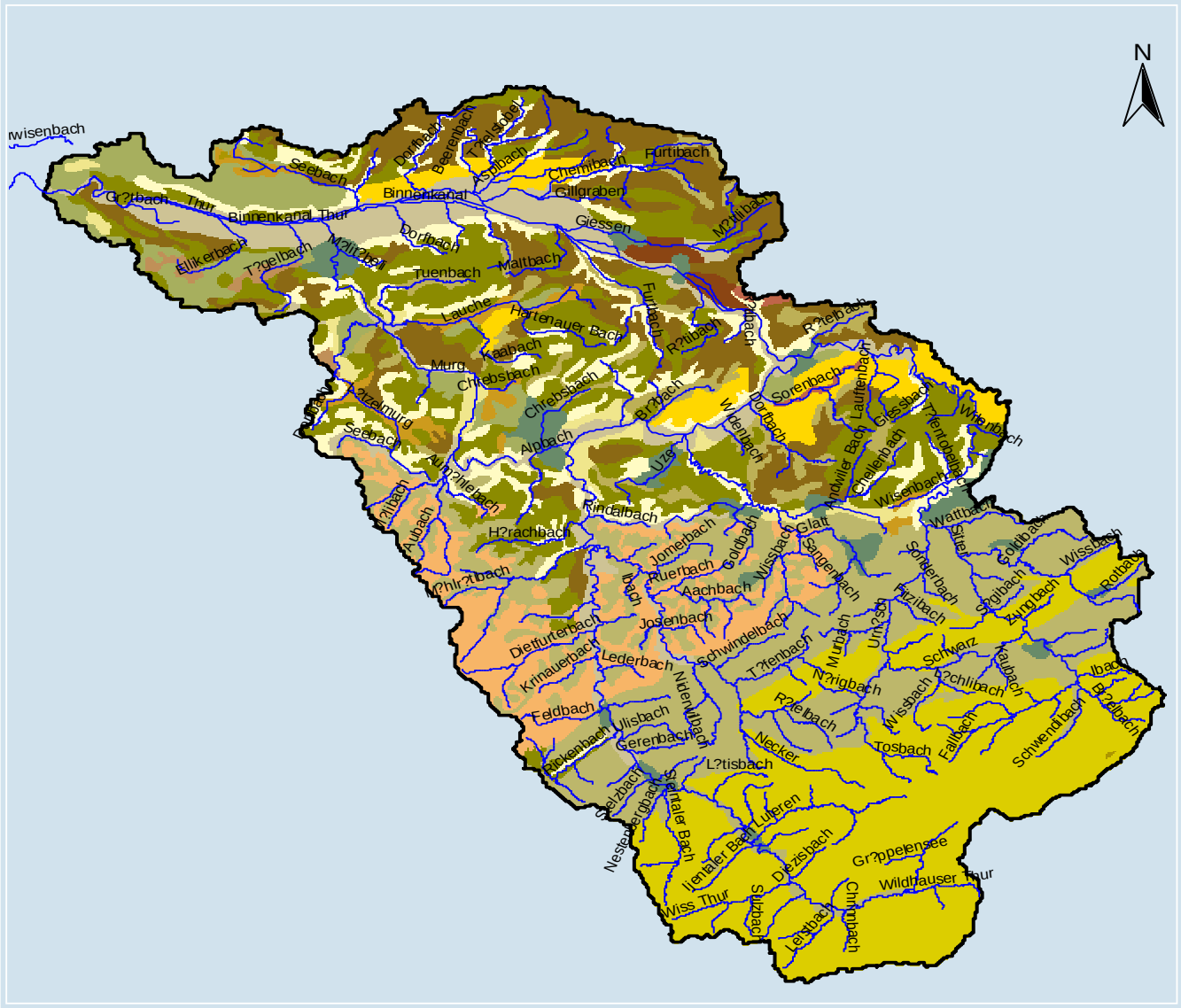
- Time constraint

  (makes some projects impossible to build and run)

Parameterization

-Which parameters to use?

- How to regionalize the parameters



Parameterization

X__<parname>.<ext>__<hydrogrp>__<soltext>__<landuse>__<subbsn>__Slope

Where x=

v__ means the existing parameter value is replaced by a given value,

a__ means the given value is added to the existing parameter value, and

r__ means the existing parameter value is multiplied by (1+the given value);

Parameterization

Soil parameters

Parameter identifiers	Description
r__SOL_K(1).sol	K of Layer 1 of all HRUs
r__SOL_K(1-3).sol	K of Layer 1,2,3 of all HRUs
r__SOL_K().sol	K of All layers and all HRUs
r__SOL_K(1).sol____FSL	K of layer 1 of HRUs with soil texture FSL
r__SOL_K(1).sol____FSL__PAST	K of layer 1 of HRUs with soil texture FSL and landuse PAST
r__SOL_K(1).sol_____PAST__1-3	K of layer 1 of subbasin 1,2, and 3 with HRUs containing landuse PAST
v__SOL_K(1).sol_____0-10	K of layer 1 for HRUs with slope 0-10

Parameterization

Management parameters

Parameter identifiers	Description
v__HEAT_UNITS{rotation no,operation no}	Management parameters that are subject to operation/rotation must have both specified
v__CNOP{[],1}.mgt	change an operation's parameters in all rotations [] means every rotation that has the specified operation.
v__CNOP{2,1,plant_id=33}.mgt v__CNOP{[],1,plant_id=33}.mgt	Operation filters could be applied as shown The changes are applied to crop 33 only
v__CNOP{[],1,plant_id=33}.000010001.mgt	To modify just one file, it could be given as shown

Parameterization

Rainfall parameters

Parameter identifiers	Description
v__precipitation(1){1977300}.pcp1.pcp	(1) means column number 1 in the pcp file {1977300} specifies year and day
v__precipitation(1-3){1977300}.pcp1.pcp	(1-3) means column 1, 2, and3 {1977300} specifies year and day
v__precipitation( ){1977300,1977301}.pcp	( ) means all columns (all stations) {1977300,1977301} means 1977 days 300 and 301
v__precipitation( ){1977001-1977361,1978001-1978365,1979003}.pcp	( ) means all columns from day 1 to day 361 of 1977, and from day 1 to day 365 of 1978, and day 3 of 1979

Parameterization

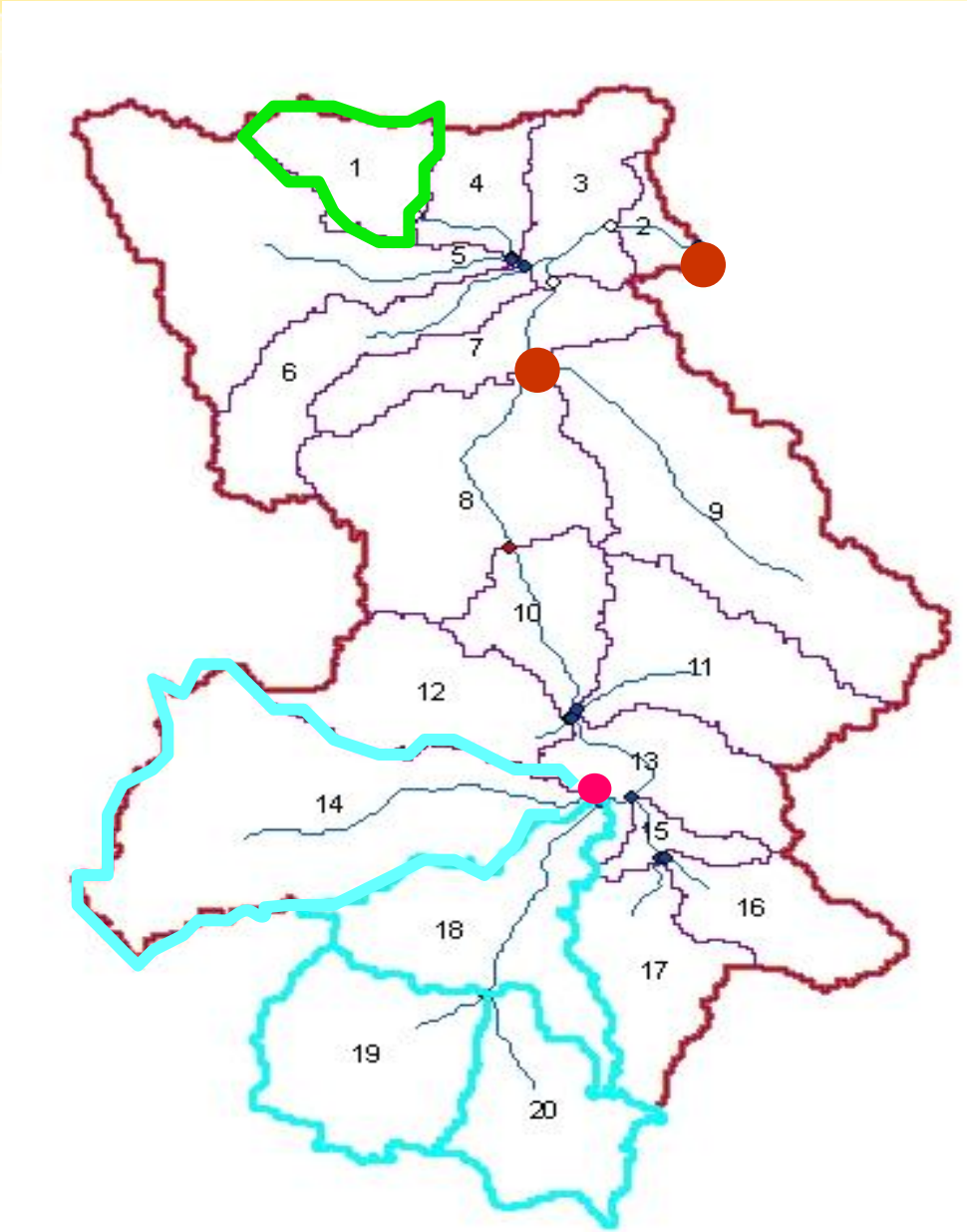
Crop parameters

Parameter identifiers	Description
V__T_OPT{30}.CROP.DAT	Parameter T_OPT for crop number 30 in the crop.dat file
v__PLTNFR(1){3}.CROP.DAT	Nitrogen uptake parameter #1 for crop number 3 in crop.dat file

Parameterization

par_inf.txt

r__CN2.mgt	0.5	0.9
v__ALPHA_BF.gw	0.4	1.4
v__GW_DELAY.gw	0.0	100.0
v__GWQMN.gw	0.0	0.0
v__GW_REVAP.gw	0.02	0.1
v__ESCO.hru	0.02	0.1
v__OV_N.hru	0.02	0.1
v__SLSUBBSN.hru	1.0	8.0
v__HRU_SLP.hru	0.3	0.8
v__CH_N2.rte	0.01	0.1
v__CH_K2.rte	29.5	96.7
v__ALPHA_BNK.rte	0.38	1.16
r__SOL_AWC(1).sol	-0.1	0.02
r__SOL_K(1).sol	-0.8	0.8


1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

Parameterization

par_inf.txt

```
r__CN2.mgt________14,18,19,20                    -0.5    -0.1
r__SOL_BD().sol________ 14,18,19,20              -0.02    0.01
r__SOL_AWC().sol________ 14,18,19,20             -0.5    -0.3
......

r__CN2.mgt________1                       -0.5    -0.1
r__SOL_BD().sol________ 1                -0.02    0.01
r__SOL_AWC().sol________ 1               -0.5    -0.3

…..

r__CN2.mgt________ 8-13,15-17                    -0.3      0.2
r__SOL_BD().sol________ 8-13,15-17               -0.04     0.05
r__SOL_AWC().sol________ 8-13,15-17              -0.5     -0.3
```

Issues wrt Calibration of Distributed Watershed Models

- Parameterization

  (most important, difficult, and neglected aspect of calibration)

- Objective function definition

  (most surprising aspect of calibration)

- Non-uniqueness (Uncertainty)

  (most difficult part to quantify and communicate)

- Parameter conditionality

  (most disappointing aspect of calibration)

- Positioning observed outlets in SWAT

  (causes the biggest headache in calibration)

- Time constraint

  (makes some projects impossible to build and run)

Objective Function Definition

Different objective functions produce different calibration results

S-MSR

$$g(\mathbf{B}) = w_1 \sum_{i=1}^{n_1} \left(Q_o - Q_s\right)_i^2 + w_2 \sum_{i=1}^{n_2} \left(S_o - S_s\right)_i^2 + \ldots\ldots$$

M-MSR

$$g(\mathrm{B}) = \sum_{i=1}^{n_1} \left(Q_o - Q_s\right)_i^2 * \sum_{i=1}^{n_2} \left(S_o - S_s\right)_i^2 * \ldots\ldots$$

NS

$$g(\mathbf{B}) = \left[1 - \frac{\sum_{1}^{n_1} \left(O_i - P_i\right)^2}{\sum_{1}^{n_1} \left(O_i - \overline{O}\right)^2} \right]$$

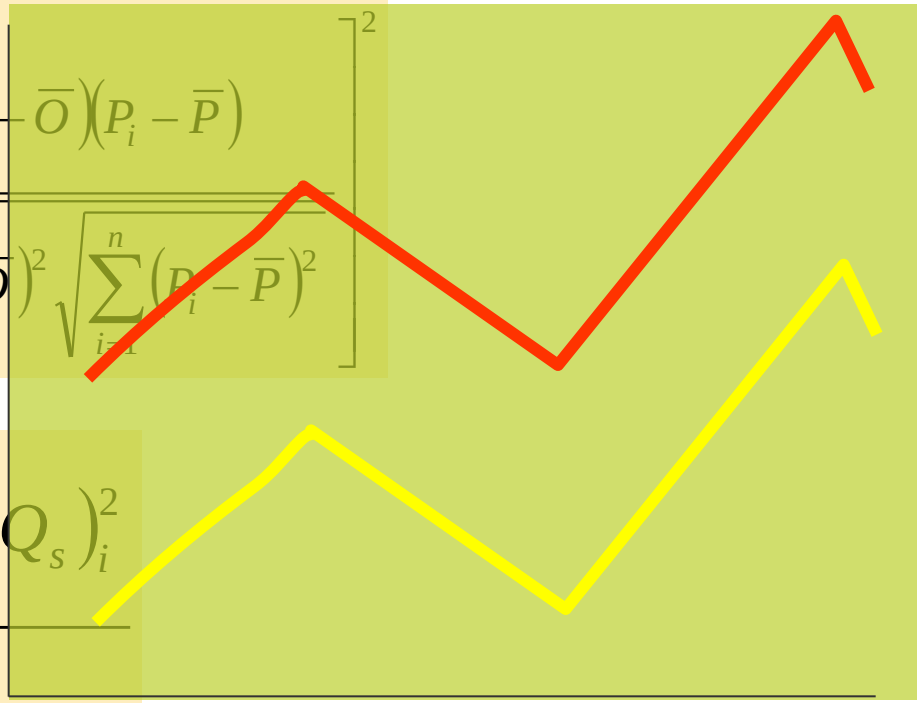
Objective Function Definition

R^2

$$g(\mathbf{B}) = \left[\frac{\sum_{i=1}^{n} (O_i - \bar{O})(P_i - \bar{P})}{\sqrt{\sum_{i=1}^{n} (O_i - \bar{O})^2} \sqrt{\sum_{i=1}^{n} (P_i - \bar{P})^2}} \right]^2$$

Chi 2

$$\chi^2 = \frac{\sum_i (Q_m - Q_s)_i^2}{\sigma_Q^2}$$



bR^2

$$g(\mathbf{B}) = \begin{cases} |b|.R^2 & for \;\; b \le 1 \\ |b|^{-1}.R^2 & for \;\; b > 1 \end{cases}$$

PBIAS

$$PBIAS = 100 * \frac{\sum_{i=1}^{n} (Q_m - Q_s)_i}{\sum_{i=1}^{n} Q_{m,i}}$$

RSR

$$RSR = \frac{\sqrt{\sum_{i=1}^{n} (Q_m - Q_s)_i^2}}{\sqrt{\sum_{i=1}^{n} (Q_m - \overline{Q}_m)^2}}$$

Objective Function Definition

The SSQR method aims at the fitting of the frequency distributions of the observed and the simulated series. After independent ranking of the measured and the simulated values, new pairs are formed and the SSQR is calculated as

SSQR

$$SSQR = \sum_{j=1,n} \left[Q_{j,measured} - Q_{j,simulated} \right]^2$$

Objective Function Definition

Likelihood function in a Bayesian inference using Box-Cox transformation and continuous time auto regressive function:

$$f_{\mathbf{Y}^M|\boldsymbol{\Theta}}(\mathbf{y}|\boldsymbol{\theta}) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma}\exp\left(-\frac{1}{2}\frac{\left[g(y_{t_0}) - g\left(y_{t_0}^M(\boldsymbol{\theta})\right)\right]^2}{\sigma^2}\right)\cdot\left|\frac{dg}{dy}\bigg|_{y=y_{t_0}}\right|$$

$$\cdot\prod_{i=1}^{n}\left[\frac{1}{\sqrt{2\pi}}\frac{1}{\sigma\sqrt{1-\exp\left(-2\frac{t_i - t_{i-1}}{\tau}\right)}}\exp\left(-\frac{1}{2}\frac{\left[\begin{array}{l} g(y_{t_i}) - g\left(y_{t_i}^M(\boldsymbol{\theta})\right) \\ -\left[g(y_{t_{i-1}}) - g\left(y_{t_{i-1}}^M(\boldsymbol{\theta})\right)\right]\exp\left(-\frac{t_i - t_{i-1}}{\tau}\right)\end{array}\right]^2}{\sigma^2\left(1-\exp\left(-2\frac{t_i - t_{i-1}}{\tau}\right)\right)}\right)\cdot\left|\frac{dg}{dy}\bigg|_{y=y_{t_i}}\right|\right]$$

Yang et al., 2007, WRR, JHydrol

Issues wrt Calibration of Distributed Watershed Models

- Parameterization

  (most important, difficult, and neglected aspect of calibration)

- Objective function definition

  (most surprising aspect of calibration)

- Non-uniqueness (uncertainty)

  (most difficult part to quantify and communicate)

- Parameter conditionality

  (most disappointing aspect of calibration)

- Positioning observed outlets in SWAT

  (causes the biggest headache in calibration)

- Time constraint

  (makes some projects impossible to build and run)

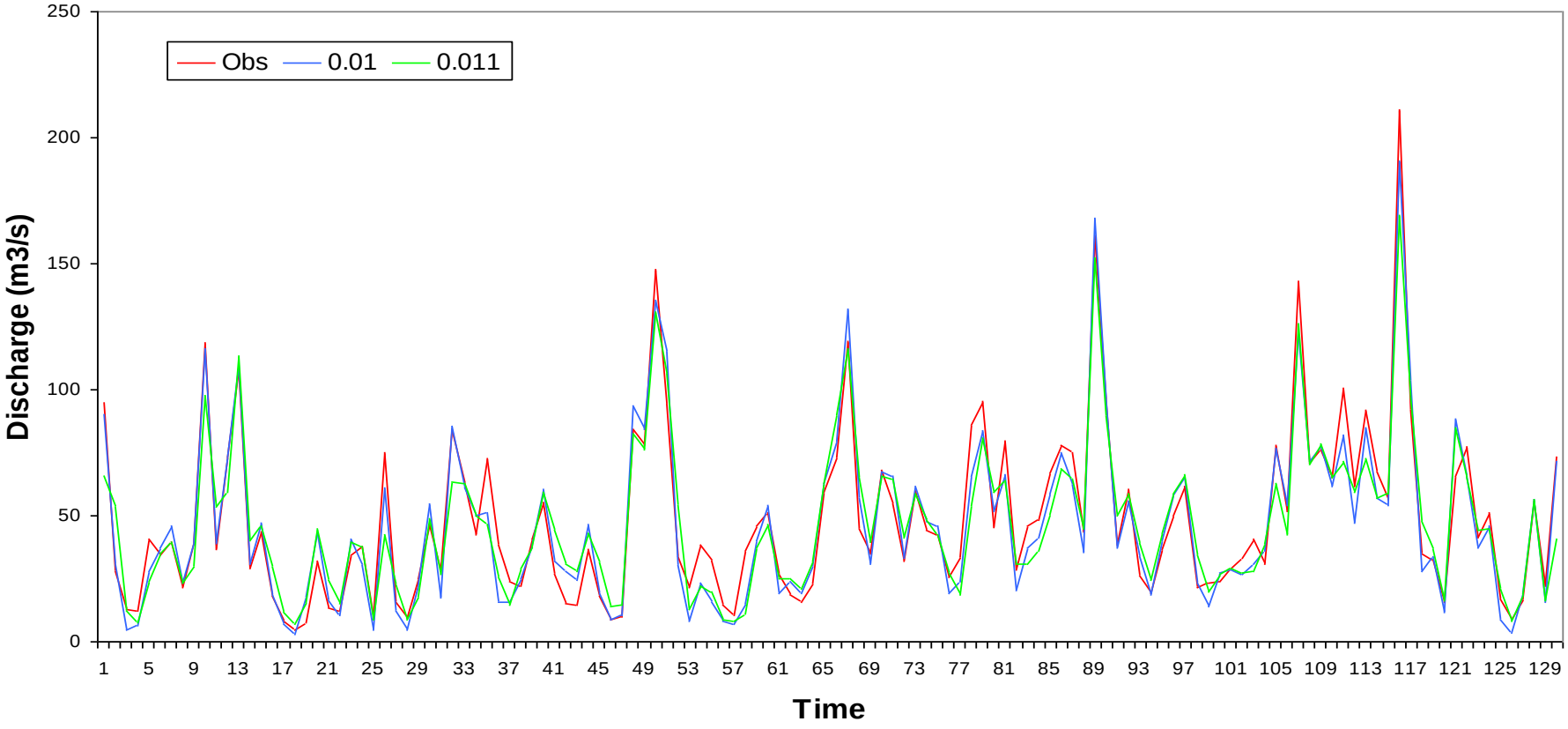
Non-uniqueness

Direct (deterministic) Modelling:

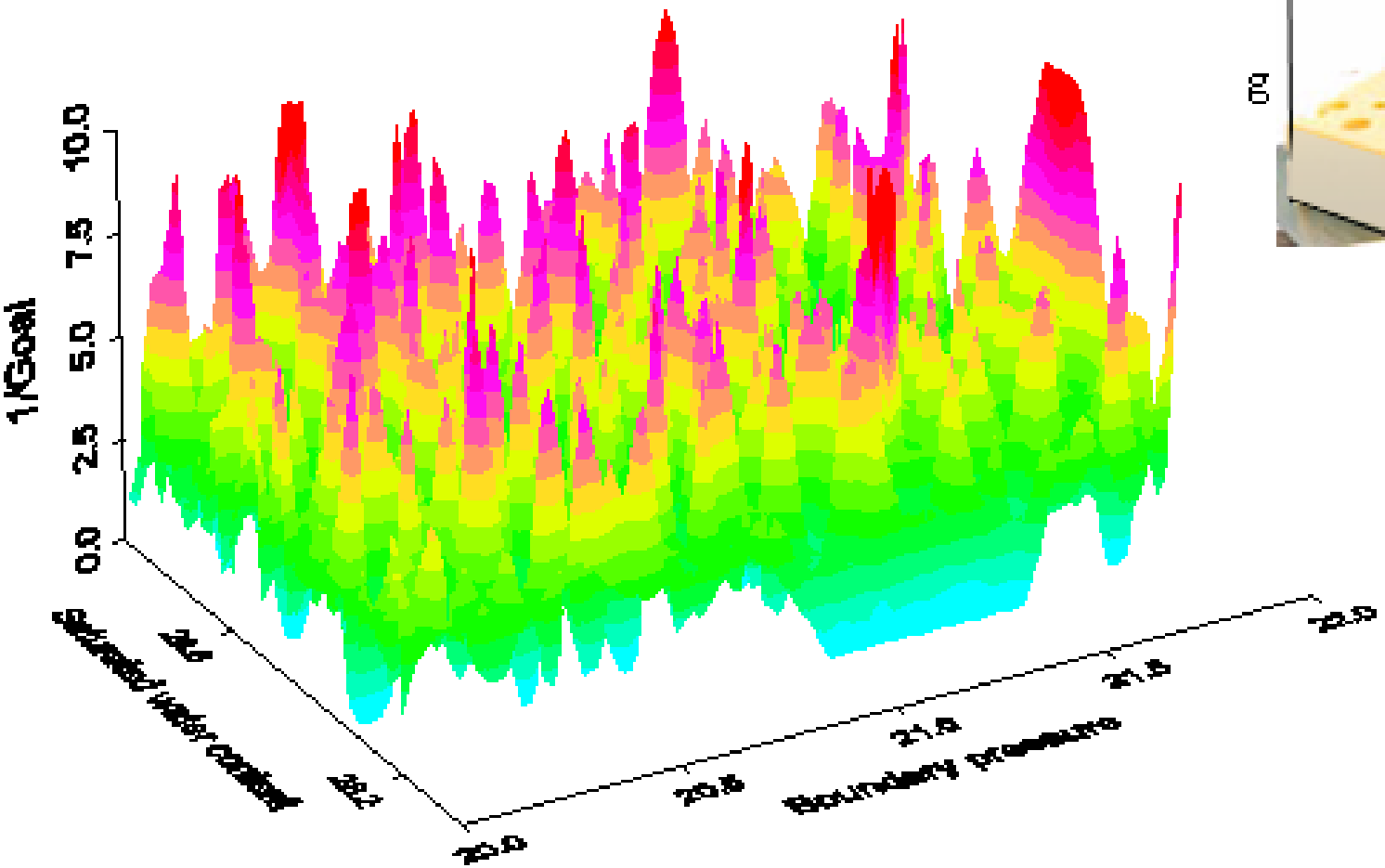
Inverse Modelling:

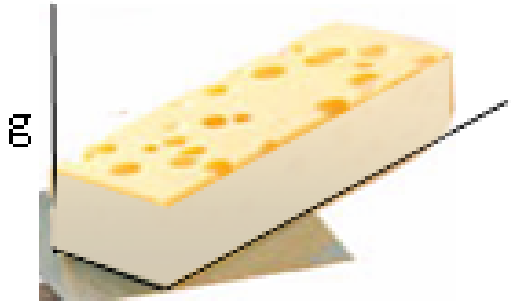
Non-uniqueness

GW_DELAY	CH_N2	CN2	REVAPMN	Sol_AWC	g
3.46	0.0098	50	0.8	0.11	0.010
0.34	0.131	20	2.4	0.2 3	0.011



The Swiss Cheese Effect (multimodality of the objective function)





Issues wrt Calibration of Distributed Watershed Models

- Parameterization

  (most important, difficult, and neglected aspect of calibration)

- Objective function definition

  (most surprising aspect of calibration)

- Non-uniqueness

  (most difficult part to quantify and communicate)

- Parameter conditionality

  (most disappointing aspect of calibration)

- Positioning observed outlets in SWAT

  (causes the biggest headache in calibration)

- Time constraint

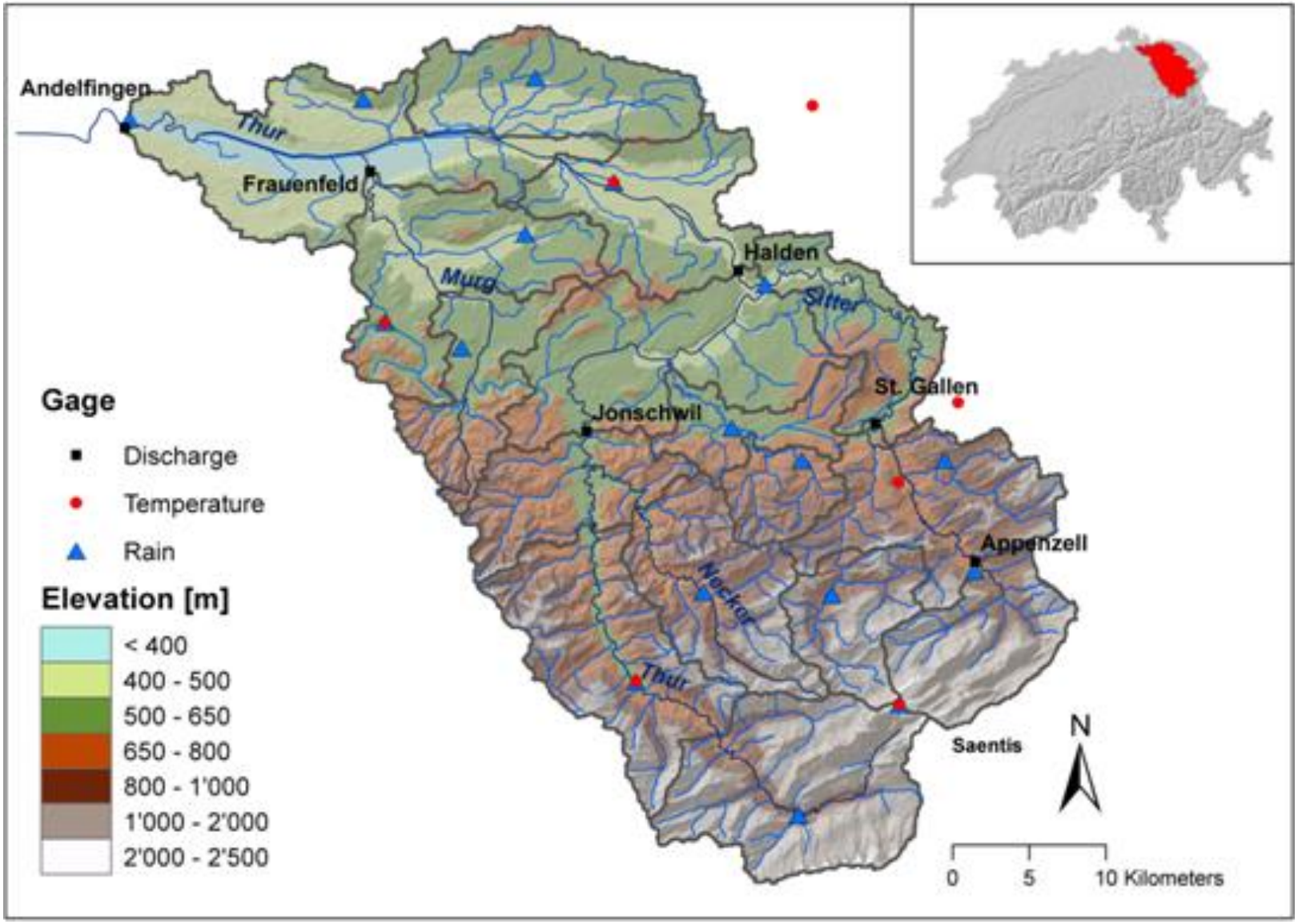
  (makes some projects impossible to build and run)

Parameter Conditionality

(B)

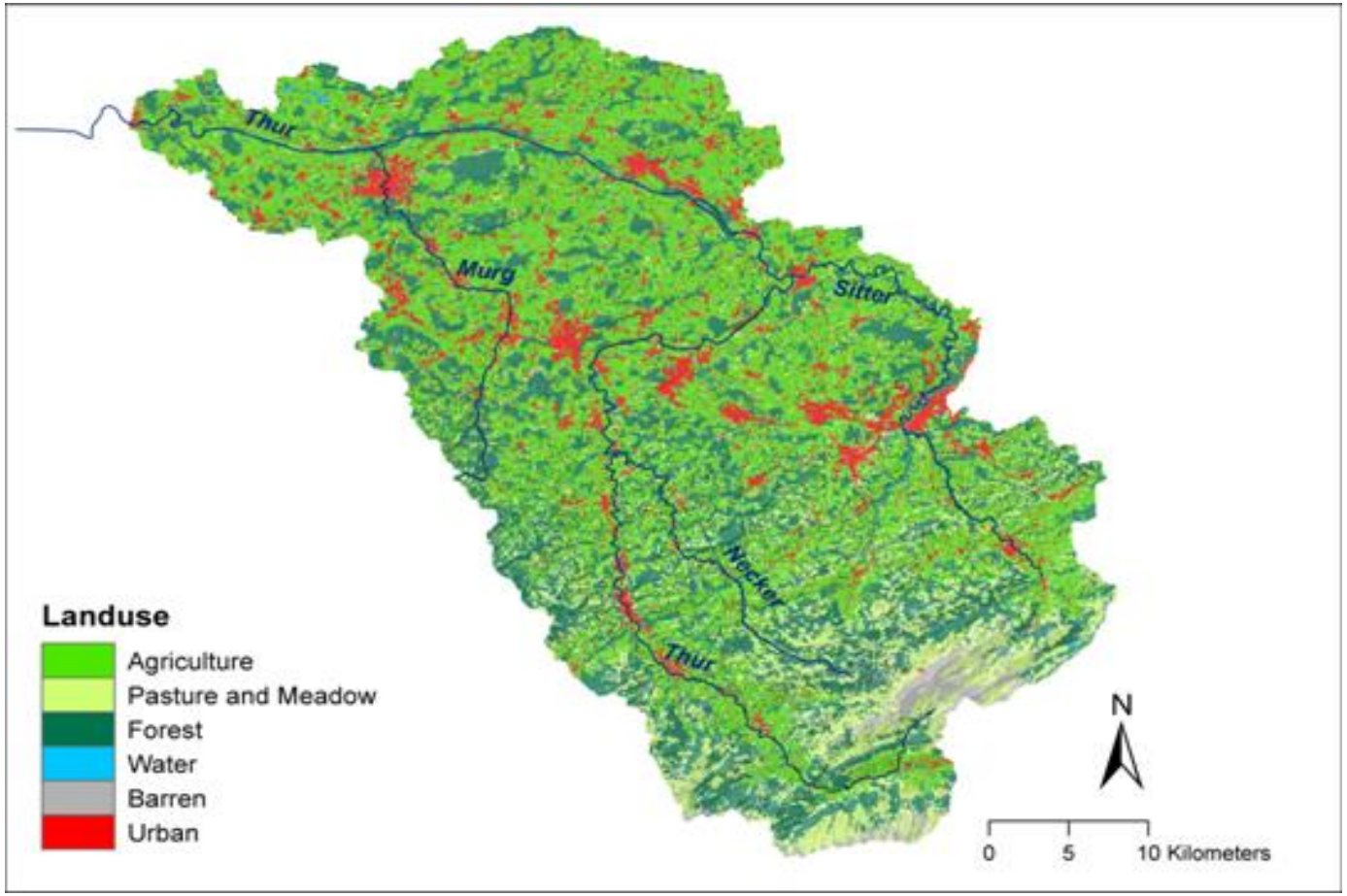
- watershed parameterization
- type of the objective function
- weights in the objective function
- conceptual model (model structure)
- experimental procedure (to collect the calibrating data)
- input (driving or forcing) data
- number and type of variables (in the objective function)
- location of outlets
- .....

Model Conditionality: Example Thur



Model Conditionality: Example Thur

$$g = w_1 \sum_{i=1}^{n} (Q_m - Q_s)_i^2 + w_2 \sum_{i=1}^{n} (S_m - S_s)_i^2 + w_3 \sum_{i=1}^{n} (N_m - N_s)_i^2 + w_4 \sum_{i=1}^{n} (P_m - P_s)_i^2$$



Model Conditionality: Example Thur

$$g = w_1 \sum_{i=1}^{n} (Q_m - Q_s)_i^2 + w_2 \sum_{i=1}^{n} (S_m - S_s)_i^2 + w_3 \sum_{i=1}^{n} (N_m - N_s)_i^2 + w_4 \sum_{i=1}^{n} (P_m - P_s)_i^2$$

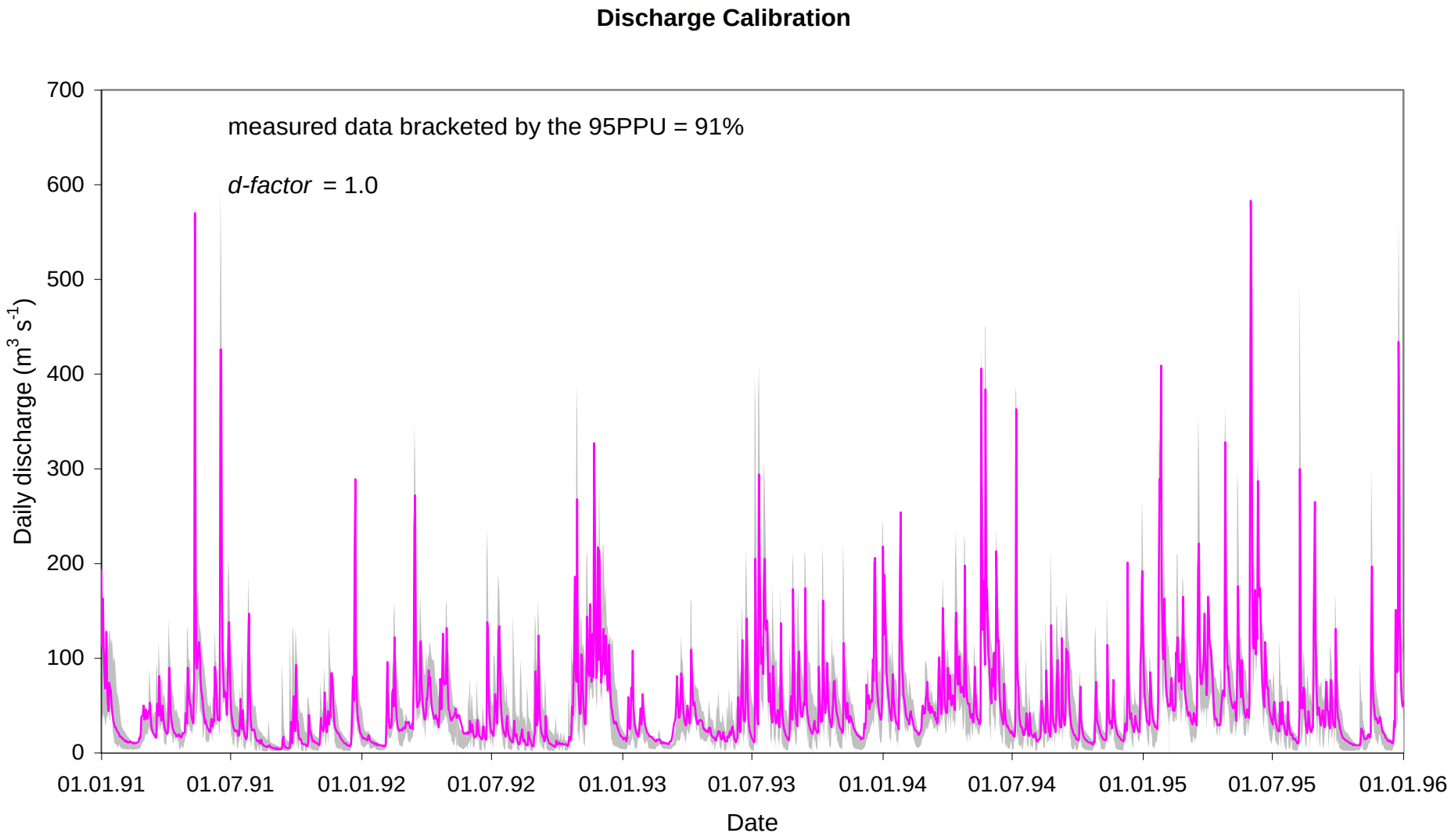
$2.2 < N_{forest} < 16$

$19 < N_{agricultural} < 47$

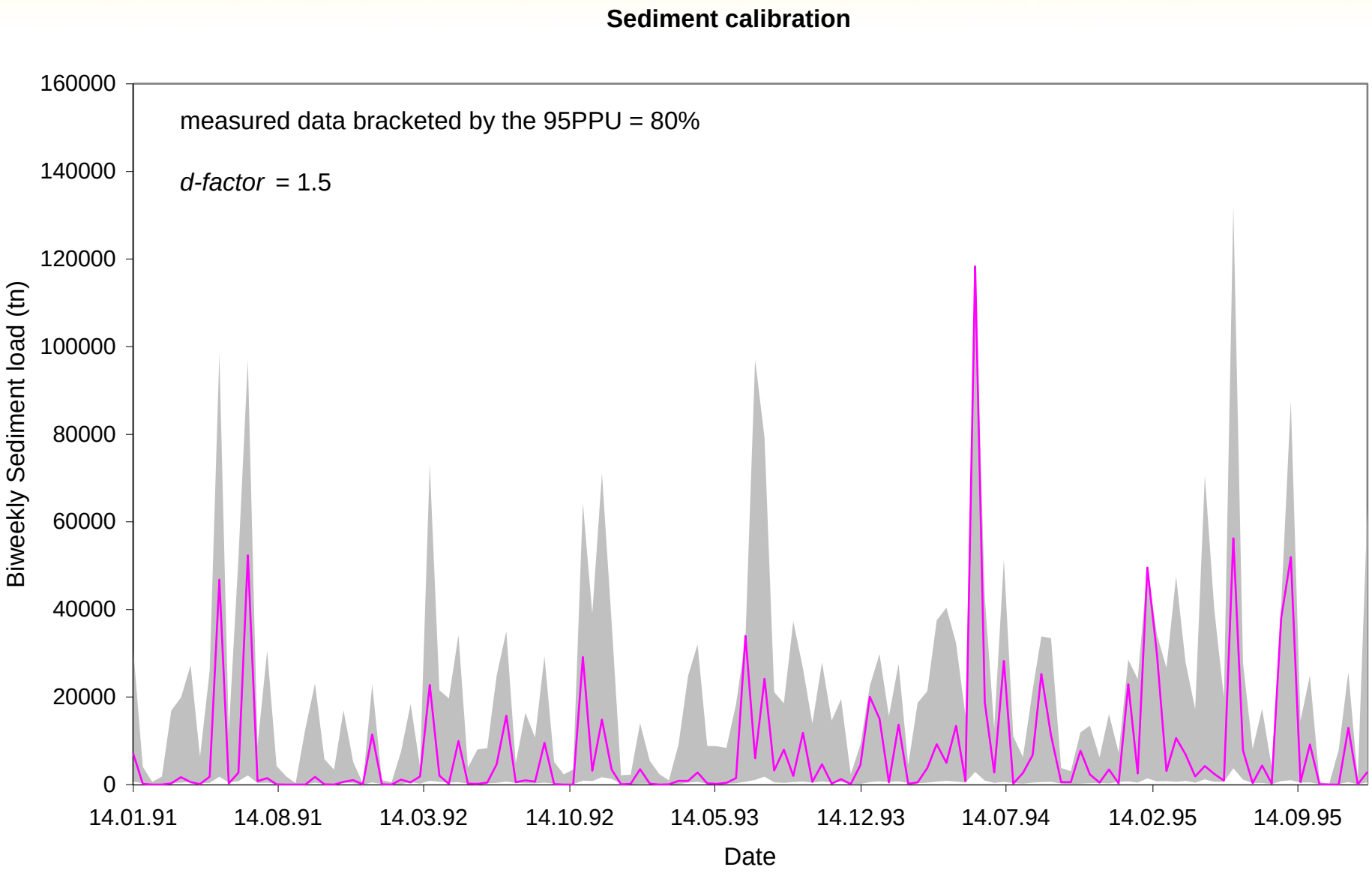
$15 < N_{pasture} < 25$

……..

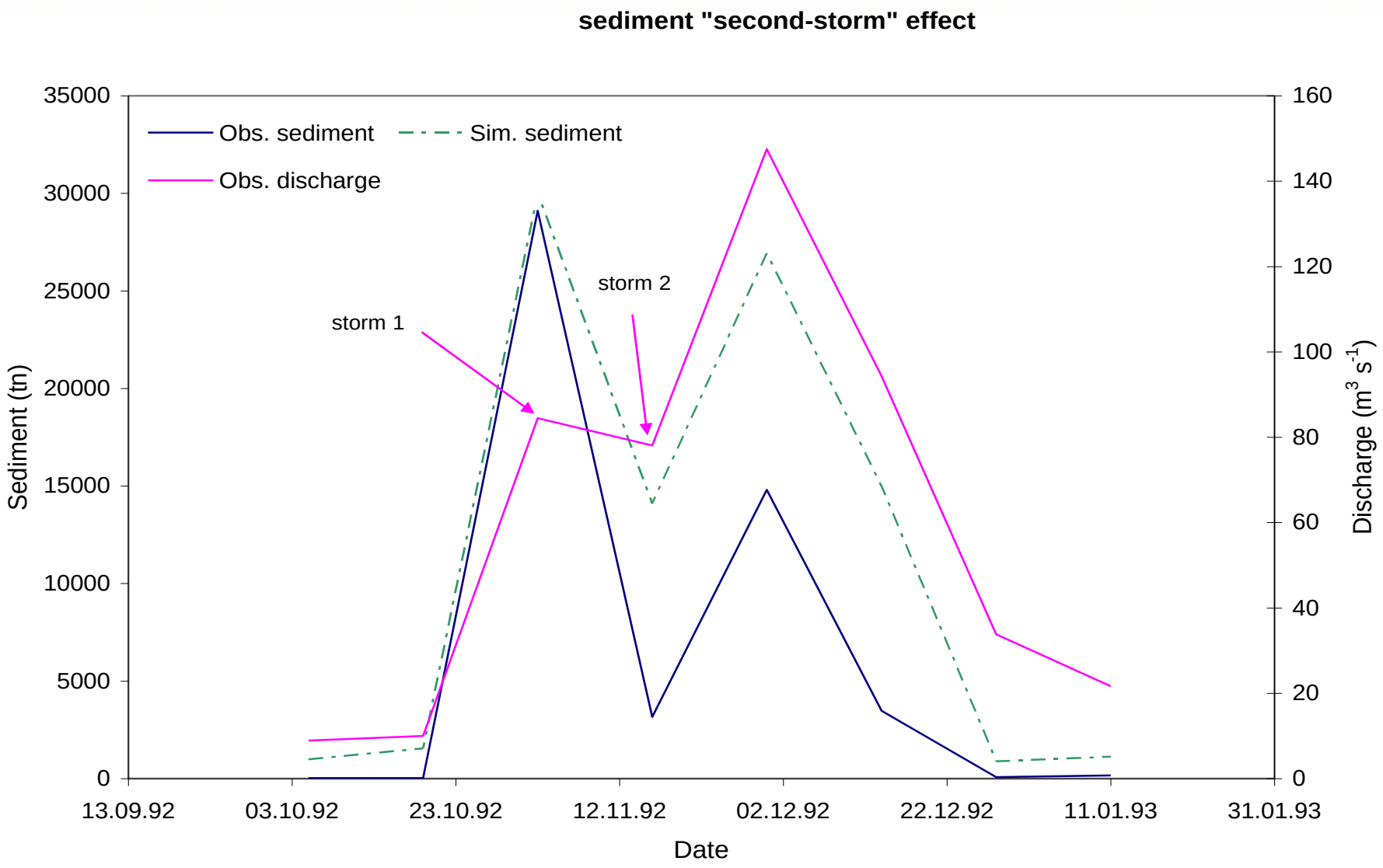
Model Conditionality: Example Thur



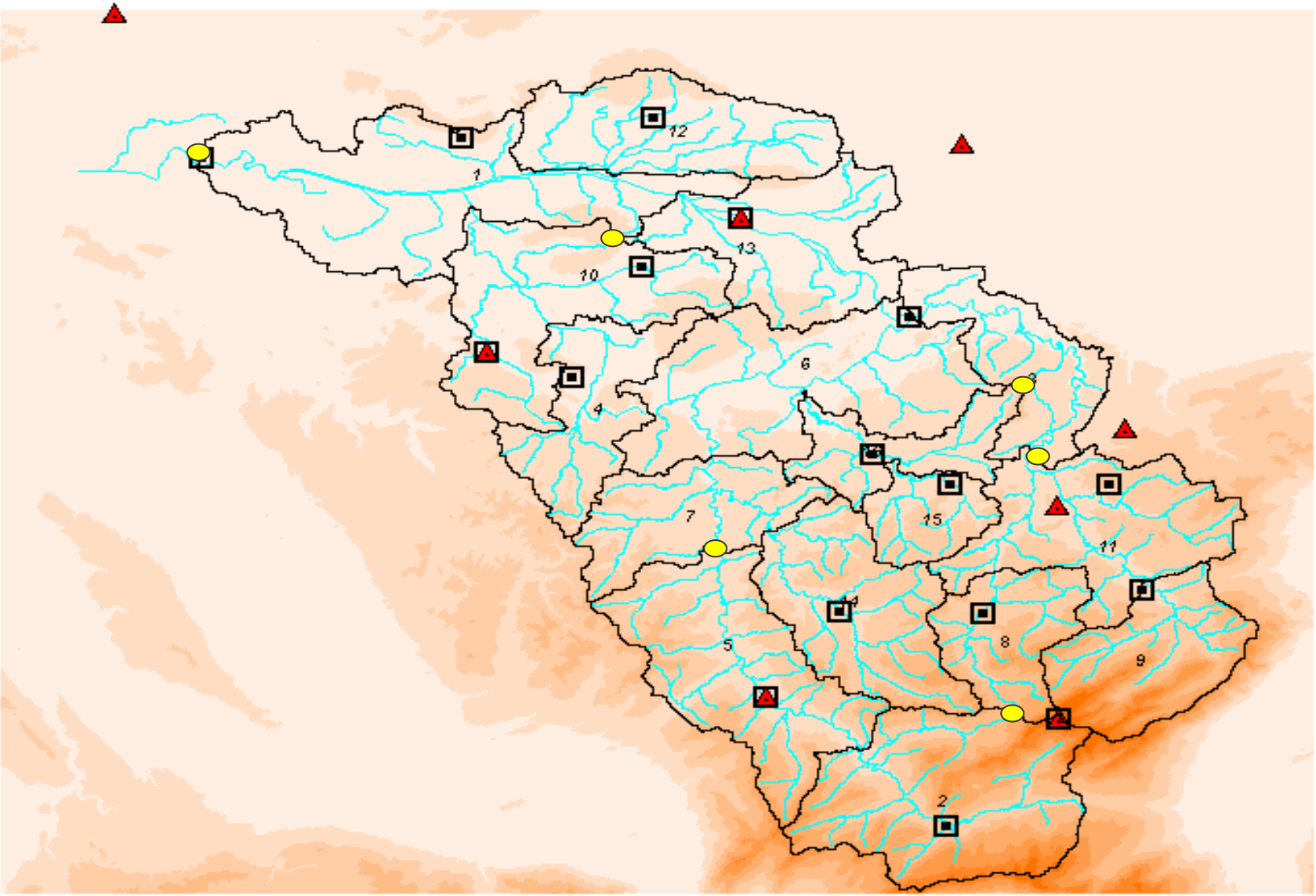
Model Conditionality: Example Thur



Model Conditionality: Example Thur



Model Conditionality: Example Thur



Model Conditionality: Example Thur

A calibrated model is always conditioned on the situation that it was calibrated for and care must be taken to apply it to outside this boundary

Issues wrt Calibration of Distributed Watershed Models

- Parameterization

  (most important, difficult, and neglected aspect of calibration)

- Objective function definition

  (most surprising aspect of calibration)

- Non-uniqueness

  (most difficult part to quantify and communicate)

- Parameter conditionality

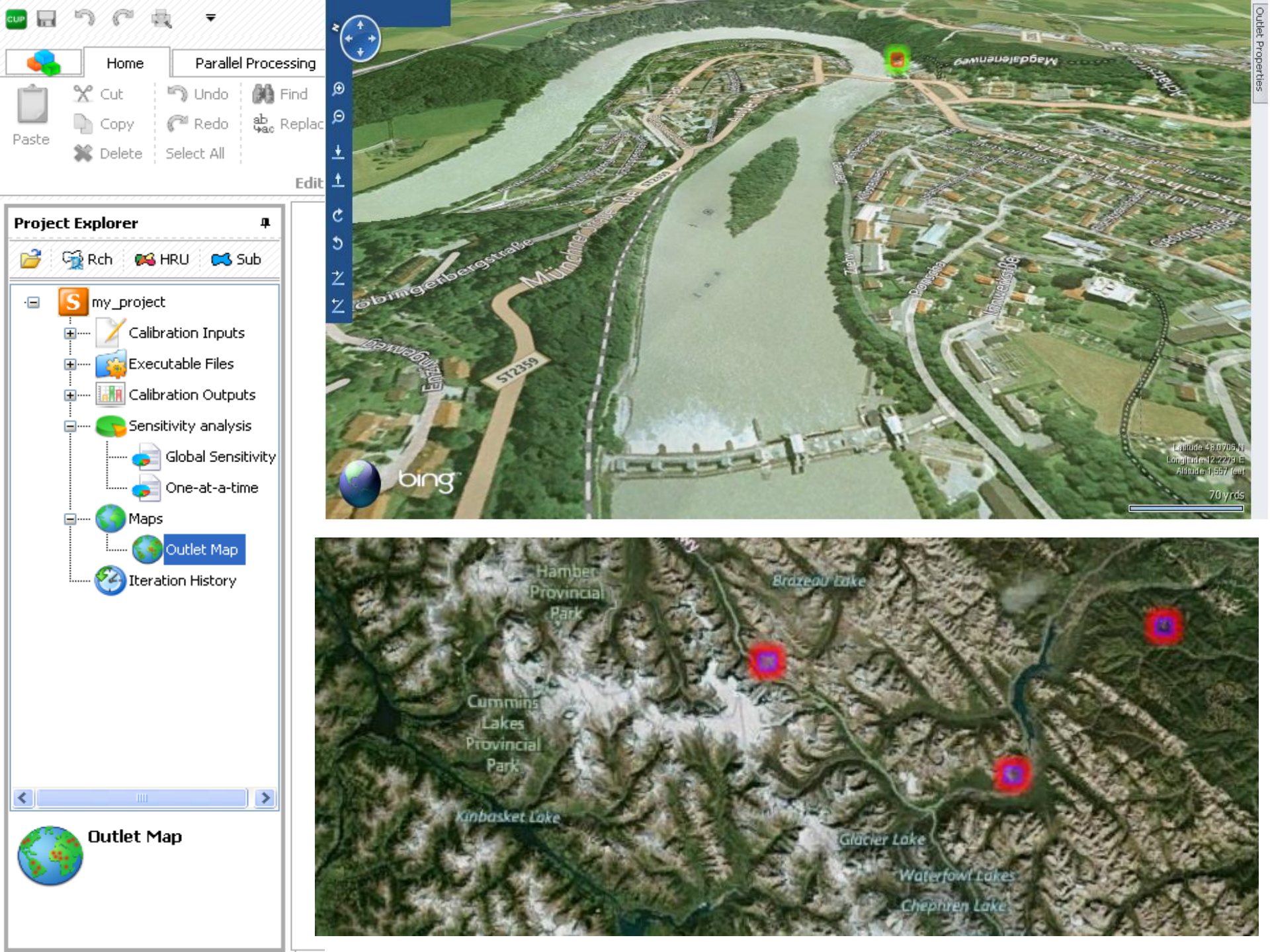
  (most disappointing aspect of calibration)

- Positioning observed outlets in SWAT

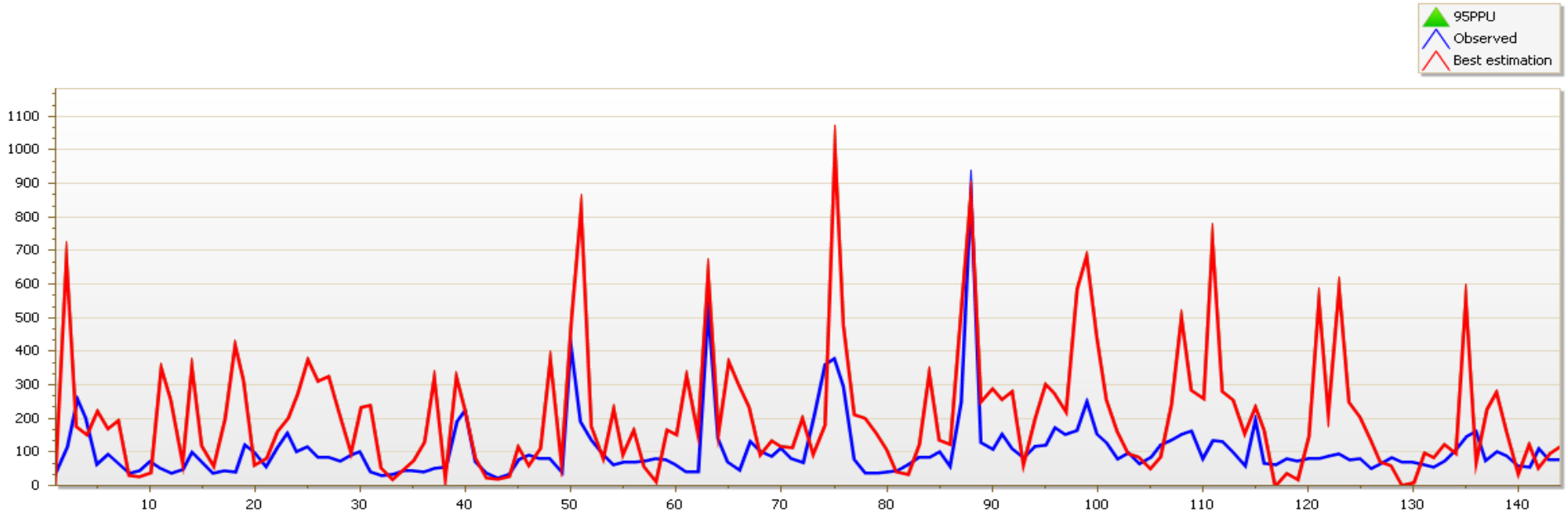
  (causes the biggest headache in calibration)

- Time constraint

  (makes some projects impossible to build and run)

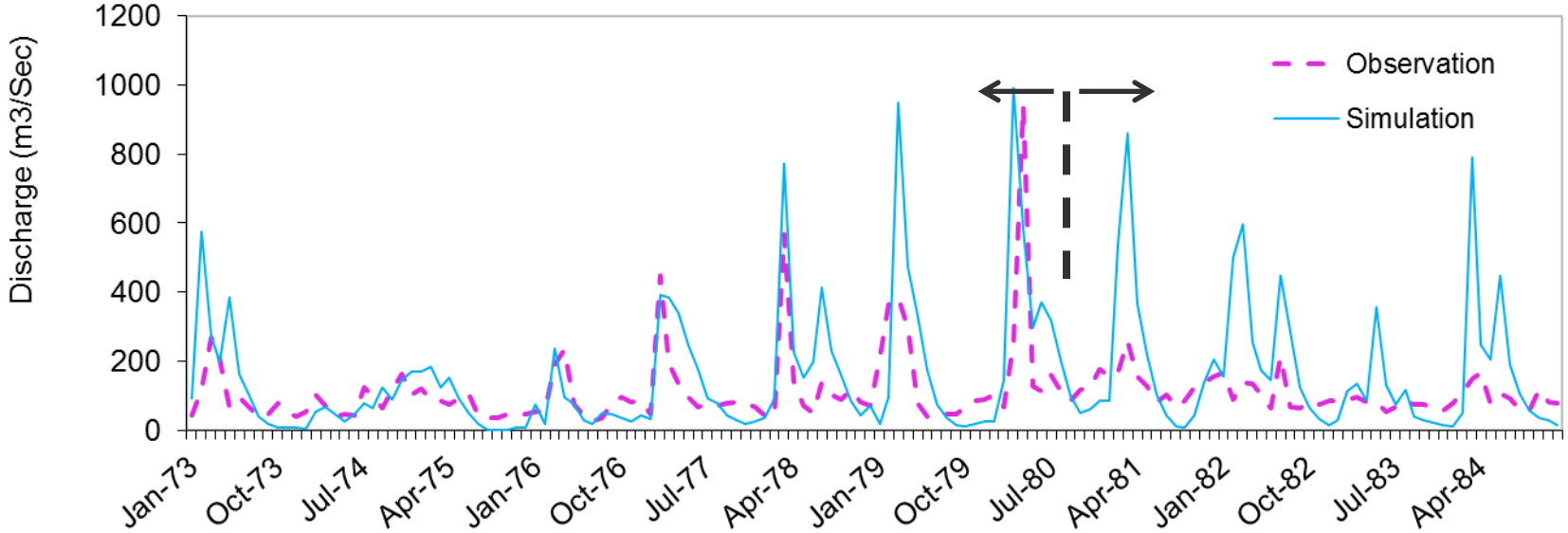

Home
Parallel Processing
Cut
Copy
Delete
Undo
Redo
Select All
Find
Replac
Paste
Edit
Project Explorer
Rch
HRU
Sub
my_project
Calibration Inputs
Executable Files
Calibration Outputs
Sensitivity analysis
Global Sensitivity
One-at-a-time
Maps
Outlet Map
Iteration History
Outlet Map
Outlet Properties
bing
70 yrds
Hamber Provincial Park
Brazeau Lake
Cummins Lakes Provincial Park
Kinbasket Lake
Glacier Lake
Waterfowl Lakes
Chephren Lake

q_5842

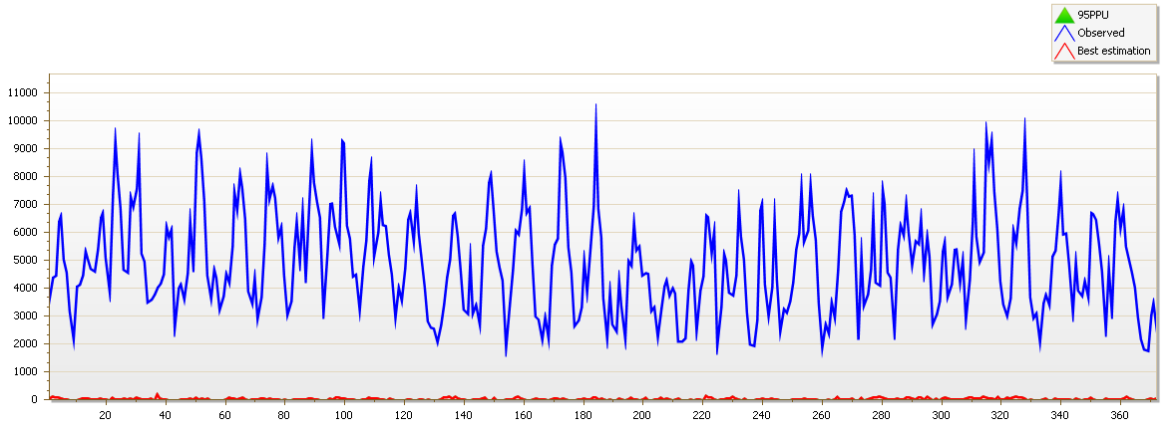

95PPU
Observed
Best estimation
1100
1000
900
800
700
600
500
400
300
200
100
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140

R06
bing
Latitude 47.7092 N
Longitude 31.2422 E
Altitude 25 feet
300 yrds

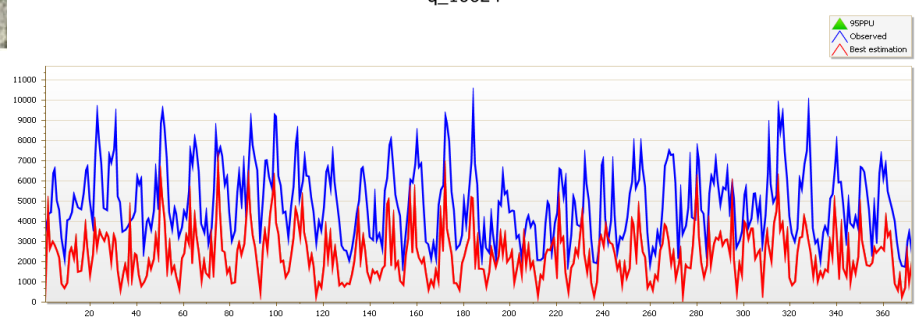
River Discharge (Q_5842, Southern Bug), Aleksandrovka reservoir



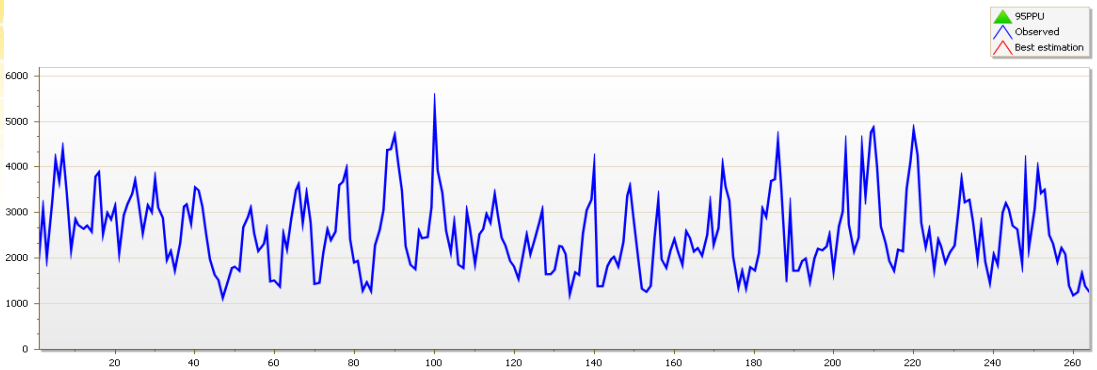
q_10565

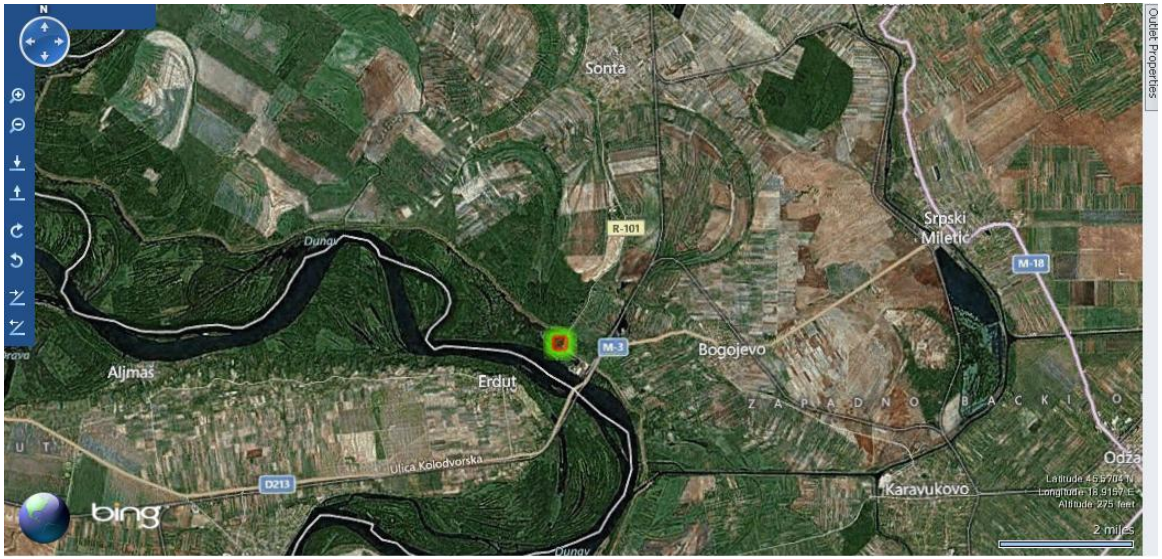


q_10624

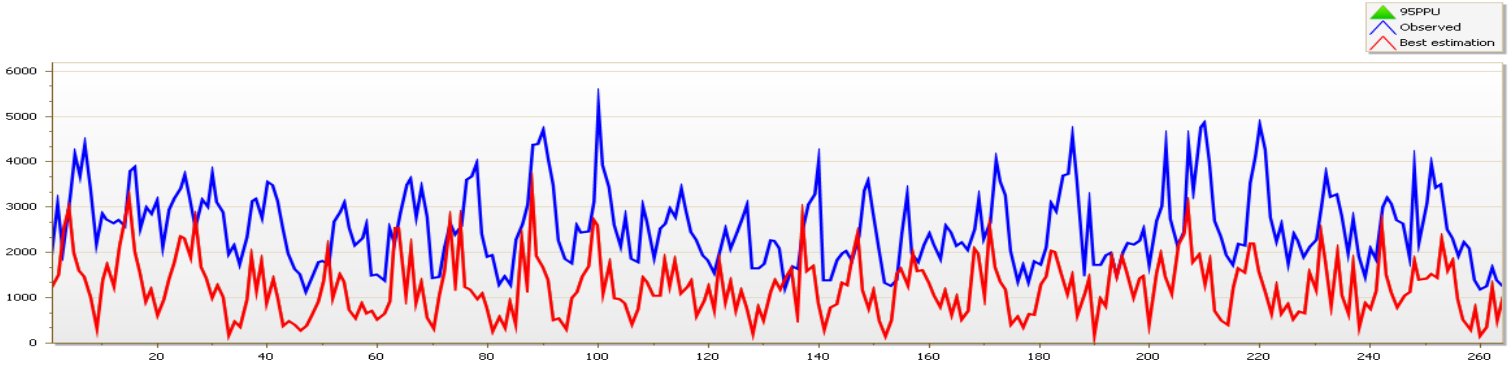


q_10137





q_10140



Issues wrt Calibration of Distributed Watershed Models

- Parameterization

  (most important, difficult, and neglected aspect of calibration)

- Objective function definition

  (most surprising aspect of calibration)

- Non-uniqueness

  (most difficult part to quantify and communicate)

- Parameter conditionality

  (most disappointing aspect of calibration)

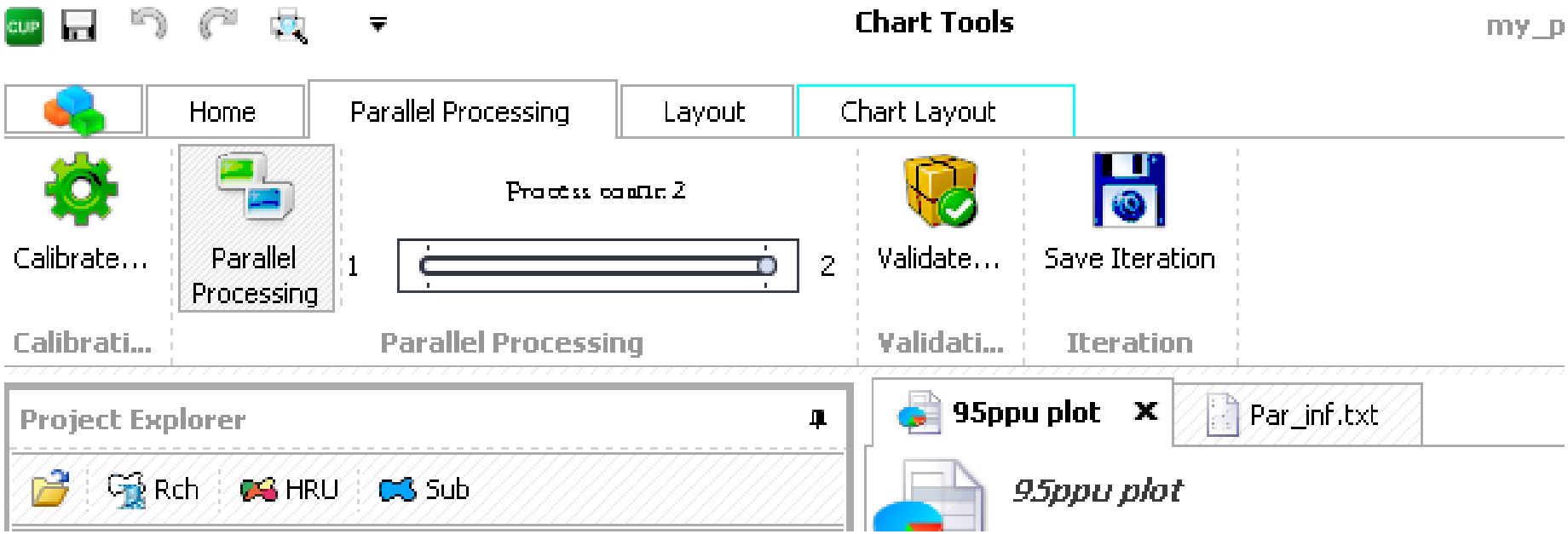
- Positioning observed outlets in SWAT

  (causes the biggest headache in calibration)

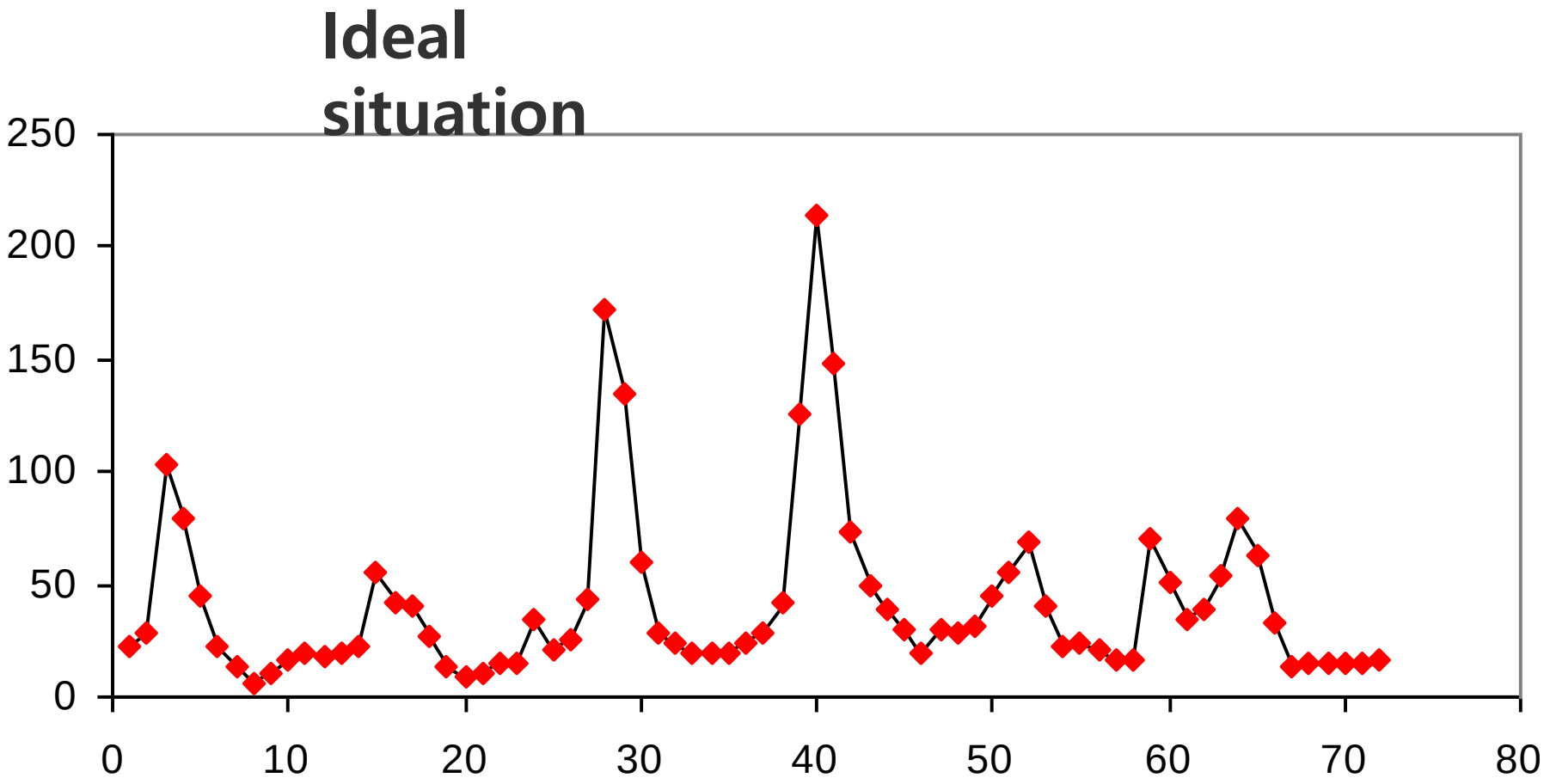
- Time constraint

  (makes some projects impossible to build and run)

- Parallel Processing



Model Uncertainty



Sources of Model Uncertainty

Errors in:

- Input data (rainfall, landuse,discharge……)
- Model parameters
- Conceptual model

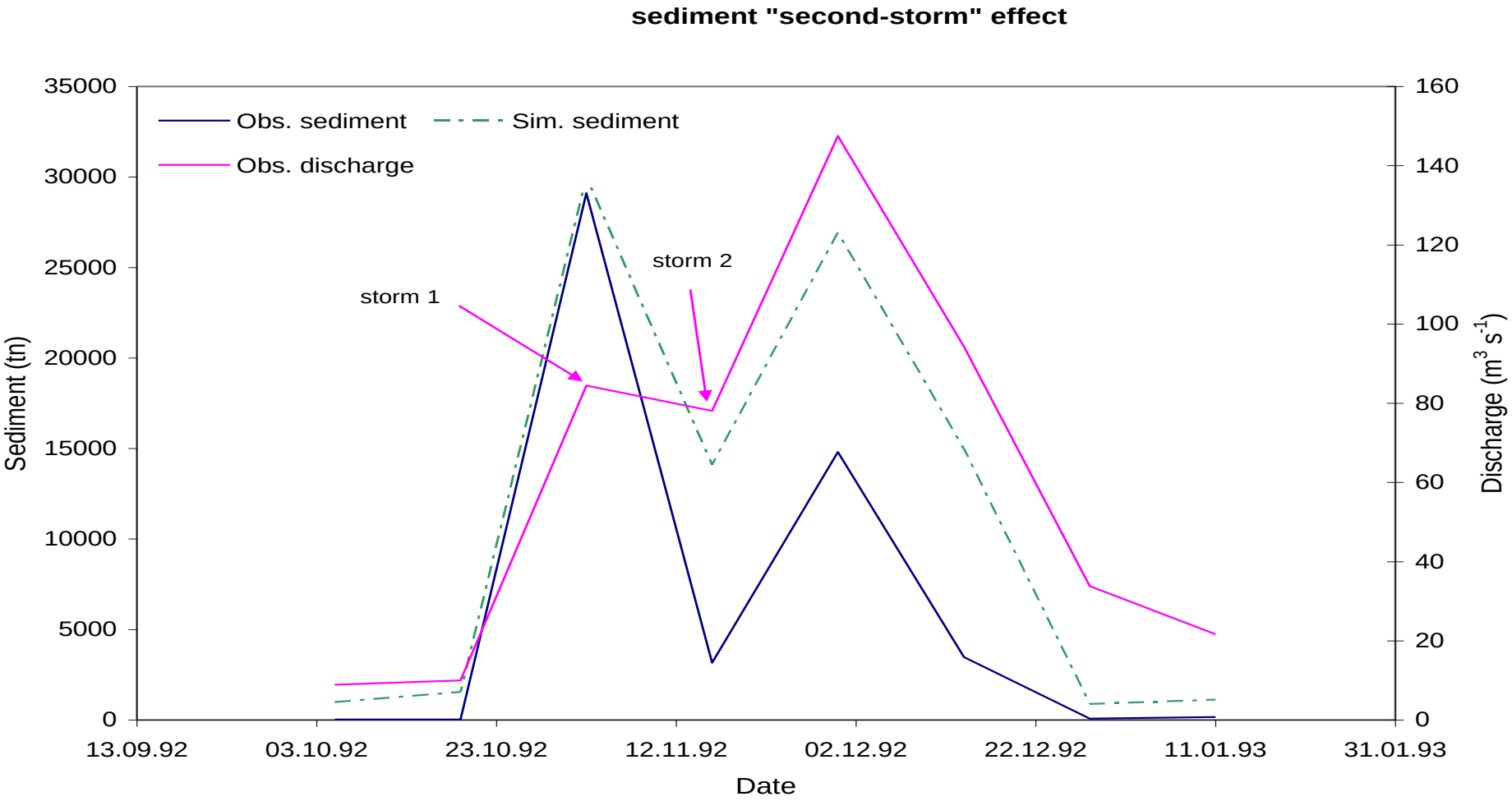
Conceptual model uncertainty

“All models are wrong - but some models are useful”
G. Box

processes occurring in the watershed but not accounted for, or not accurately accounted for in the model (wetland processes, glacier melting…)

processes accounted for in the model , but their occurrences are not known in the watershed (water transfers, unusual erosion,….)

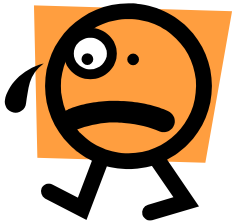
Conceptual model uncertainty



Sources of Model Uncertainty….

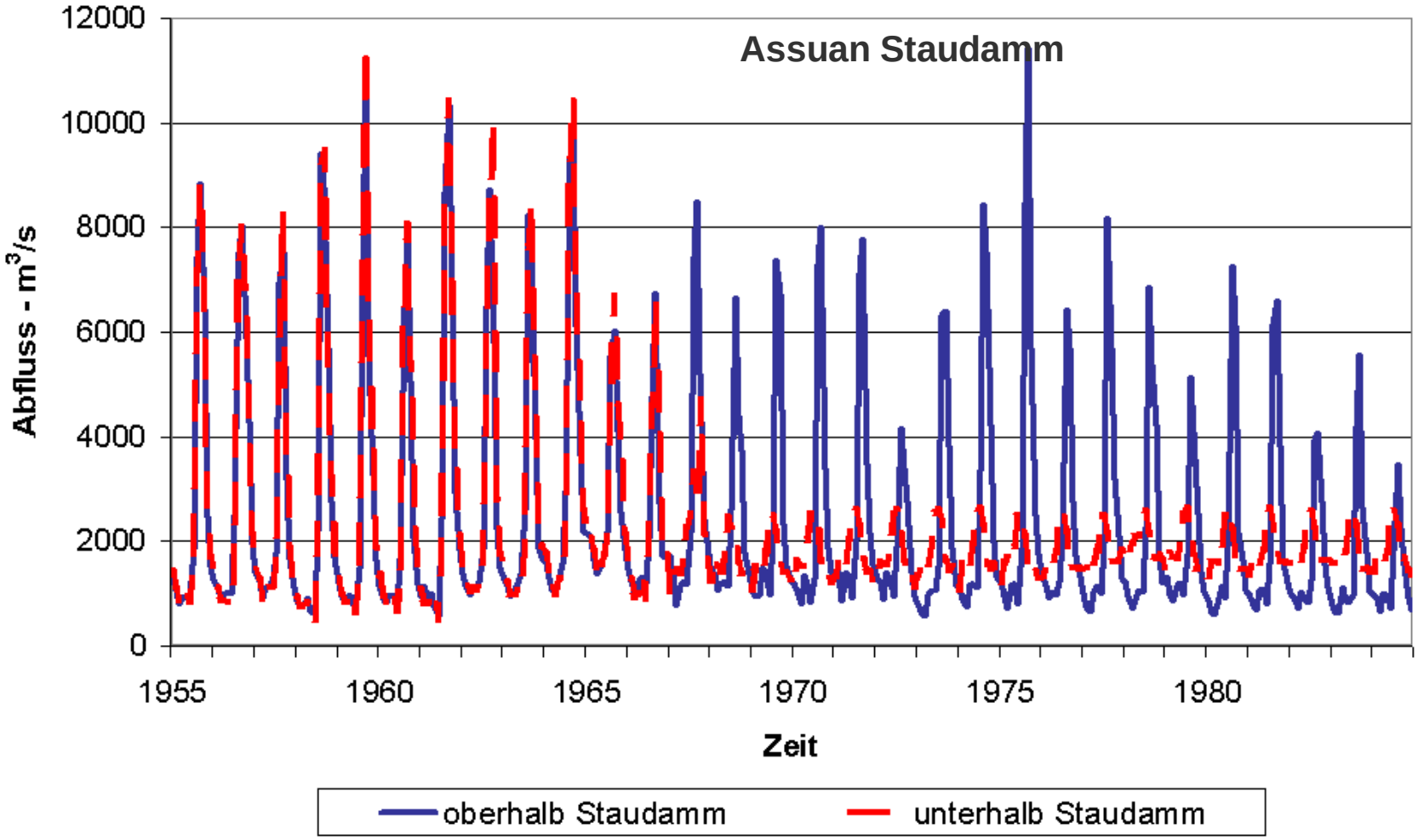
Finally…

Modeler!



5 2 2006

Effect of Aswan dam on downstream discharge



SWAT-CUP

http://www.eawag.ch/forschung/siam/software/swat/index

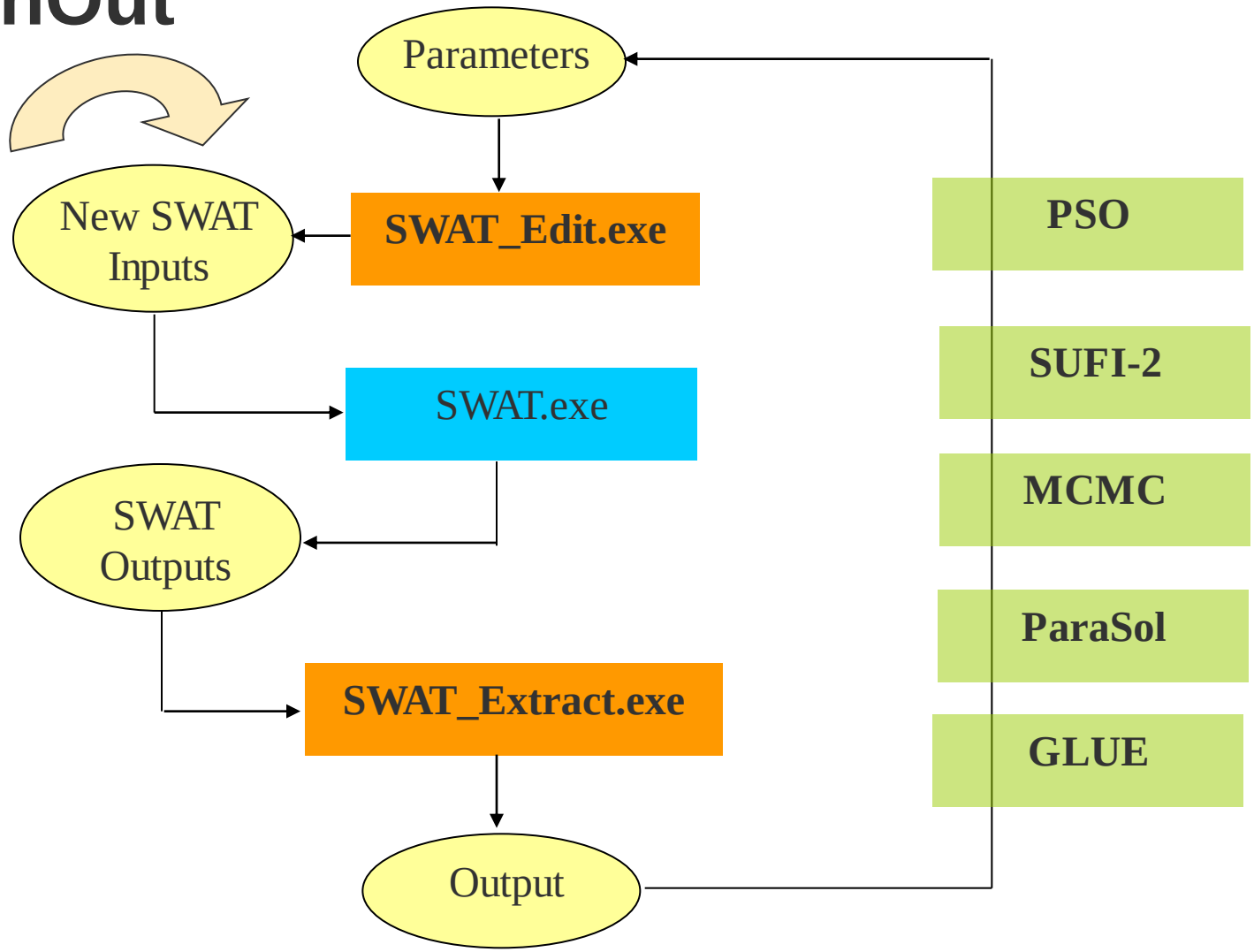
SWAT-CUP

SWAT Calibration and Uncertainty analysis Procedures

- Calibration
- Validation
- One-at-a-time and global Sensitivity analysis
- Uncertainty analysis
- Visualize the watershed and outlet locations
- Perform parallel processing
- Utility programs
    - upstream subbasins
    - make_observation
    - make elevation band

SWAT-CUP

TxtInOut



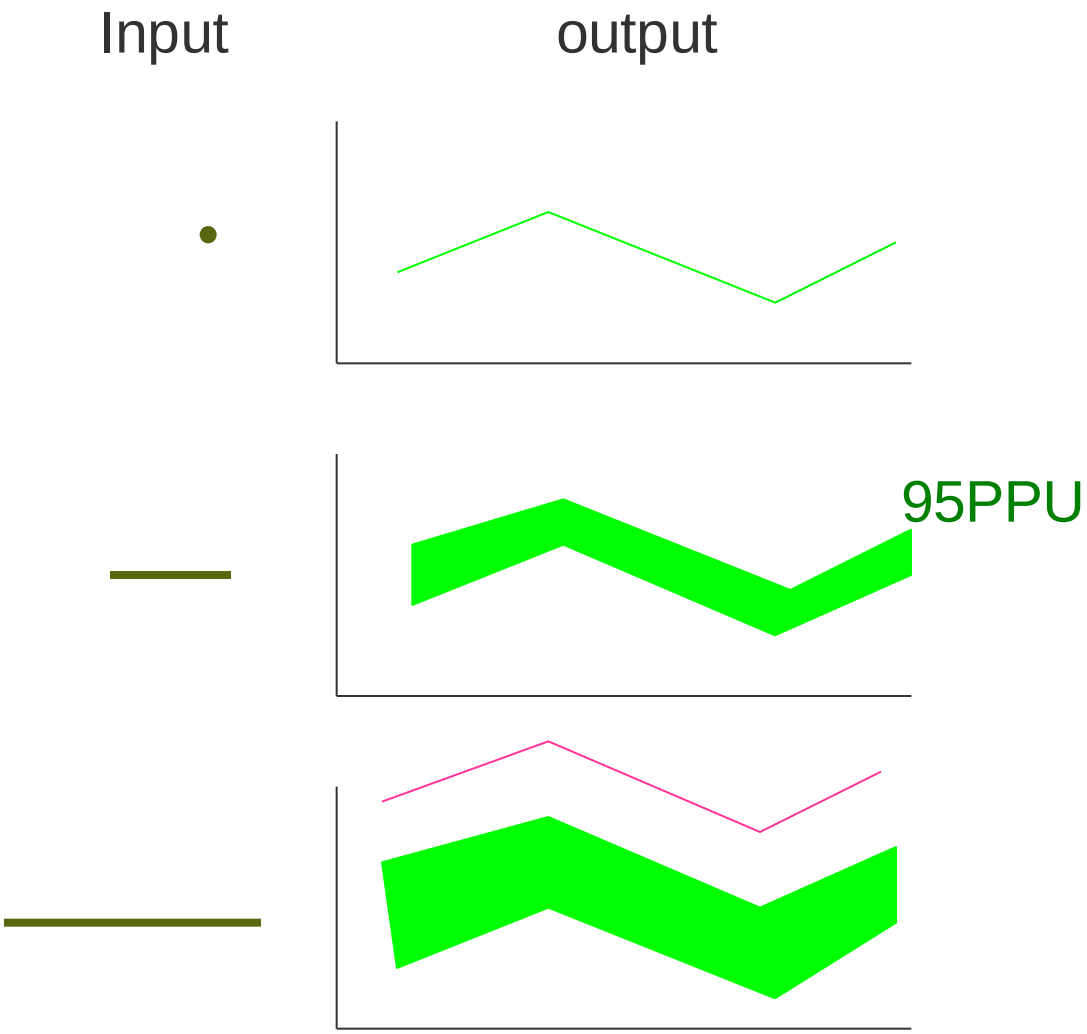
Latest version of SWAT-CUP could be downloaded from:

http://www.eawag.ch/forschung/siam/software/swat/index

http://swatmodel.tamu.edu

http://neprashtechnology.ca/

SUFI2



SUFI2 Concept

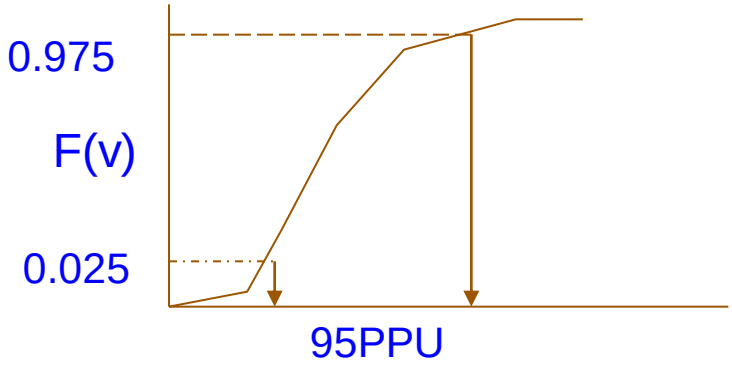
- Combines calibration and uncertainty analysis

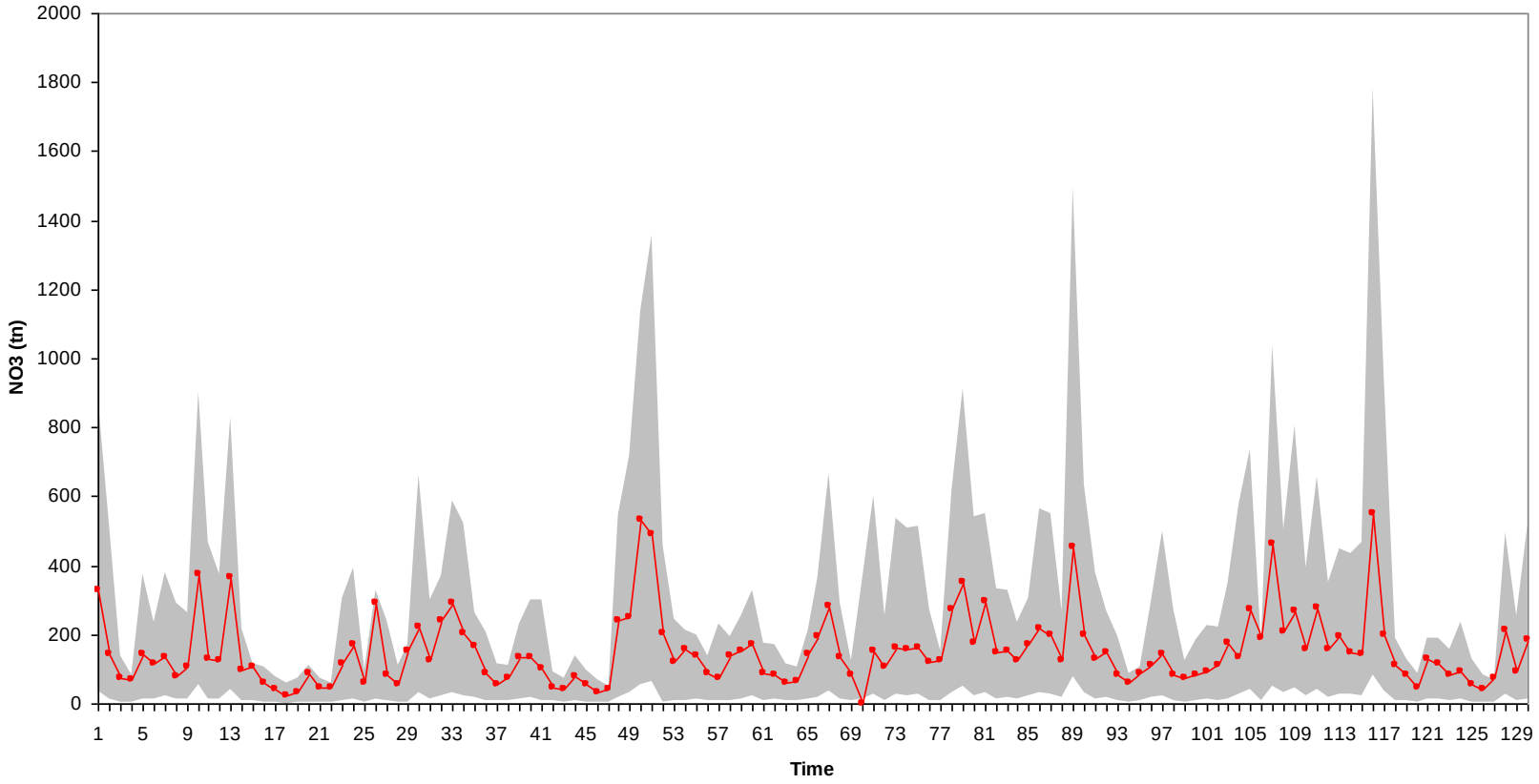
- Accounts for all uncertainties combined and maps them onto the parameters

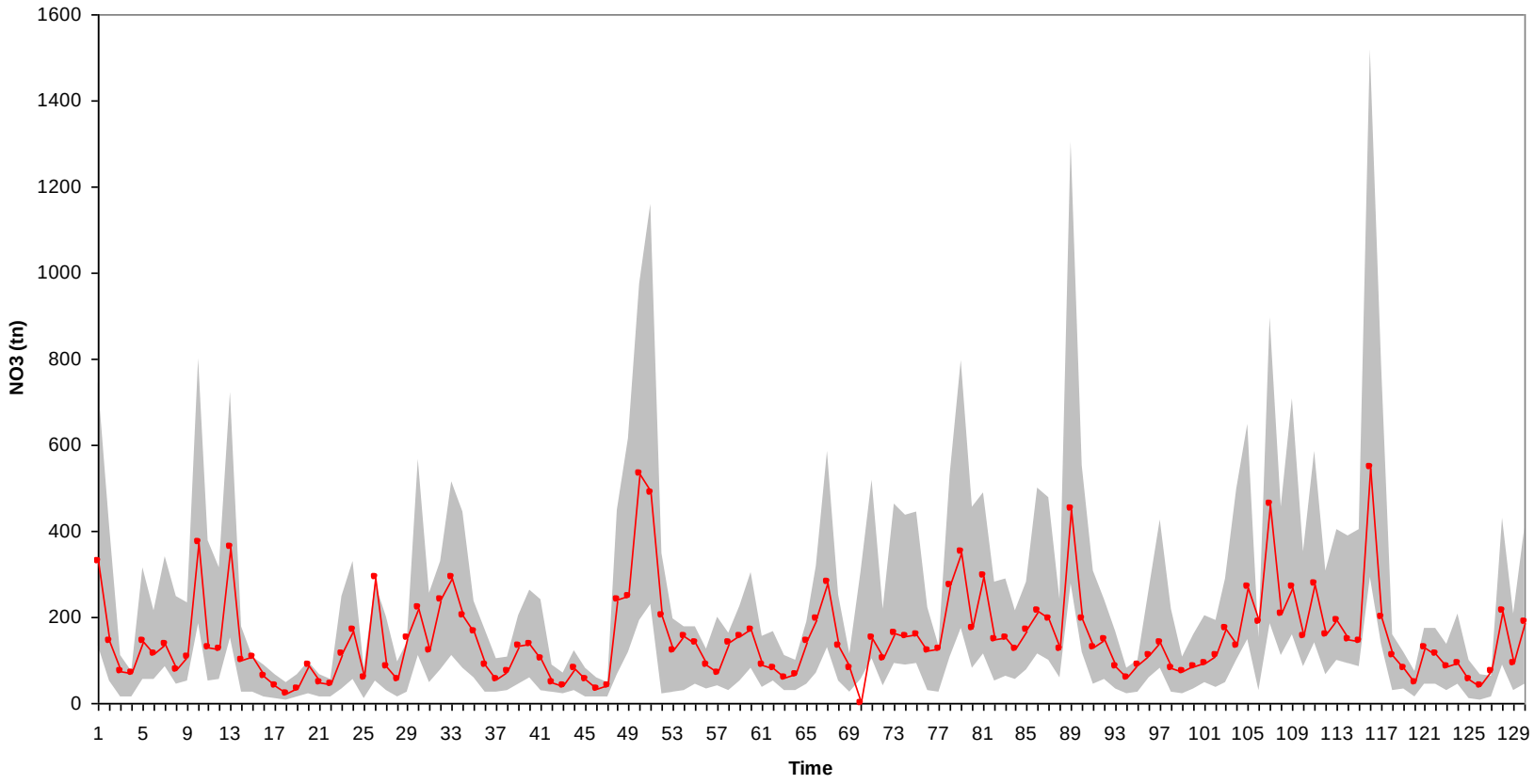
- Parameter uncertainty is depicted as an interval (uniform distribution)

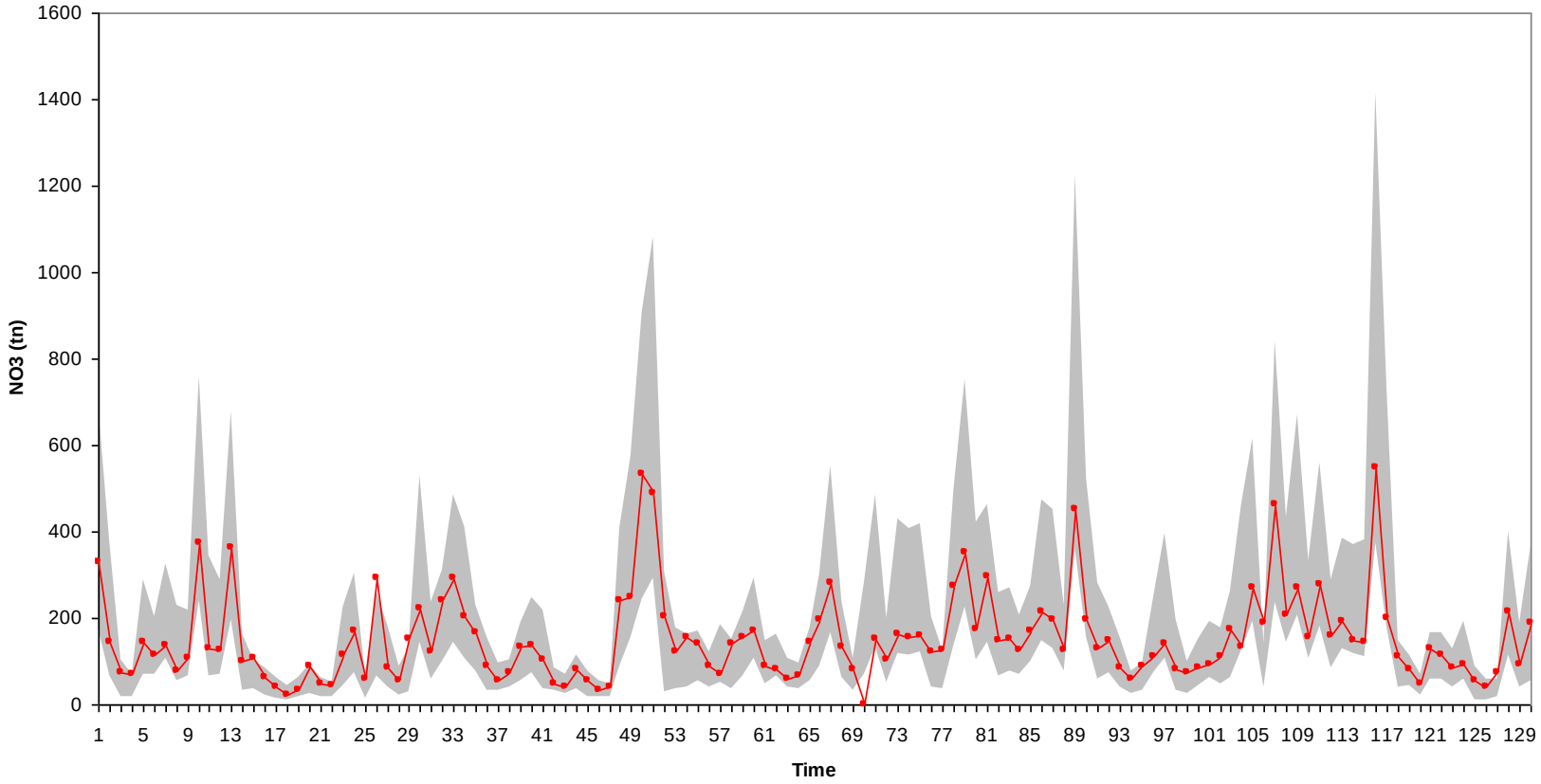
- Output uncertainty is quantified as the 95% prediction uncertainty (95PPU) calculate at the 2.5% and 97.5% levels

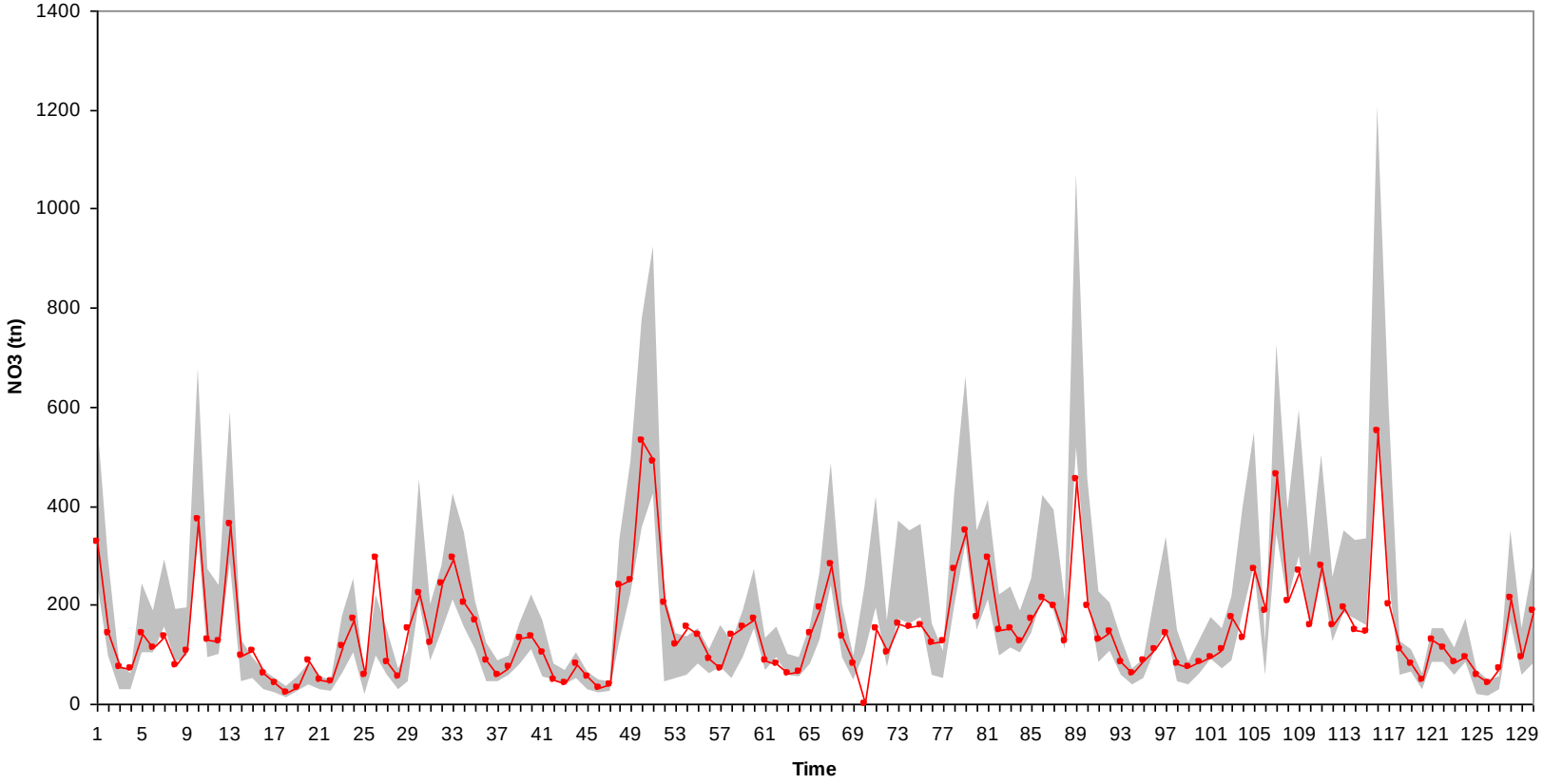
parameter uncertainty → Latin Hypercube simulation → Model →

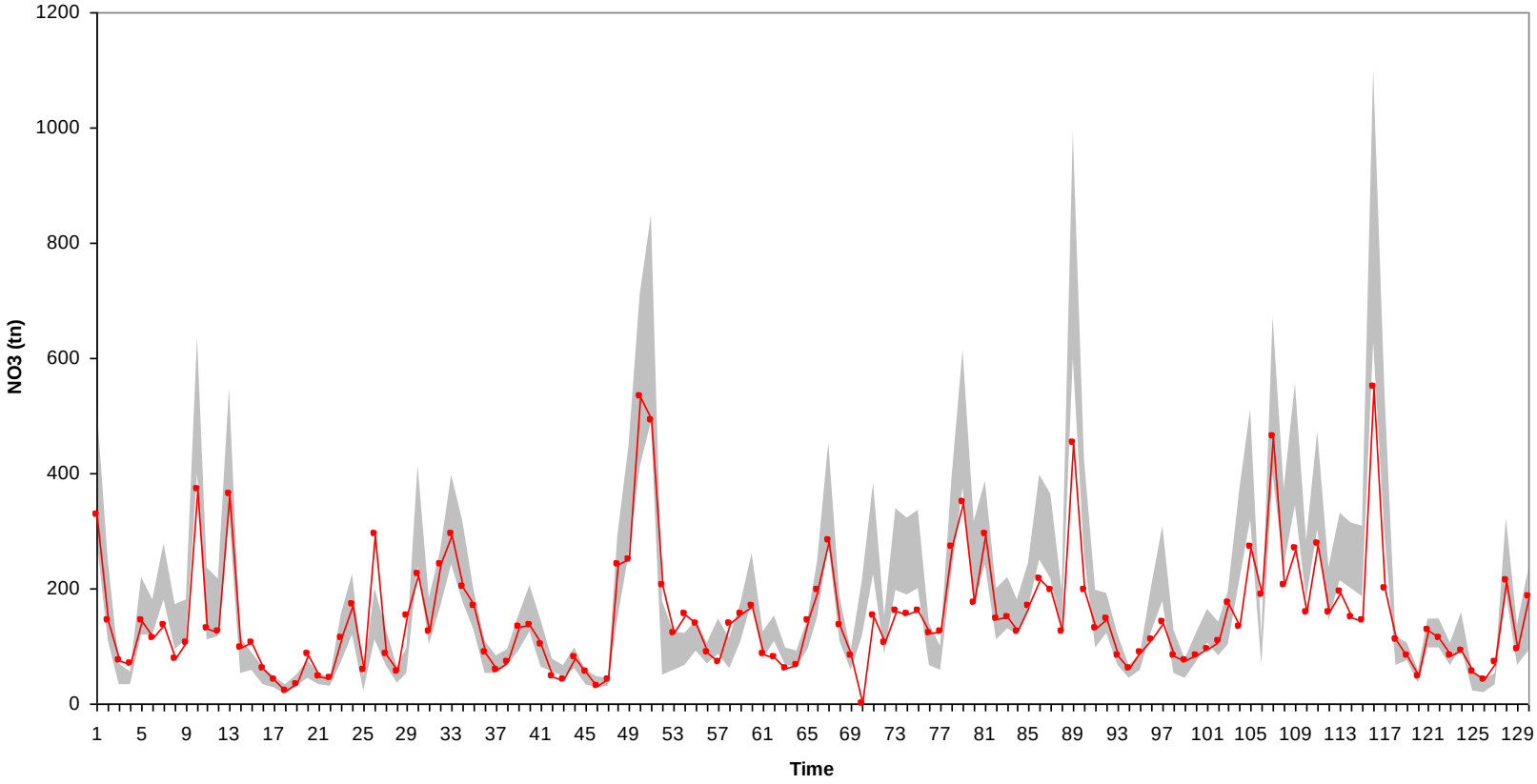


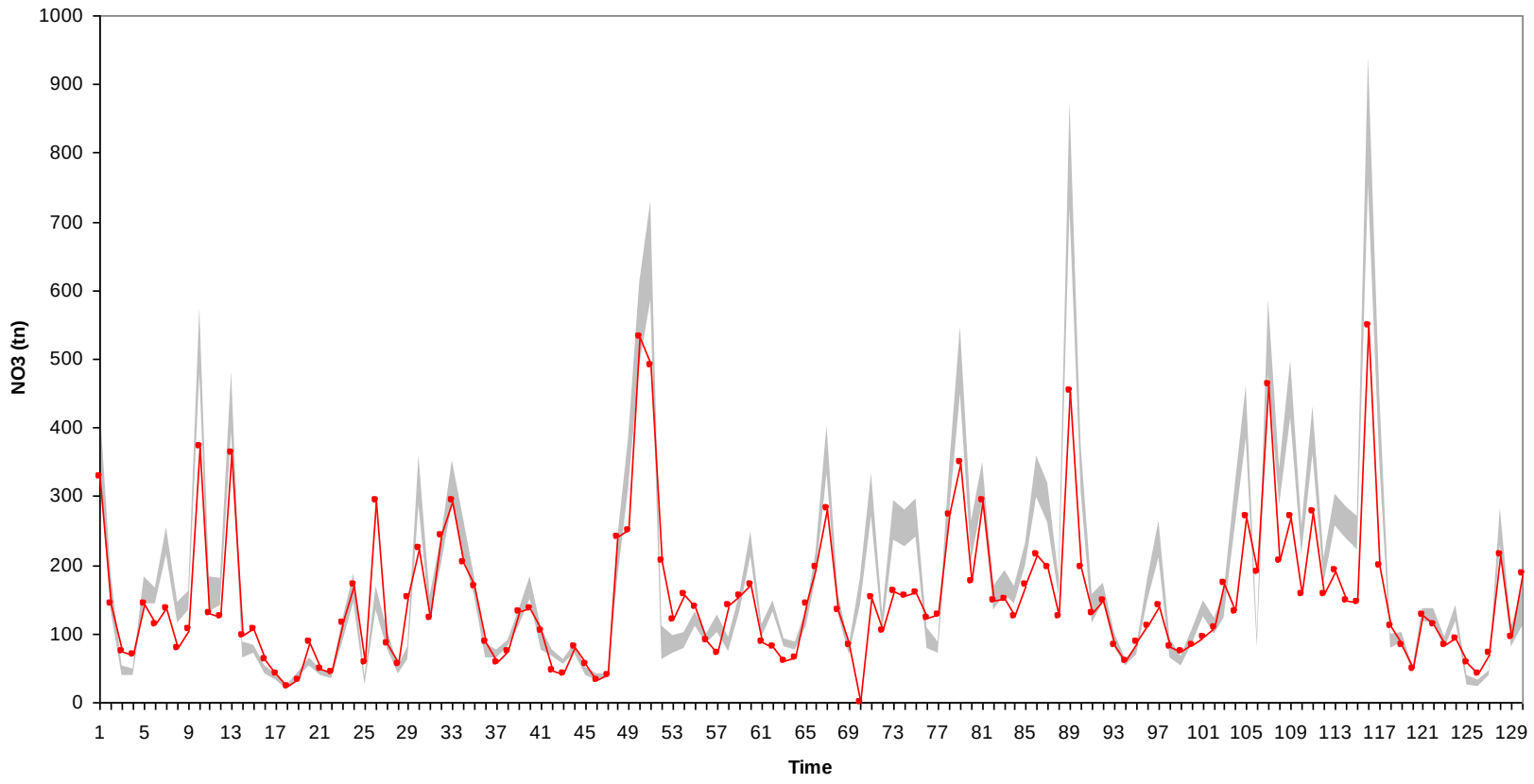

NO3 (tn)
2000
1800
1600
1400
1200
1000
800
600
400
200
0
1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77 81 85 89 93 97 101 105 109 113 117 121 125 129
Time

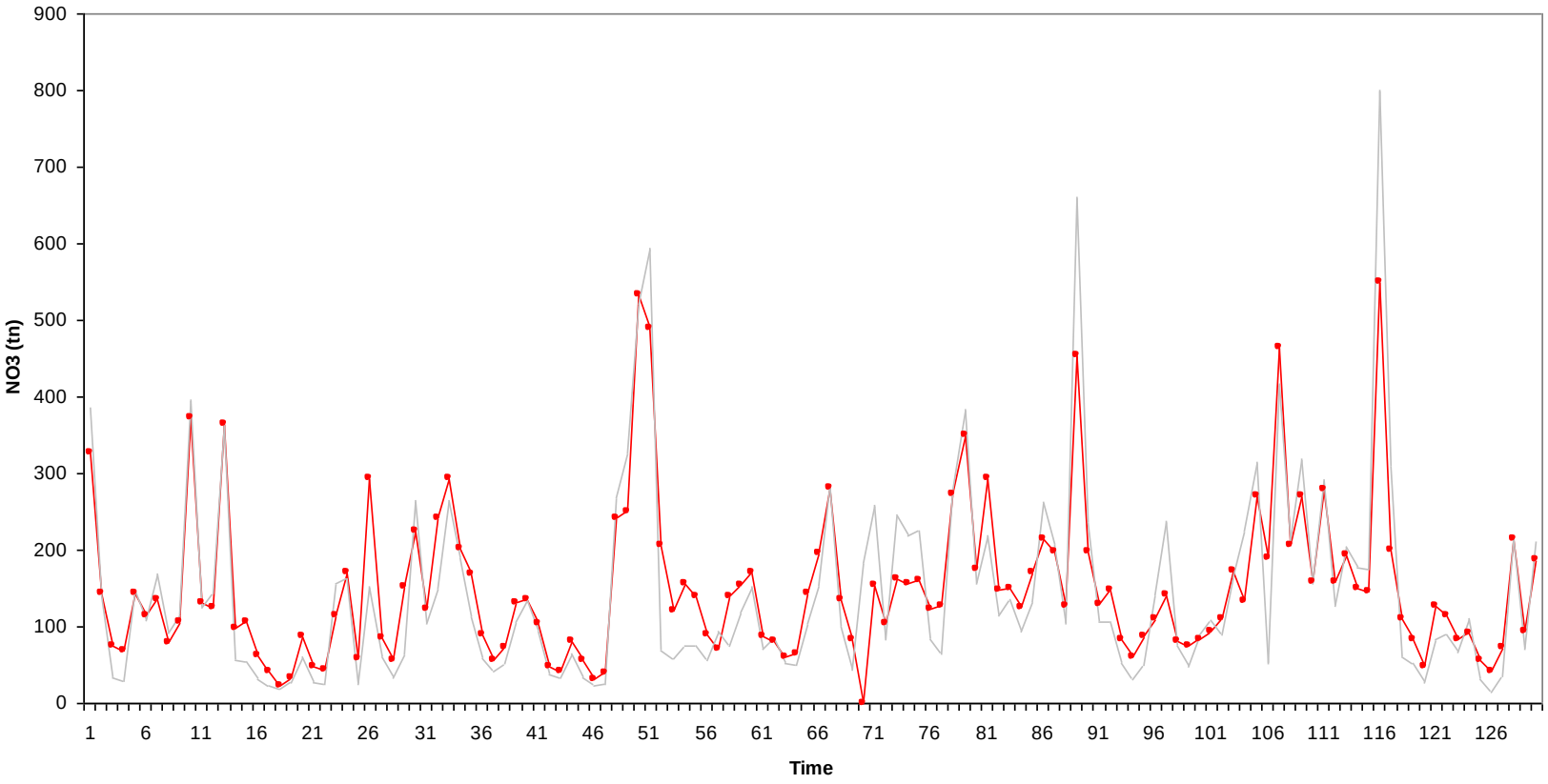

1600
1400
1200
1000
800
600
400
200
0
NO3 (tn)
1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77 81 85 89 93 97 101 105 109 113 117 121 125 129
Time


1600
1400
1200
1000
800
600
400
200
0
NO3 (tn)
1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77 81 85 89 93 97 101 105 109 113 117 121 125 129
Time


1400
1200
1000
800
600
400
200
0
NO3 (tn)
1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77 81 85 89 93 97 101 105 109 113 117 121 125 129
Time


1200
1000
800
600
400
200
0
NO3 (tn)
1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77 81 85 89 93 97 101 105 109 113 117 121 125 129
Time


1000
900
800
700
600
500
400
300
200
100
0
NO3 (tn)
1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77 81 85 89 93 97 101 105 109 113 117 121 125 129
Time


900
800
700
600
500
400
300
200
100
0
NO3 (tn)
1
6
11
16
21
26
31
36
41
46
51
56
61
66
71
76
81
86
91
96
101
106
111
116
121
126
Time

Important to realize that

Observations reflect the net effect of all the true processes in a watershed….

The goal of calibration is to capture observations

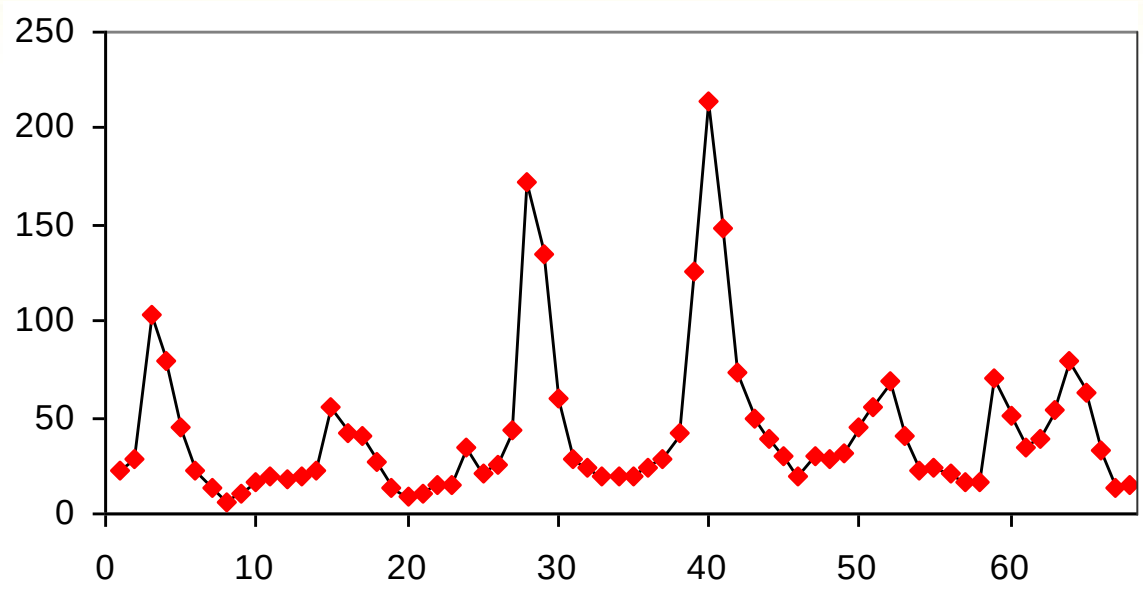
Uncertainty Analysis Definition

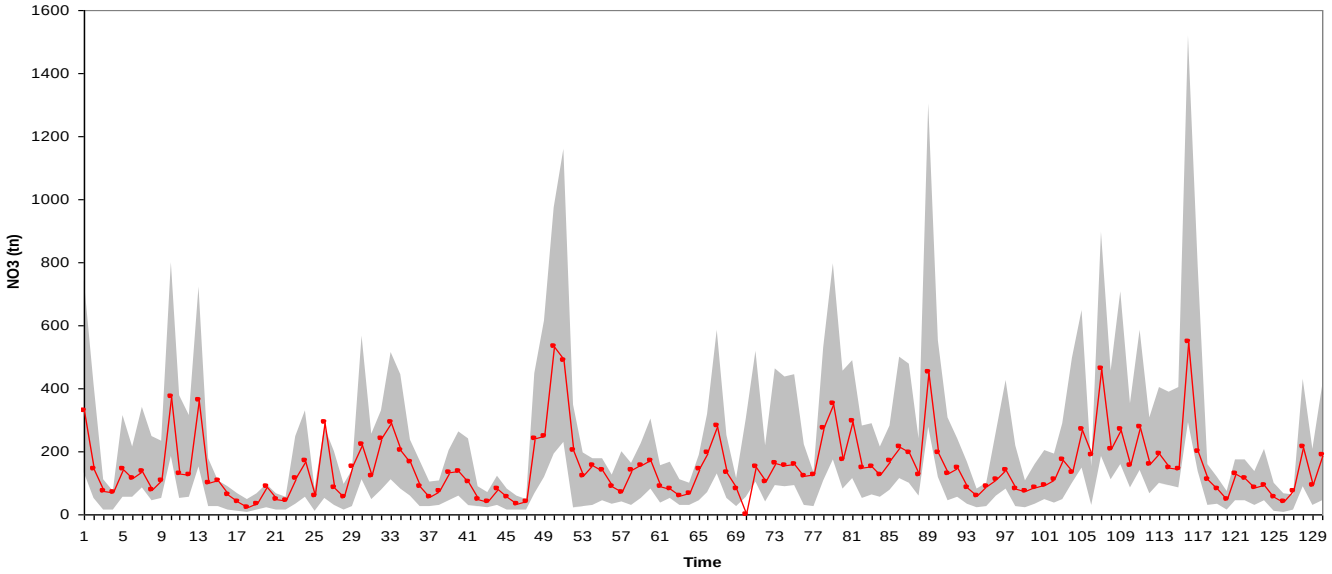
Uncertainty analysis:

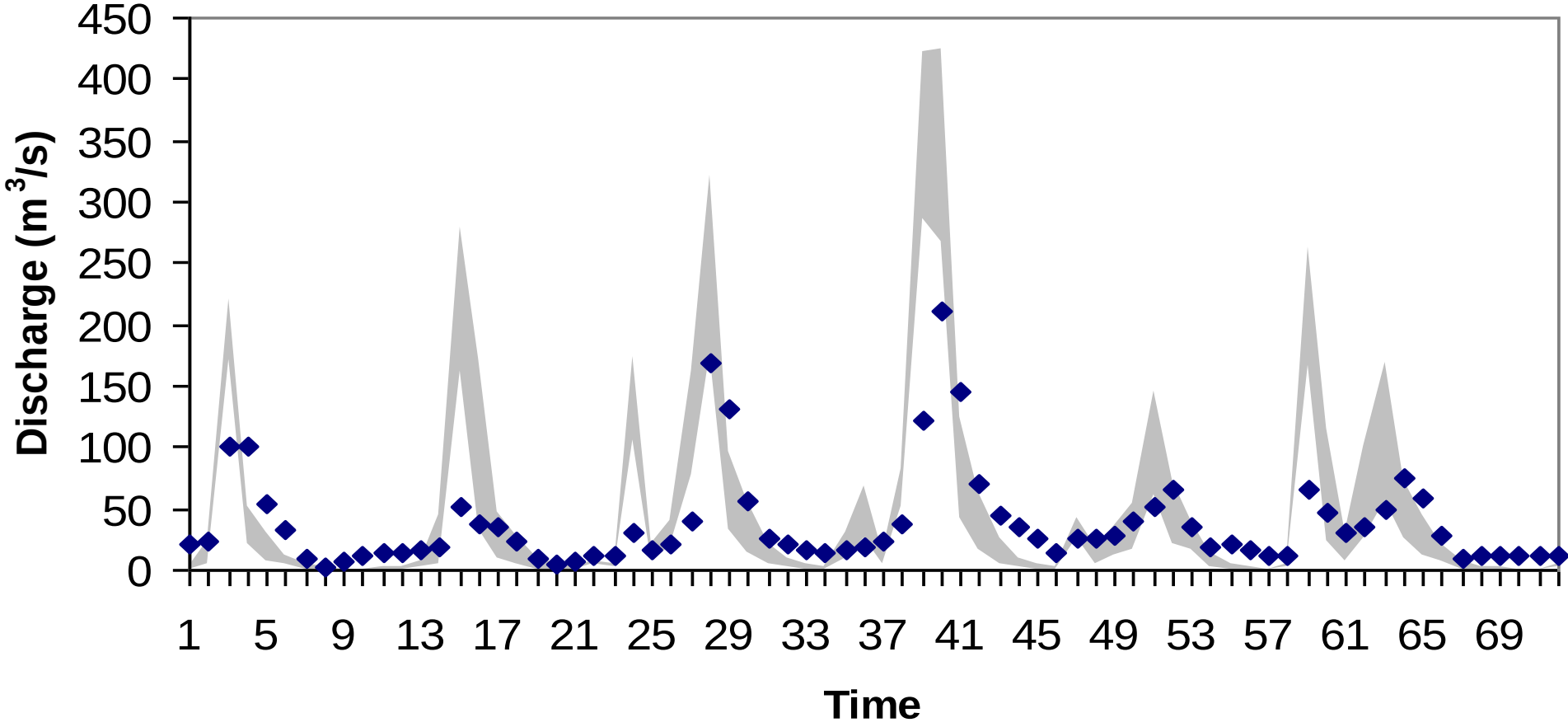
To obtain a range of parameters such that upon propagation the 95PPU brackets “most” of the observed points

Model Uncertainty

Ideal situation







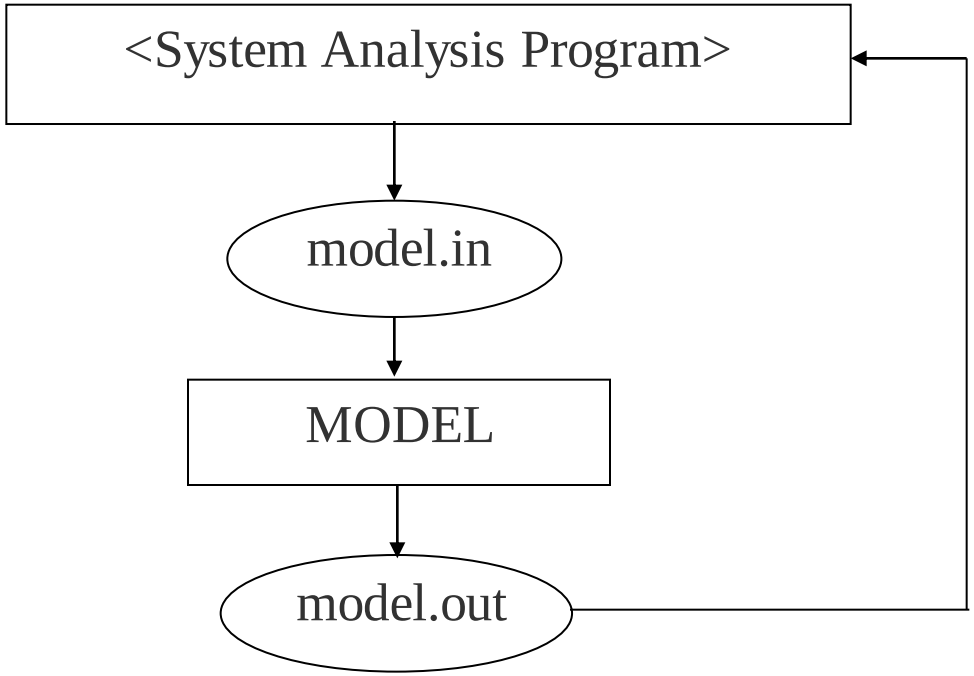
p-factor

% observed data bracketed by the 95PPU (⟶ 1)

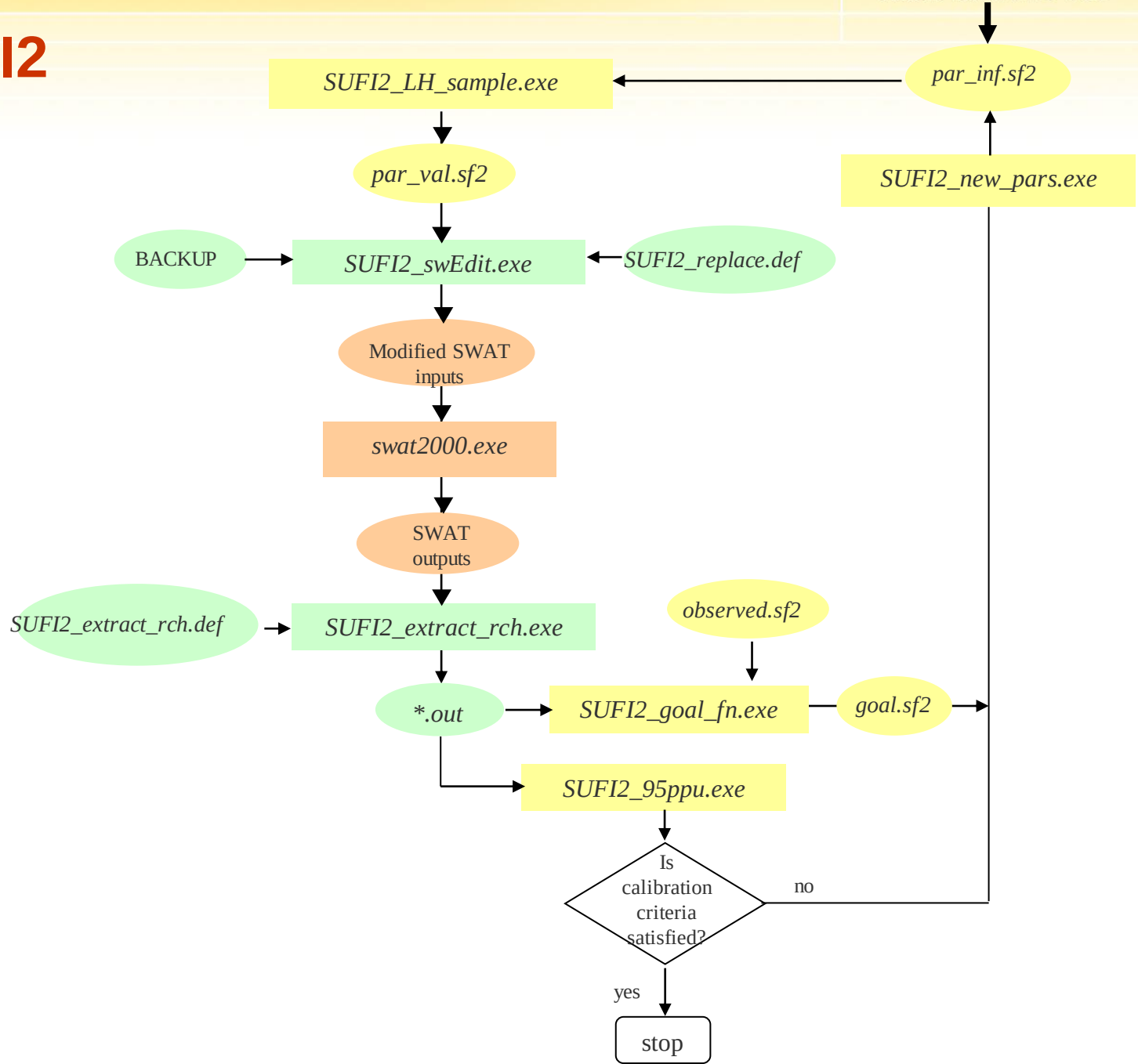
d-factor

The ratio of the average distance between the 95PPU band by the standard deviation of the measured data (⟶ 0)

Structure of the Interface



SWAT-SUFI2


par_inf.sf2
SUFI2_LH_sample.exe
par_val.sf2
SUFI2_new_pars.exe
BACKUP
SUFI2_swEdit.exe
SUFI2_replace.def
Modified SWAT inputs
swat2000.exe
SWAT outputs
SUFI2_extract_rch.def
SUFI2_extract_rch.exe
observed.sf2
*.out
SUFI2_goal_fn.exe
goal.sf2
SUFI2_95ppu.exe
Is calibration criteria satisfied?
no
yes
stop

Particle Swarm Optimization (PSO)

- PSO is a robust stochastic optimization technique based on the movement and intelligence of swarms

- PSO applies the concept of social interaction to problem solving. It was developed in 1995 by James Kennedy (social-psychologist) and Russell Eberhart (electrical engineer).

-It uses a number of agents (particles) that constitute a swarm moving around in the search space looking for the best solution.

- Each particle is treated as a point in a N-dimensional space which adjusts its “flying” according to its own flying experience as well as the flying experience of other particles.

Particle Swarm Optimization (PSO)

- Each particle keeps track of its coordinates in the solution space which are associated with the best solution (fitness) that has achieved so far by that particle. This value is called personal best , ***pbest***.

- Another best value that is tracked by the PSO is the best value obtained so far by other particles in the neighborhood of that particle. This value is called ***gbest***.

- The basic concept of PSO lies in accelerating each particle toward its *pbest* and the *gbest* locations, with a random weighted acceleration at each time step as shown in Fig.1

Particle Swarm Optimization (PSO)

s^k : current searching point.

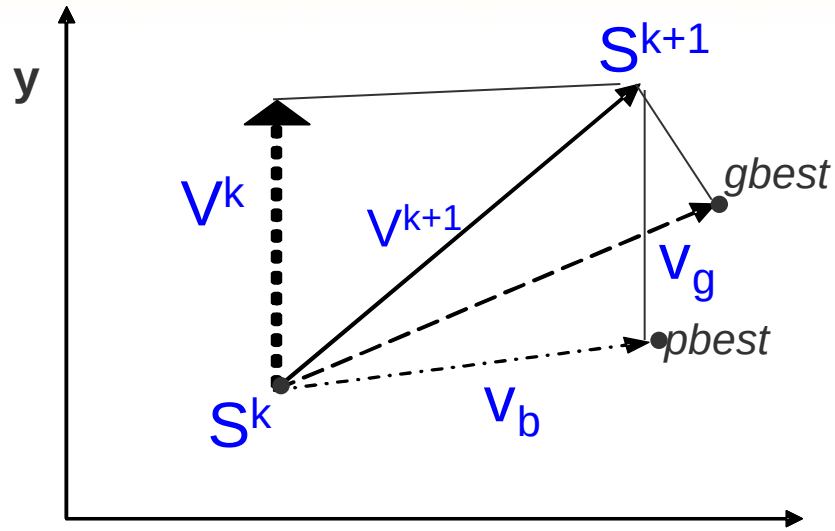
s^{k+1}: modified searching point.

v^k: current velocity.

v^{k+1}: modified velocity.

v_b : velocity based on pbest.

v_g : velocity based on gbest



$$V_i^{k+1} = wV_i^k + c_1 rand()(P_{bi} - s_i^k) + c_2 rand()(G_b - s_i^k)$$

v_i^k : velocity of agent i at iteration k,

w: weighting function,
c_j : weighting factor,
$rand$: uniformly distributed random number between 0 and 1,
s_i^k : current position of agent i at iteration k,
P_{bi} : pbest of agent i, G_b: gbest of the group.

GLUE
(Generalized Likelihood Uncertainty Estimation)

Bayesian Methods

	GLUE	MCMC
1. Prior distribution	Subjective assessment	Subjective assessment
2. Likelihood distribution	General	Statistical
3. Sampling technique	Random sampling	Metropolis algorithm

GLUE

- 1) Define a "likelihood measure", L(θ). A Commonly use likelihood is Nash-Sutcliffe

$$L(\theta) = NS = 1 - \frac{\sum_{i=1}^{n} (y_i^M(\theta) - y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

2) Take a large number of random samples from the prior parameter distributions

3) Run the model, each parameter set is assessed as either "behavioral" or "non-behavioral" through a comparison of the "likelihood measure" with a given threshold value (i.e., NS=0.7)

GLUE

4) Each behavioral parameter is given a “likelihood weight” which measures how good the corresponding simulation is:

$$w_i = \frac{L(\theta_i)}{\sum_{k=1}^{N} L(\theta_k)}$$

5) Finally, the prediction uncertainty is described as prediction quantile from the cumulative distribution realized from the weighted behavioral parameter sets

MCMC
Monte Carlo Makov Chain

Basis of the Bayesian probability model is the Bayes' equation:

Likelihood distribution

Prior distribution

Posterior distribution

$$p(\boldsymbol{\theta}|i) = \frac{p(i|\boldsymbol{\theta}) \cdot p(\boldsymbol{\theta})}{p(i)}$$

MCMC

MCMC generates samples from a random walk which adapts to the posterior distribution

A simple sampling method is Metropolis-Hasting algorithm

Metropolis-Hastings Algorithm

In mathematics and physics, the **Metropolis-Hastings algorithm** is a rejection sampling algorithm used to generate a sequence of samples from a probability distribution that is difficult to sample from directly. This sequence can be used in Markov chain Monte Carlo simulation to approximate the distribution (i.e., to generate a histogram), or to compute an integral (such as an expected value). The algorithm was named in reference to Nicholas Metropolis, who published it in 1953 for the specific case of the Boltzmann distribution, and W.K. Hastings, who generalized it in 1970. The Gibbs sampling algorithm is a special case of the Metropolis-Hastings algorithm which is usually faster and easier to use but is less generally applicable.

The Metropolis-Hastings algorithm can draw samples from any probability distribution $P(x)$, requiring only that a function proportional to the density can be calculated at x. In Bayesian applications, the normalization factor is often extremely difficult to compute, so the ability to generate a sample without knowing this constant of proportionality is a major virtue of the algorithm. The algorithm generates a Markov chain in which each state $xt + 1$ depends only on the previous state x^t. The algorithm uses a *proposal density* $Q(x';xt)$, which depends on the current state x^t, to generate a new proposed sample x'. This proposal is 'accepted' as the next value ($x^t + 1=x'$) if α drawn from $U(0,1)$ isproposal is 'accepted' as the next value ($x^{t+1}=x'$) if α drawn from $U(0,1)$ is

$$\alpha < \frac{P(x')Q(x^t|x')}{P(x^t)Q(x'|x^t)}.$$

Metropolis-Hastings Algorithm

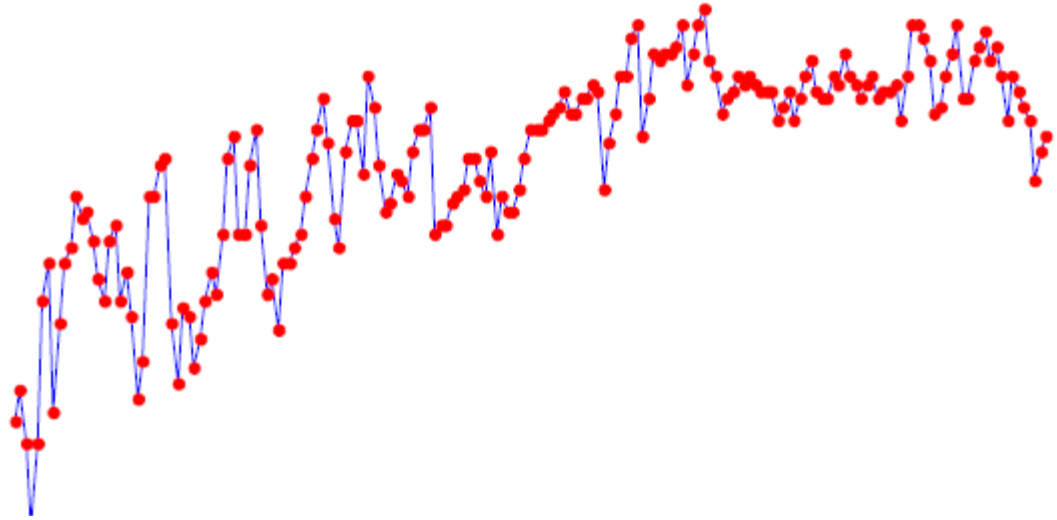
If the proposal is not accepted, then the current value of x is retained: $x^{t+1} = x^t$.
For example, the proposal density could be a Gaussian function centered on the current state x^t:

$$Q(x'; x^t) \sim N(x^t, \sigma^2 I)$$

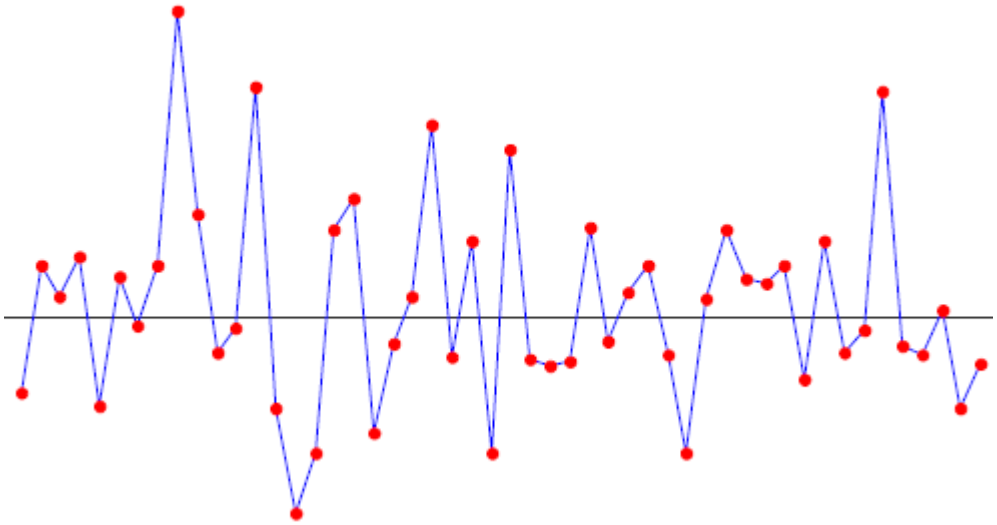
reading $Q(x';x^t)$ as the probability density function for x' given the previous value x^t. This proposal density would generate samples centred around the current state with variance $\sigma 2I$. The original Metropolis algorithm calls for the proposal density to be symmetric ($Q(x;y) = Q(y;x)$); the generalization by Hastings lifts this restriction. It is also permissible for $Q(x',x^t)$ not to depend on x' at all, in which case the algorithm is called "Independence Chain Metropolis-Hastings" (as opposed to "Random Walk Metropolis-Hastings"). The Independence Chain M-H algorithm with a suitable proposal density function can offer higher accuracy than the random walk version, but it requires some *a priori* knowledge of the distribution.

Independent and identically distributed (iid) residuals

Not iid residual



iid residual



MCMC

Likelihood function in a Bayesian inference using Box-Cox transformation and continuous time auto regressive function. This function ensures an iid residual distribution for discharge in a watershed in China (see Yang et al., WRR, JHydrol, 2007)

$$f_{\mathbf{Y}^M|\boldsymbol{\Theta}}(\mathbf{y}|\boldsymbol{\theta}) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma}\exp\left(-\frac{1}{2}\frac{\left[g(y_{t_0}) - g\left(y_{t_0}^M(\boldsymbol{\theta})\right)\right]^2}{\sigma^2}\right)\cdot\left|\frac{dg}{dy}\bigg|_{y=y_{t_0}}\right|$$

$$\cdot\prod_{i=1}^{n}\left[\frac{1}{\sqrt{2\pi}}\frac{1}{\sigma\sqrt{1-\exp\left(-2\frac{t_i - t_{i-1}}{\tau}\right)}}\exp\left(-\frac{1}{2}\frac{\left[\begin{array}{c} g(y_{t_i}) - g\left(y_{t_i}^M(\boldsymbol{\theta})\right) \\ -\left[g(y_{t_{i-1}}) - g\left(y_{t_{i-1}}^M(\boldsymbol{\theta})\right)\right]\exp\left(-\frac{t_i - t_{i-1}}{\tau}\right)\end{array}\right]^2}{\sigma^2\left(1-\exp\left(-2\frac{t_i - t_{i-1}}{\tau}\right)\right)}\right)\cdot\left|\frac{dg}{dy}\bigg|_{y=y_{t_i}}\right|\right]$$

MCMC

1) An initial starting point in the parameter space is chosen through Shuffle Complex, which approximates the maximum of the likelihood

2) A candidate for the next point is proposed (perturbation or mutation,...)

$$\theta_{k+1} = \theta_k + rand(f_{jump})$$

3) The acceptance of the candidate depends on the ratio r:
   r > 1 accept, else reject

$$r = \frac{f(\boldsymbol{\theta}^*_{k+1} | i)}{f(\boldsymbol{\theta}_k | i)}$$

Parasol
(Parameter Solution)

ParaSol uses Shuffled-Complex optimization, which is based on simplex procedure with the concept of a controlled random search

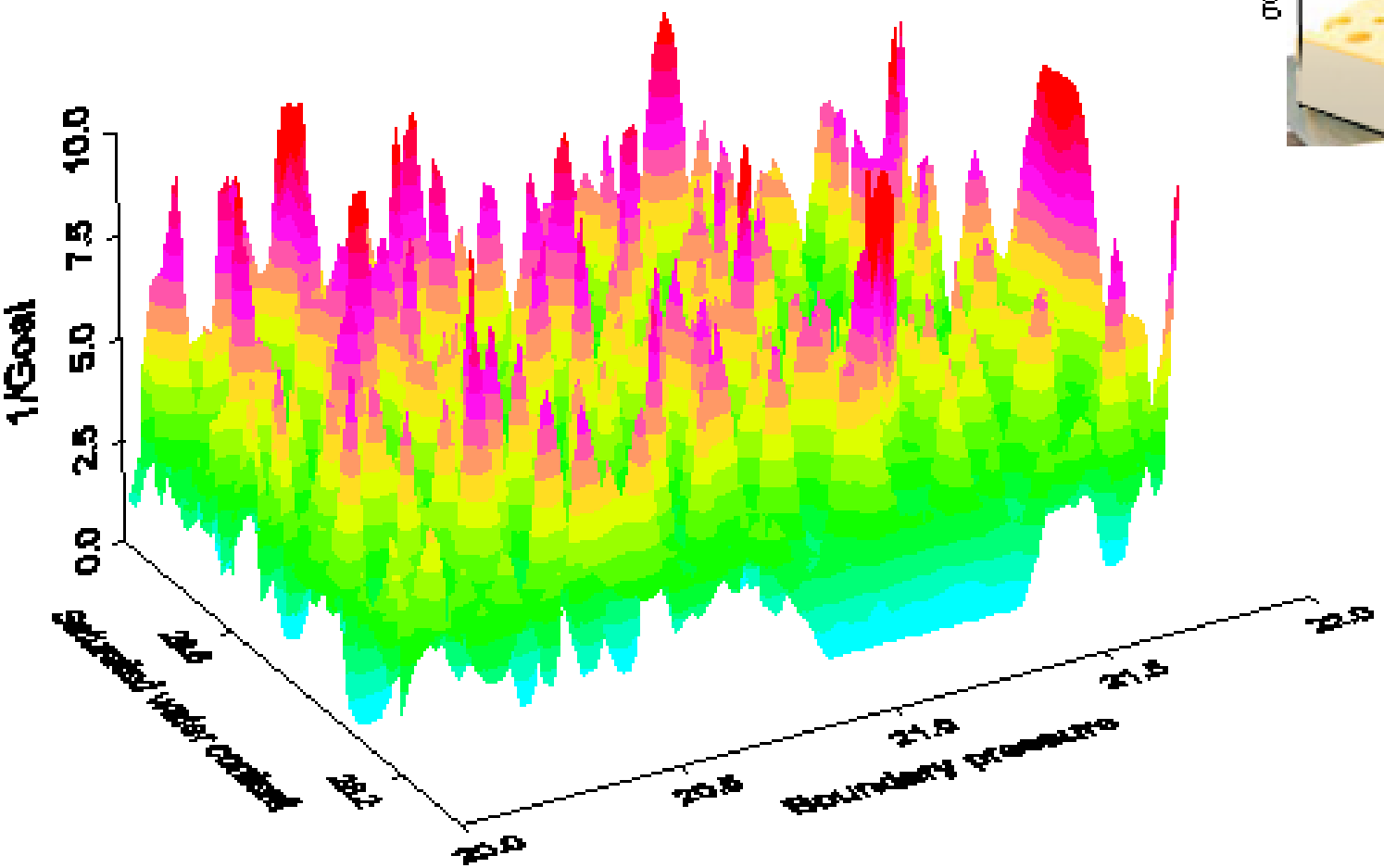
1. Select an initial population by random search

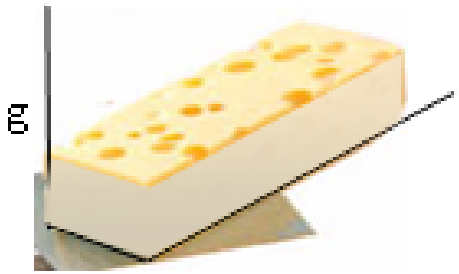
2. Partition the population into several “complexes”

3. Each complex evolves independently using the simplex algorithm. The complexes are shuffled periodically

4. Check convergence criteria is satisfied, stop; or go back to 2

The Swiss Cheese Effect (multimodality of the objective function)





Criterion	GLUE	ParaSol	SUFI-2	Bayesian inference with cont. autoregr. error model	
				MCMC	IS
Goal function	Nash-Sutcliffe	Nash-Sutcliffe	Nash-Sutcliffe	post. prob. density	post. prob. density
a__CN2.mgt	-16.8 (-29.6, -9.8)[1]	-21.0 (-21.9, -20.1)	-26.9 (-30.0, -7.2)	-14.2 (-16.8, -11.6)	-19.60
v__ESCO.hru	0.76 (0.02, 0.97)	0.67 (0.65, 0.69)	0.82 (0.43, 1.0)	0.74 (0.63, 0.75)	0.62
v__EPCO.hru	0.22 (0.04, 0.90)	0.16 (0.13, 0.20)	1 (0.34, 1.0)	0.94 (0.39, 0.98)	0.27
r__SOL_K.sol	-0.16 (-0.36, 0.78)	-0.37 (-0.41, -0.34)	-0.1 (-0.58, 0.34)	-0.29 (-0.31, 0.78)	0.01
a__SOL_AWC.sol	0.11 (0.01, 0.15)	0.07 (0.08, 0.08)	0.07 (0.05, 0.15)	0.12 (0.1, 0.13)	0.05
v__ALPHA_BF.gw	0.12 (0.06, 0.97)	0.12 (0.08, 0.13)	0.51 (0.23, 0.74)	0.14 (0.11, 0.15)	0.91
v__GW_DELAY.gw	159.58 (9.7, 289.3)	107.7 (91.2,115.2)	190.07 (100.2, 300)	25.5 (17.8, 33.3)	33.15
r__SLSUBBSN.hru	-0.45 (-0.56, 0.46)	-0.59 (-0.60, -0.58)	-0.52 (-0.60, 0.03)	-0.55 (-0.56, 0.15)	0.58
a__CH_K2.rte	78.19 (6.0, 144.8)	35.70 (27.72,37.67)	83.95 (69.4, 150.0)	78.3 (68.0, 86.2)	147.23
a__OV_N.hru	0.05 (0.00, 0.20)	0.11 (0.07, 0.10)	0.06 (0.00, 0.11)	0.12 (0.00, 0.19)	0.08
[2]σ_{dry}	-	-	-	0.93 (0.81, 1.10)	0.87
[2]σ_{wet}	-	-	-	2.81 (2.4, 3.9)	2.30
[2]τ_{dry}	-	-	-	38.13 (29.5, 53.8)	28.47
[2]τ_{wet}	-	-	-	3.42 (2.4, 8.0)	0.92
NS for cal (val)	0.80 (0.78)	0.82 (0.81)	0.80 (0.75)	0.77 (0.77)	0.64 (0.71)
R^2 for cal (val)	0.80 (0.84)	0.82 (0.85)	0.81 (0.81)	0.78 (0.81)	0.70 (0.72)
[3]*p-factor* cal(val)	79% (69%)	18% (20%)	84% (82%)	85% (84%)	-
[4]*d-factor* cal(val)	0.65 (0.51)	0.08 (0.07)	1.03 (0.82)	1.47 (1.19)	-
Uncertainty described by parameter uncertainty	All sources of uncertainty	Parameter uncertainty only	All sources of uncertainty	Parameter uncertainty only	Parameter uncertainty only
Difficulty of implement.	very easy	easy	easy	more complicated	more complicated
Number of runs	10000	7500	1500 + 1500	5000 + 20’000 + 20’000	100’000

Abbaspour, K. C. E. Rouholahnejad, S. Vaghefi, R. Srinivasan, B. Klöve. 2014. Modelling hydrology and water quality of the European Continent at a subbasin scale: calibration of a high-resolution large-scale SWAT model. Journal of Hydrology, 524: 733-752.

http://www.sciencedirect.com/science/article/pii/S0022169415001985

Rouholahnejad E., K.C. Abbaspour, R. Srinivasan, V. Bacu, A. Lehmann. 2014. A high resolution spatiotemporal distribution of water resources quantity and quality in the Black Sea Basin. Water Resources Research, 50, 5866–5885 DOI: 10.1002/2013WR014132.

Vaghefi A.S., Mousavi S.J., Abbaspour K.C., Srinivasan R., Arnold J.R. 2013. Integration of Hydrologic and Water Allocation Models in Basin-Scale Water Resources Management Considering Crop Pattern and Climate Change: Karkheh River Basin in Iran. Regional Environmental Change. DOI 10.1007/s10113-013-0573-9.

Azimi M, Heshmati Gh.A., Faramarzi M., Abbaspour K.C. 2013. Modelling the impact of rangeland management on Sagebrush community in arid and semi-arid regions of Iran. Ecological Modeling. 250:1-14.

Faramarzi M, K.C. Abbaspour, S.A. Vaghefi, M.R. Farzaneh, A.J.B. Zehnder, H. Yang. 2013. Modelling impacts of climate change on freshwater availability in Africa. Journal of Hydrology. 250: 1– 14.

Rouholahnejad E, Abbaspour KC, Vejdani M, Srinivasan R, Schulin R, Lehmann A. 2012. Parallelization framework for calibration of hydrological models, *Environmental Modelling Software,* 31: 28-36.

Notter B. Hurni H., Wiesmann U., and Abbaspour K.C. 2012. Modelling water provision as an ecosystem service in a large East African river basin.. Hydrology and Earth Science System, 16:69-86.

Faramarzi, M, Yang H., Mousavi J., Schulin R., Binder CR., Abbaspour K.C. 2010. Analysis of Intra-country virtual water trade strategy to alleviate water scarcity in Iran. Hydrol. Earth Syst. Sci. 14: 1417-1433.

Faramarzi, M, Yang H., Schulin R., Abbaspour K.C. 2010. Modeling wheat yield and crop water productivity in Iran: Implications of agricultural water management for wheat production. Agricultural Water Management. 97: 1861-1875.

Akhavan, S., Abedi-Koupai J., Mousavi S.F., Afyuni, M., Eslamian S.S, Abbaspour K.C. 2010. Application of SWAT model to investigate nitrate leachiing in Hamadan-Bahar watershed, Iran. Journal of Agriculture, Ecosystem, & Environment. 139:675-688.

Abbaspour, K. C., M. Faramarzi, S. S. Ghasemi, and H. Yang (2009), Assessing the impact of climate change on water resources in Iran, Water Resour. Res., 45, W10434, doi:10.1029/2008WR007615.

Faramarzi, M., K.C. Abbaspour, R. Schulin, and H. Yang. 2009. Modeling blue and green water availability in Iran. Hydrological Processes. 23(3): 486-501.

Schuol, J., Abbaspour, KC., Sarinivasan, R., Yang, H. 2008. Estimation of freshwater availability in the West African Sub-continent using the SWAT hydrologic model. Journal of Hydroloy, 352(1-2):30-49.

Schuol, J., K.C. Abbaspour, R. Srinivasan, and H.Yang. 2008. Modelling Blue and Green Water Availability in Africa at monthly intervals and subbasin level. Water Resources Research. VOL. 44, W07406, doi:10.1029/2007WR006609.

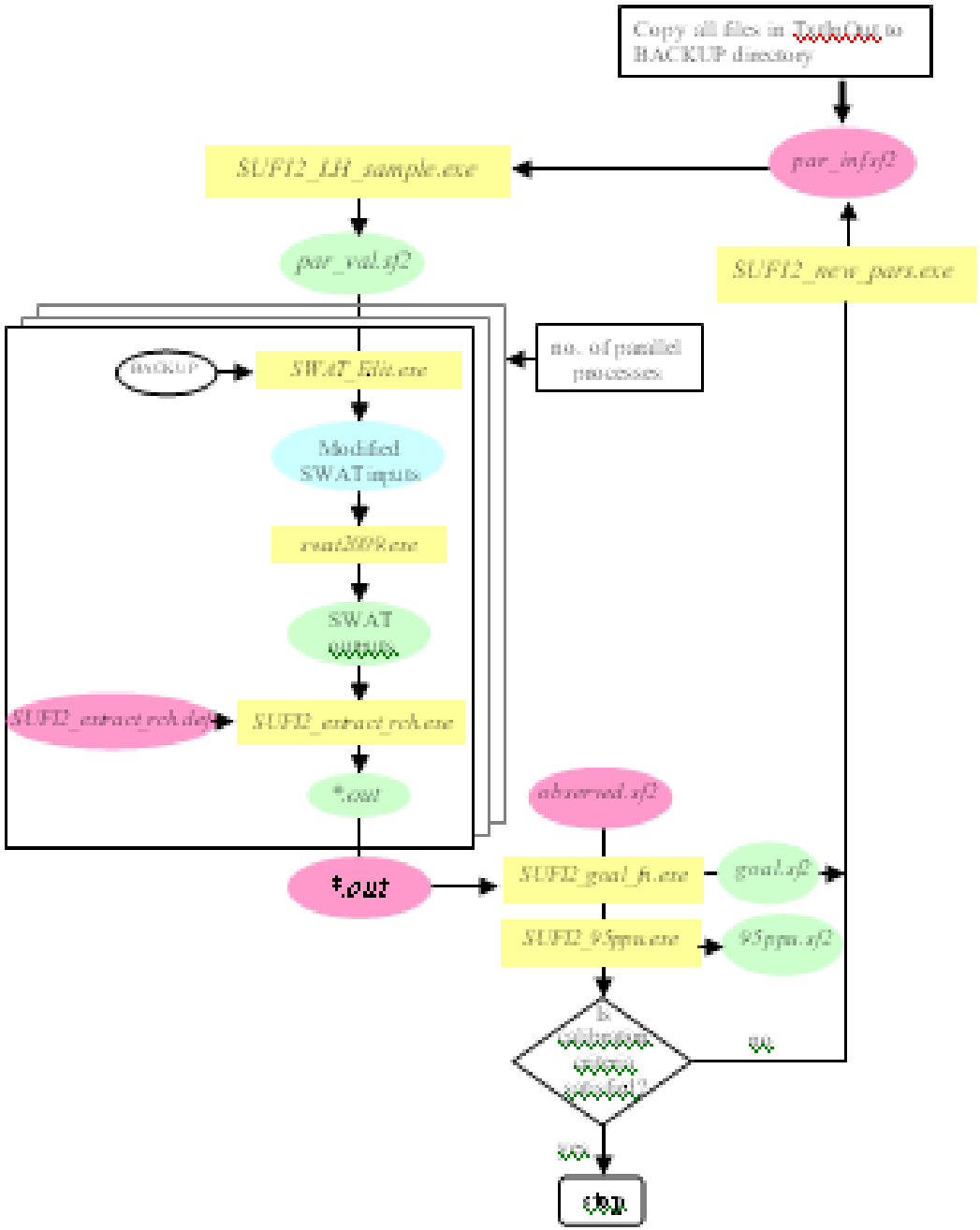
Yang, J., Abbaspour K. C., Reichert P., and Yang H. 2008. Comparing uncertainty analysis techniques for a SWAT application to Chaohe Basin in China. Journal of Hydrology. 358, 1-23.

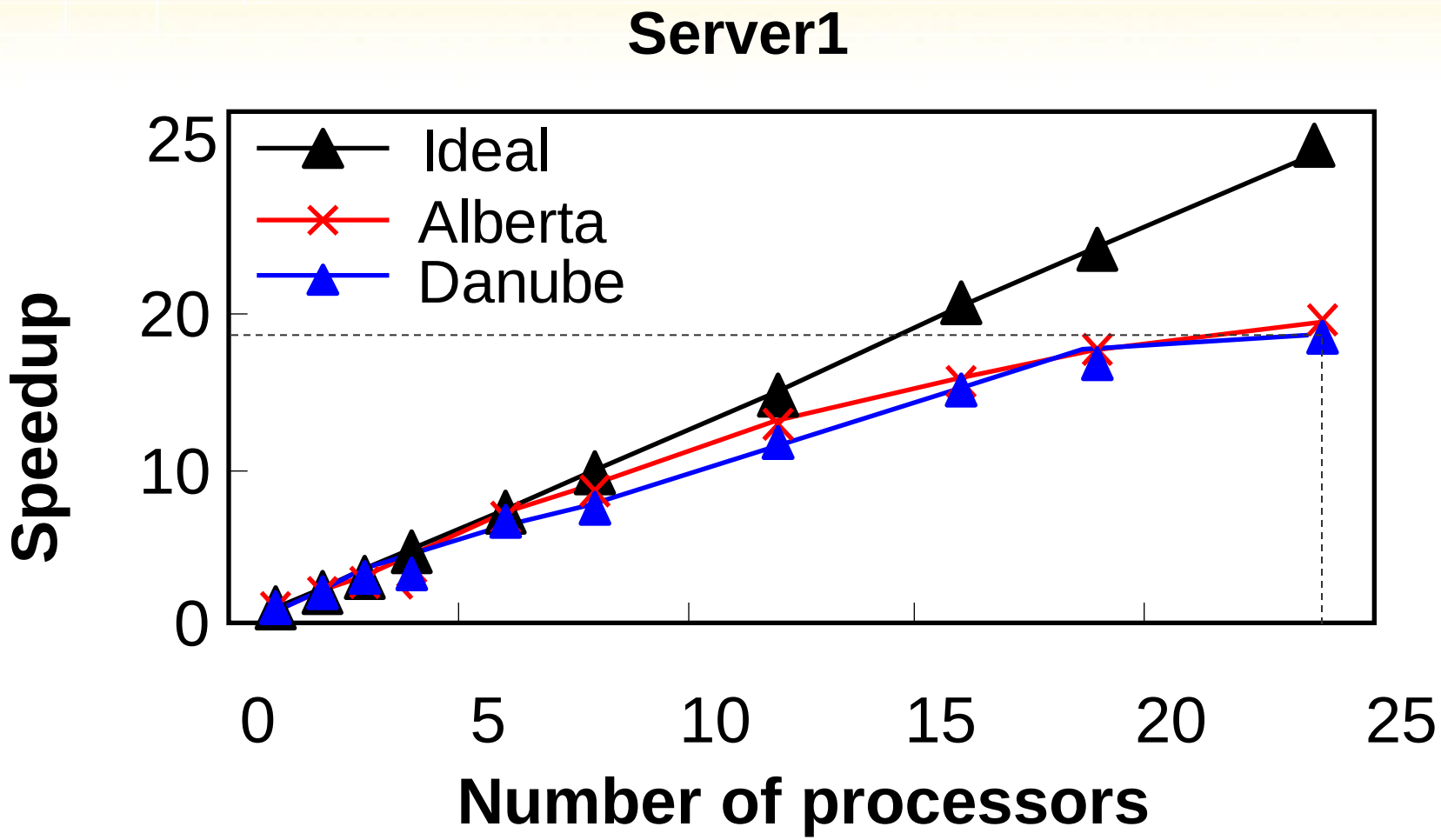
Abbaspour, K.C., J. Yang, I. Maximov,., R. Siber, K. Bogner, J. Mieleitner, J. Zobrist, R. Srinivasan. 2007. Modelling hydrology and water quality in the pre-alpine/alpine Thur watershed using SWAT. Journal of Hydrology, 333:413-430.

Yang, J., P. Reichert, and K. C. Abbaspour. 2007. Bayesian uncertainty analysis in distributed hydrologic modeling: A case study in the Thur River basin (Switzerland), Water Resour. Res., 43(10).

W10401, doi:10.1029/2006WR005497

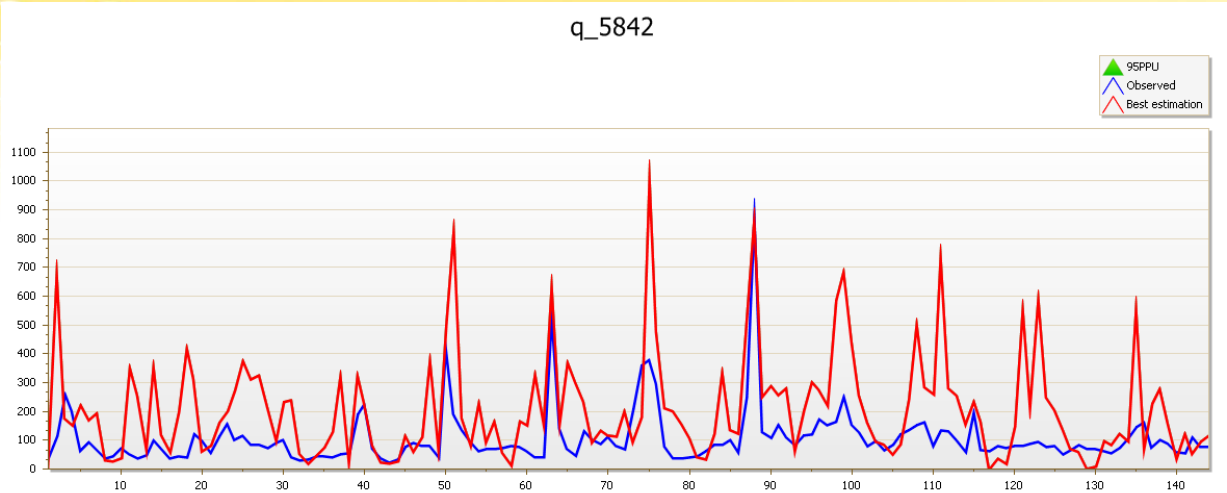
Yang, J., Reichert P., Abbaspour K. C., and Yang H. 2007. Hydrological Modelling of the Chaohe Basin in China: Statistical Model Formulation and Bayesian Inference. Journal of Hydrology. 340:167-182.


Copy all files in TxtInOut to BACKUP directory
par_inf.sf2
SUFI2_LH_sample.exe
SUFI2_new_pars.exe
par_val.sf2
no. of parallel processes
BACKUP
SWAT_Edit.exe
Modified SWAT inputs
swat2009.exe
SWAT outputs
SUFI2_extract_rch.def
SUFI2_extract_rch.exe
*.out
observed.sf2
*.out
SUFI2_goal_fn.exe
goal.sf2
SUFI2_95ppu.exe
95ppu.sf2
no
yes
stop



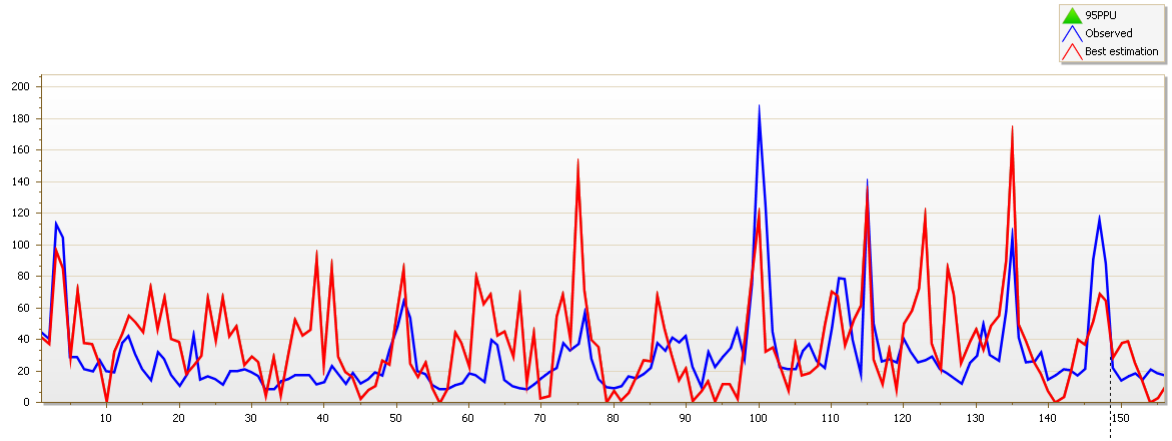
24 CPU Danube 69,875

16 GB RAM Alberta 2,698

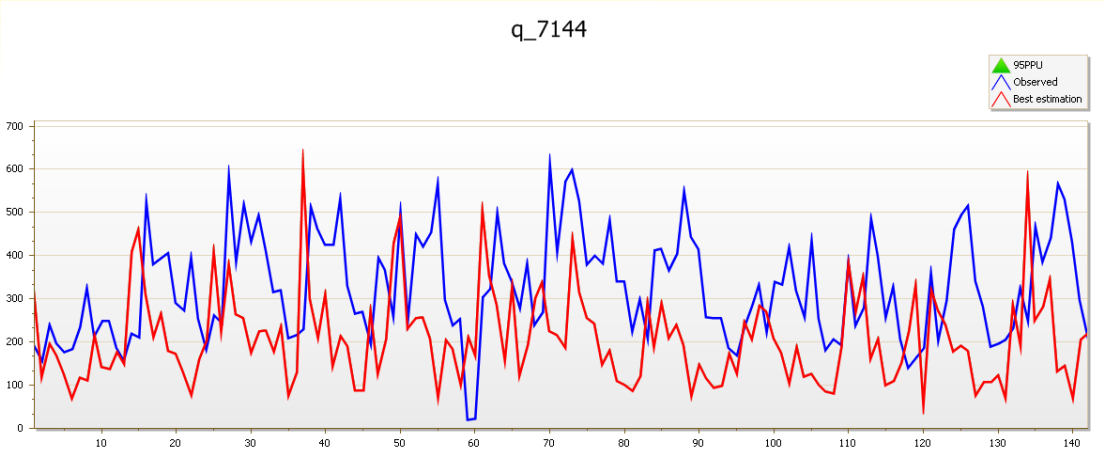

q_5842
95PPU
Observed
Best estimation
1100
1000
900
800
700
600
500
400
300
200
100
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140

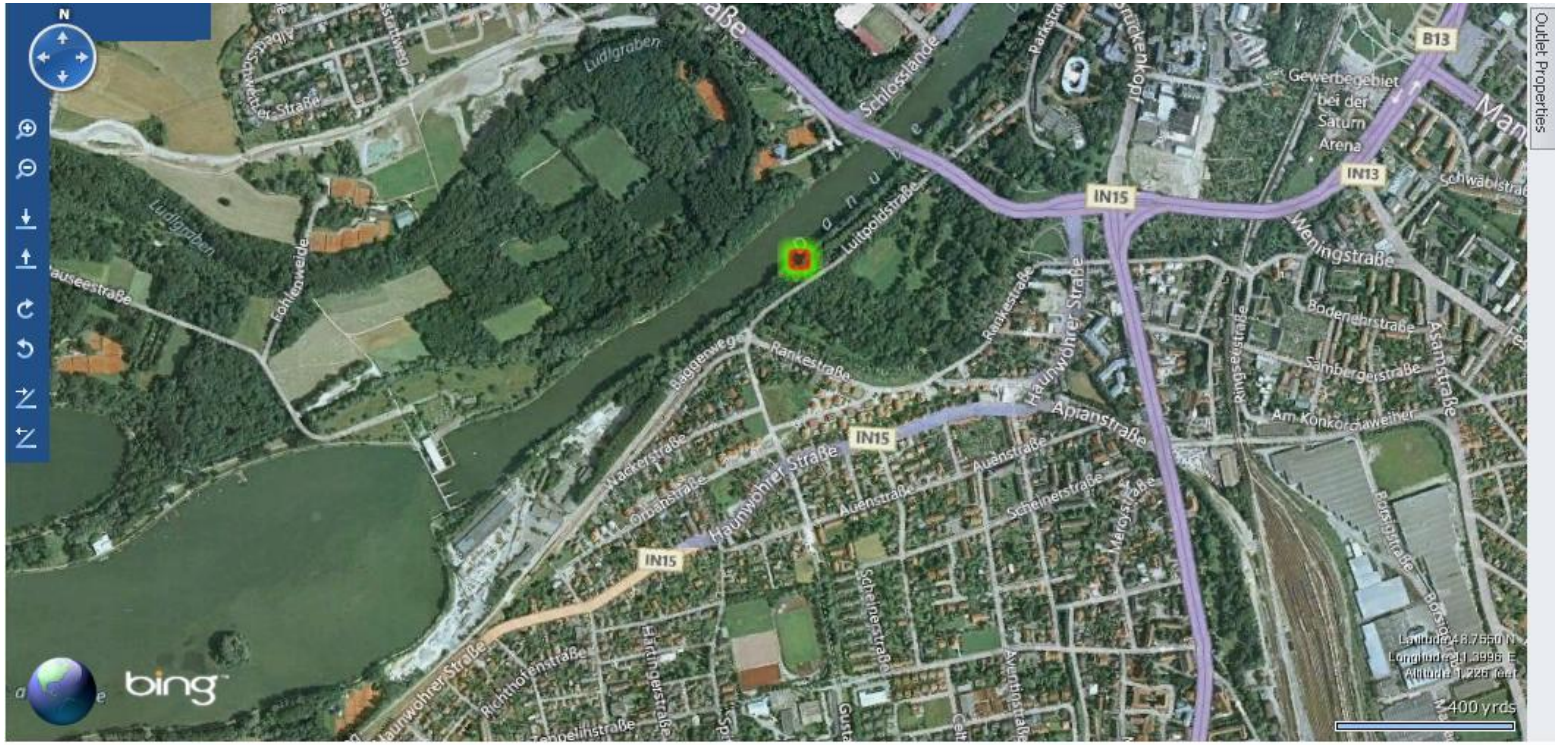
Outlet Properties
R06
Latitude 47.7092 N
Longitude 31.2422 E
Altitude 25 feet
300 yrds
Latitude 47.7342 N
Longitude 31.1760 E
Altitude 207 feet
1 miles
bing

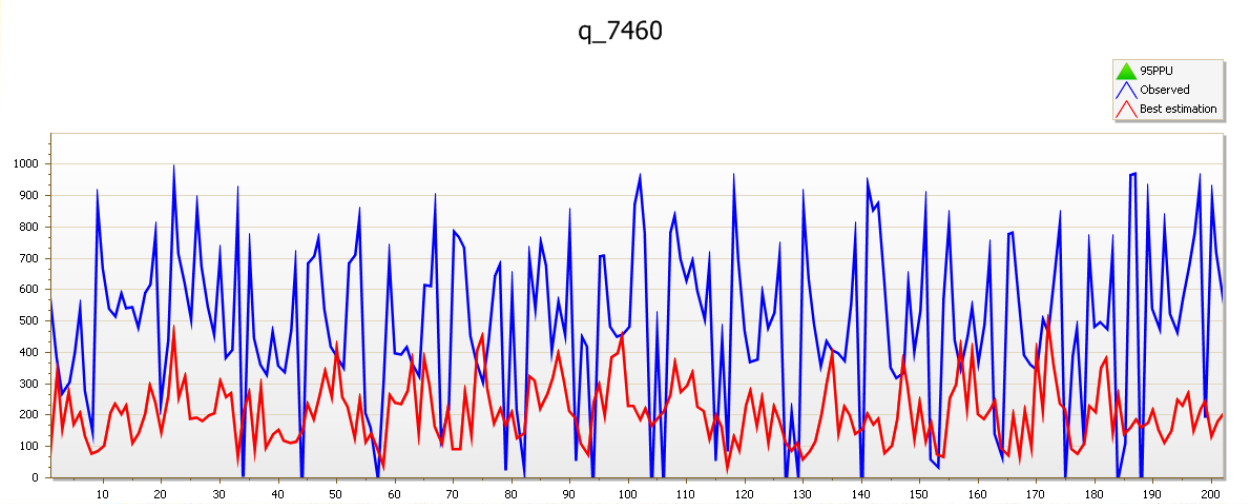
q_6726


95PPU
Observed
Best estimation
200
180
160
140
120
100
80
60
40
20
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150

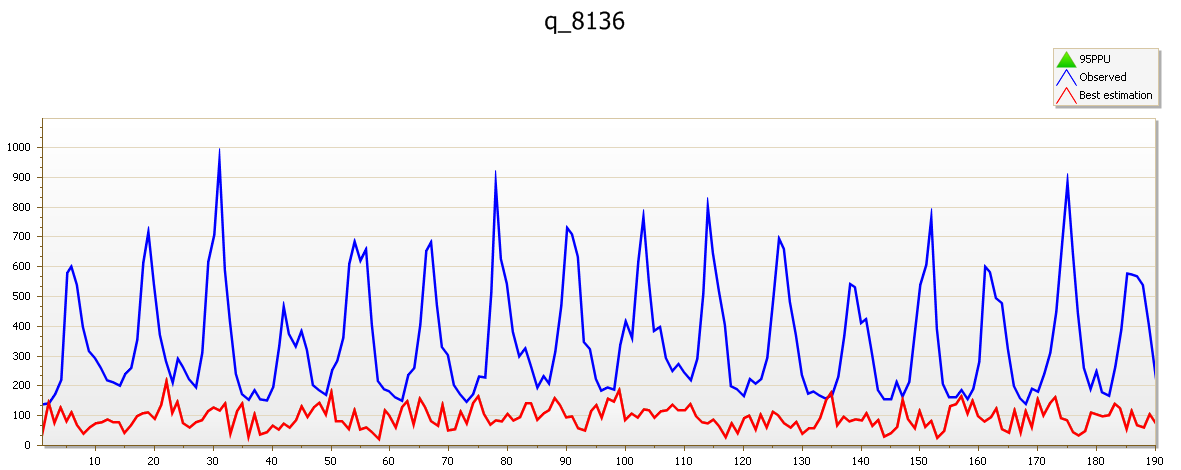
Vodni nadrz Nove
Nove Mlyny
Nove Mlyny
421
42125
421
Klentnicky Potok
bing
Latitude 48.8647 N
Longitude 16.7058 E
Altitude 535 feet
300 yrds


q_7144
95PPU
Observed
Best estimation
700
600
500
400
300
200
100
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140

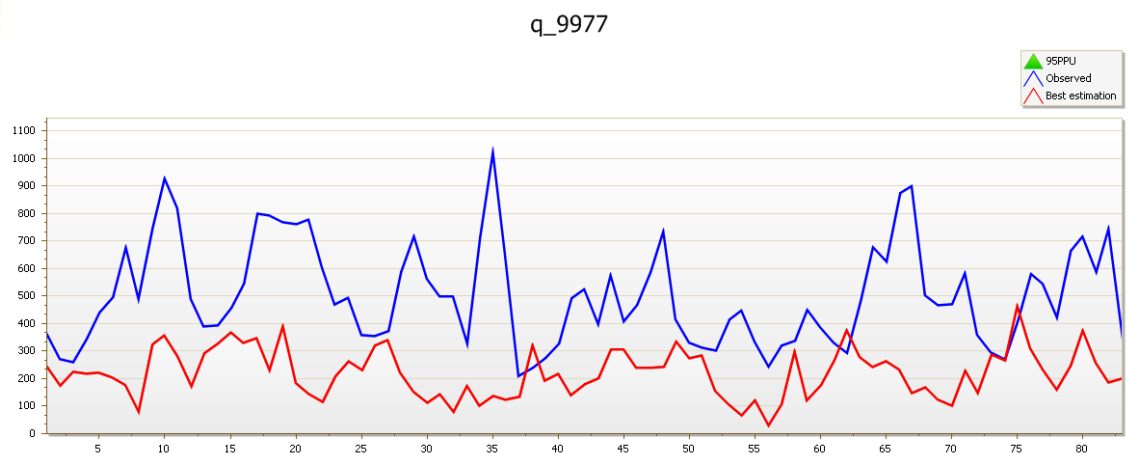

Outlet Properties
N
Ludlgraben
Schlosslände
Luitpoldstraße
Gewerbegebiet bei der Saturn Arena
B13
IN13
IN15
Wenningstraße
Schwäbistraße
Rankestraße
Baggerweg
Haunwöhrer Straße
Apianstraße
Auenstraße
Scheinerstraße
Bodenehrstraße
Sambergerstraße
Am Konkordiaweiher
Asamstraße
Melostraße
Ringseisstraße
Bürgerstraße
Eichenweiderstraße
Wackerstraße
Orbanstraße
Richthofenstraße
Barthingerstraße
Tempelhofstraße
Avenhofstraße
Latitude 48.7550 N
Longitude 11.3996 E
Altitude 1,226 feet
400 yrds
bing


q_7460
95PPU
Observed
Best estimation
1000
900
800
700
600
500
400
300
200
100
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200

Pothbauerweg
Edward-Hamm-Straße
Schiffweg
Innstraße
Ingling
Güterweg Hof
Hörl
bing
Latitude 48.5619 N
Longitude 13.4214 E
Altitude 1,258 feet
150 yrds
Outlet Properties


q_8136
95PPU
Observed
Best estimation
1000
900
800
700
600
500
400
300
200
100
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190

Outlet Properties
Münchner
Ebimgetbergstraße
ST2359
bing
Latitude 48.0706 N
Longitude 12.2279 E
Altitude 1,557 feet
70 yrds


q_9977
95PPU
Observed
Best estimation
1100
1000
900
800
700
600
500
400
300
200
100
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80

DRAVAPALKONYA
DRAVASZABOLCS
Drava
Donji Miholjac
Vukovarska
Kolodvorska
D34
D34
bing
Latitude 45.7845 N
Longitude 18.0943 E
Altitude 293 feet
1 miles