Questions:

What is calibration?

Why do we have to calibrate a groundwater model?

How would you calibrate your groundwater model?

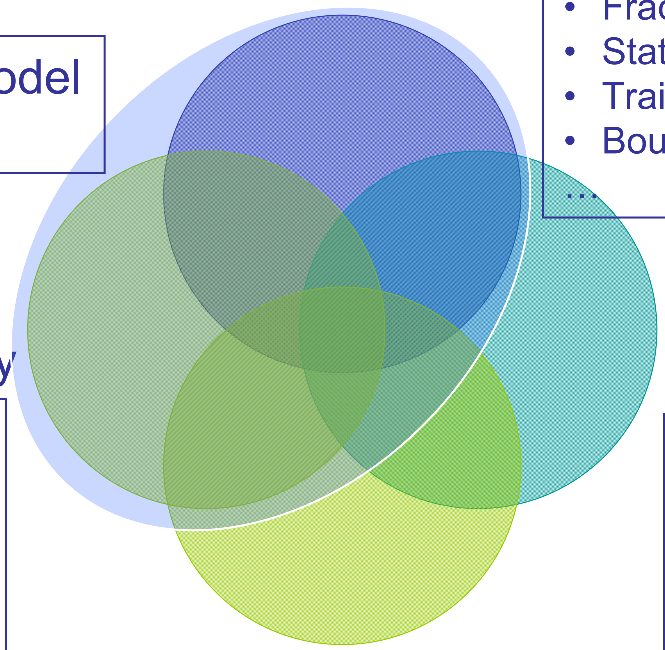
Uncertainties in groundwater models

Conceptual model uncertainty

Process uncertainty

Description of:
- groundwater-river interaction
- drain flow
- unsaturated zone flow
- Fracture flow
- Stationary flow
- Trainsient flow
- Boundary conditions

…



Structural uncertainty

Geological layers and lenses
Precipitation zones
Zones of hydraulic conductivity
Drainage zones
Boundary conditions?
…

Parameter uncertainty

Hydraulic conductivity
- horizontal
- vertical

Specific yield
Storage coefficient
Effective porosity
…

Input uncertainty

Precipitation
Potential evapotranspiration
…

Calibration →

Simulated state variables → Observed state variables

which parameter should be calibrated?

In principle:

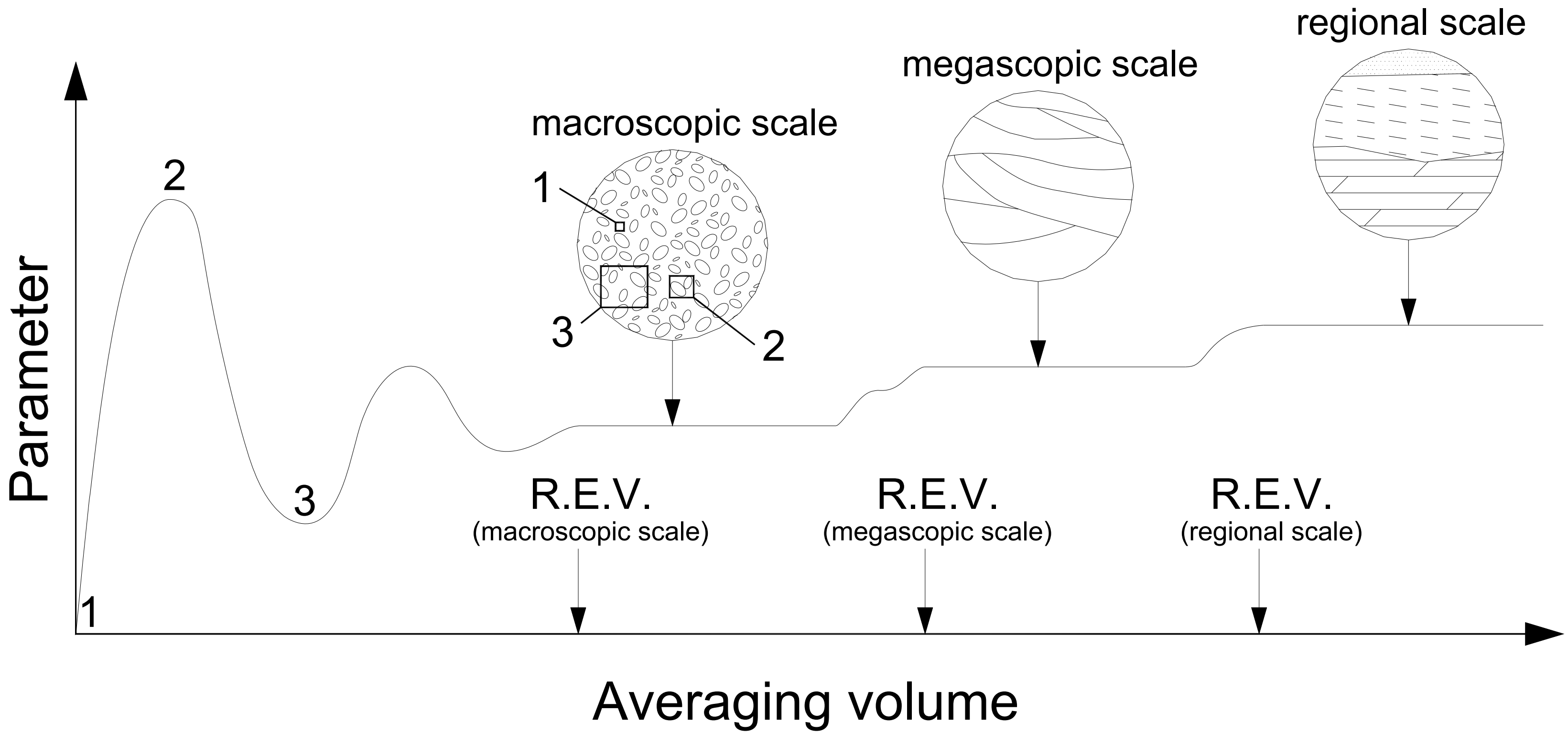
- all parameters that are uncertain

In practice:

- the most uncertain parameters
- Parameters that can be identified from the observed state variables

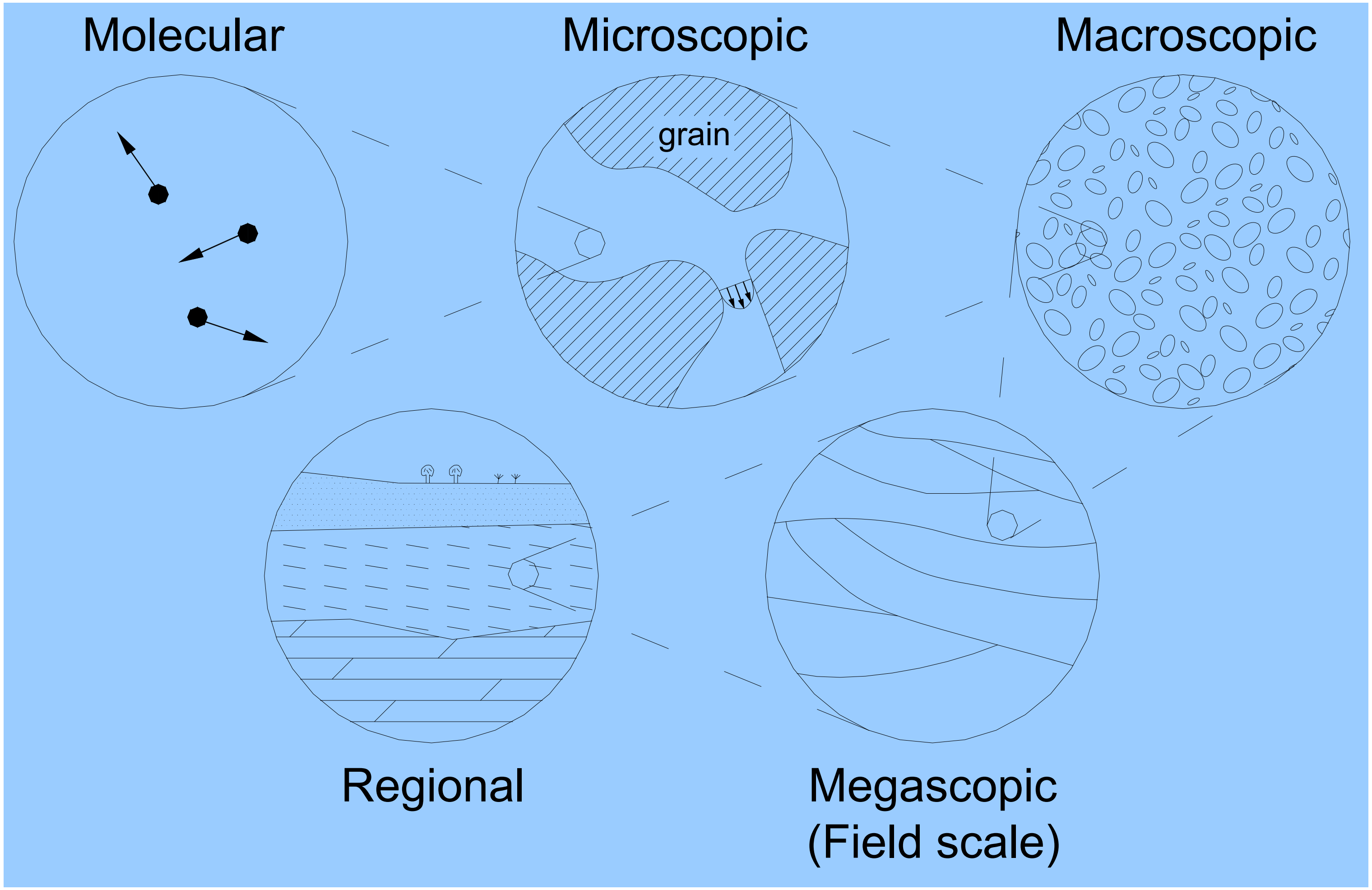
→ Hydrogeological parameters and especially hydraulic conductivity are target for calibrations

Why don't we just measure the uncertain parameters?
- A question of money and scale

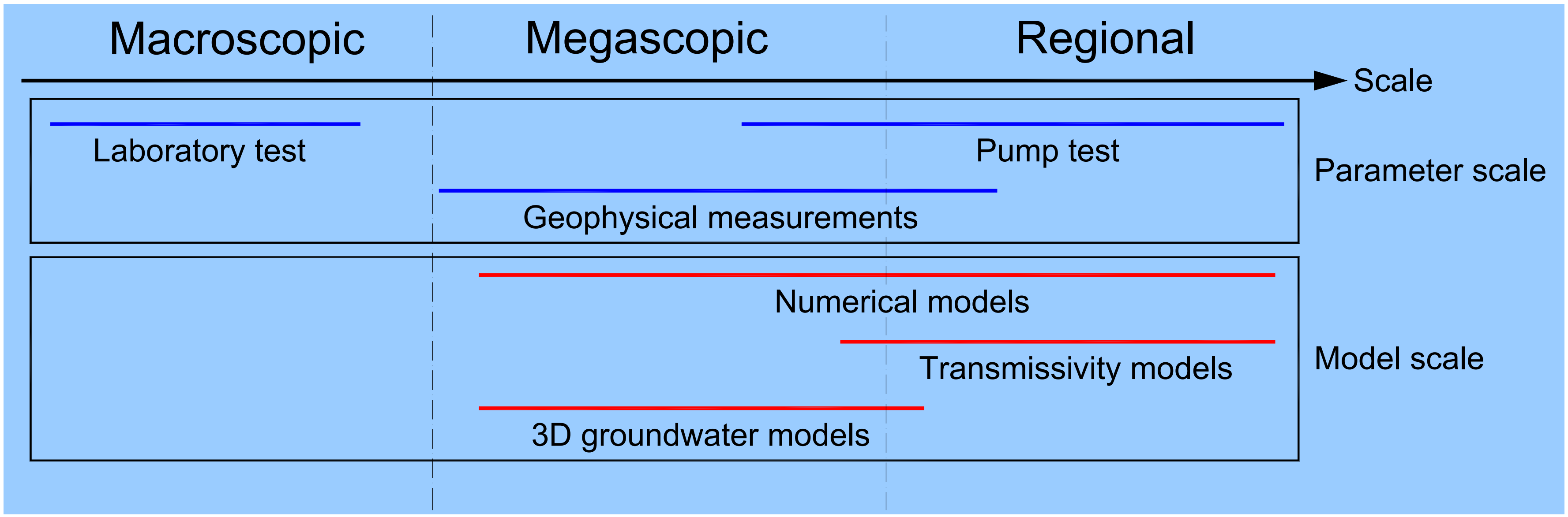


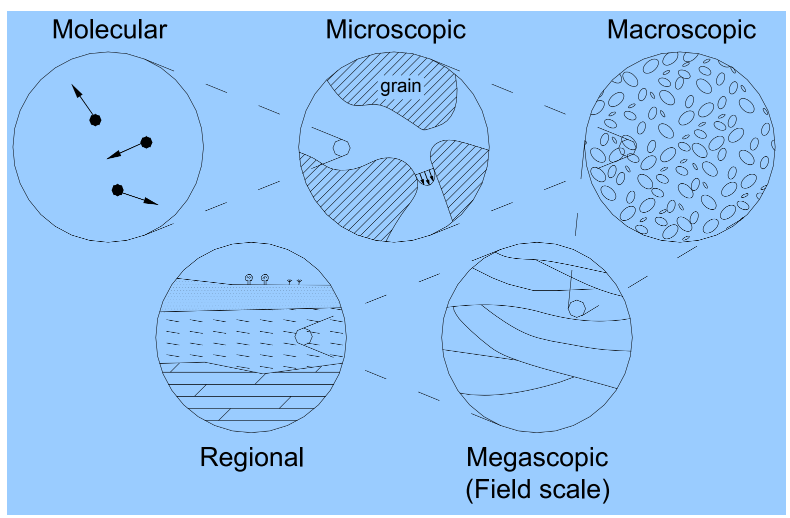
R.E.V. = Representative Elementary Volume

Different scales



At what scale do we measure the parameters and at what scale do we use the parameters?





Parameterization

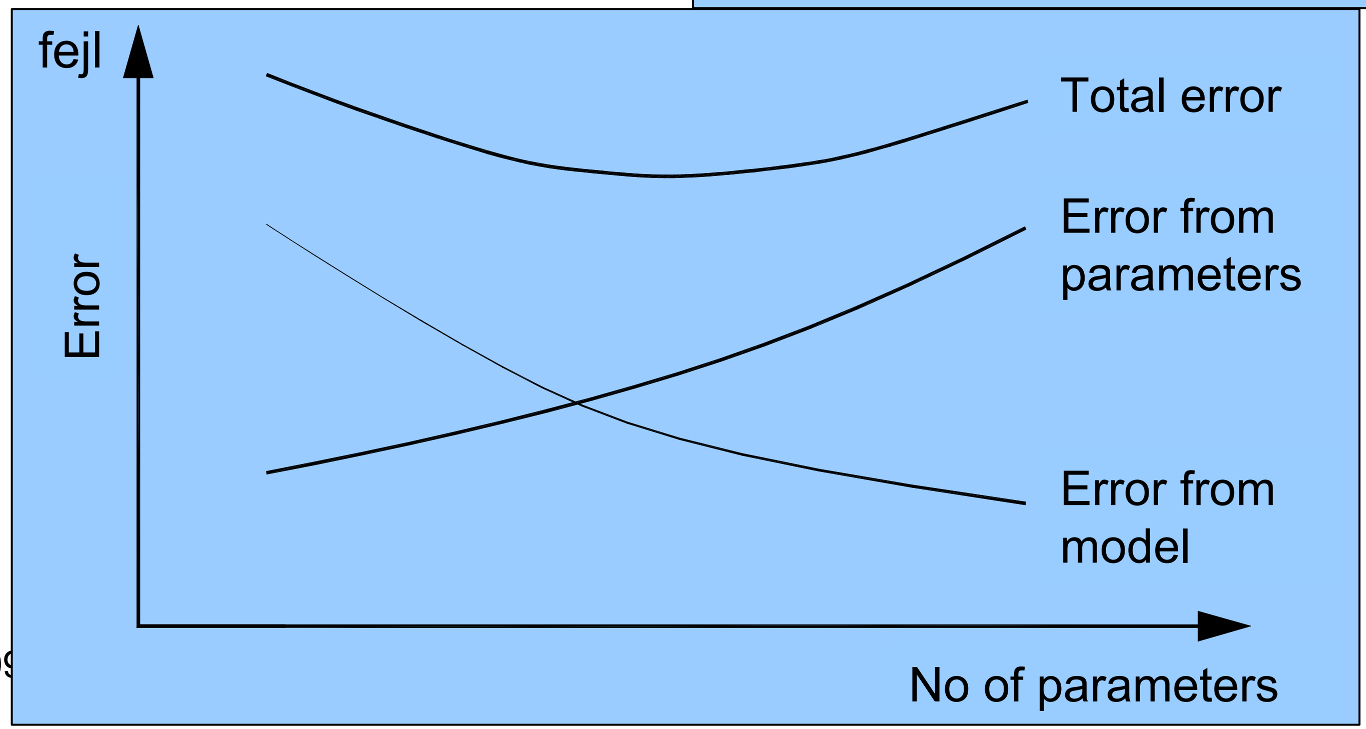
From an ”infinite” number of parameters to a “finite” number of parameters.

The highest number of parameters?

- Kx, Ky, Kz, Sy, Ss i each cell!

The smallest number of parameters?

- one value Kx, Ky, Kz, Sy, Ss in the entire model area!



Parameter estimation

Why can't we find a parameter set that gives a perfect match to the real world (observations)?
- Comparing simulated head and observed head

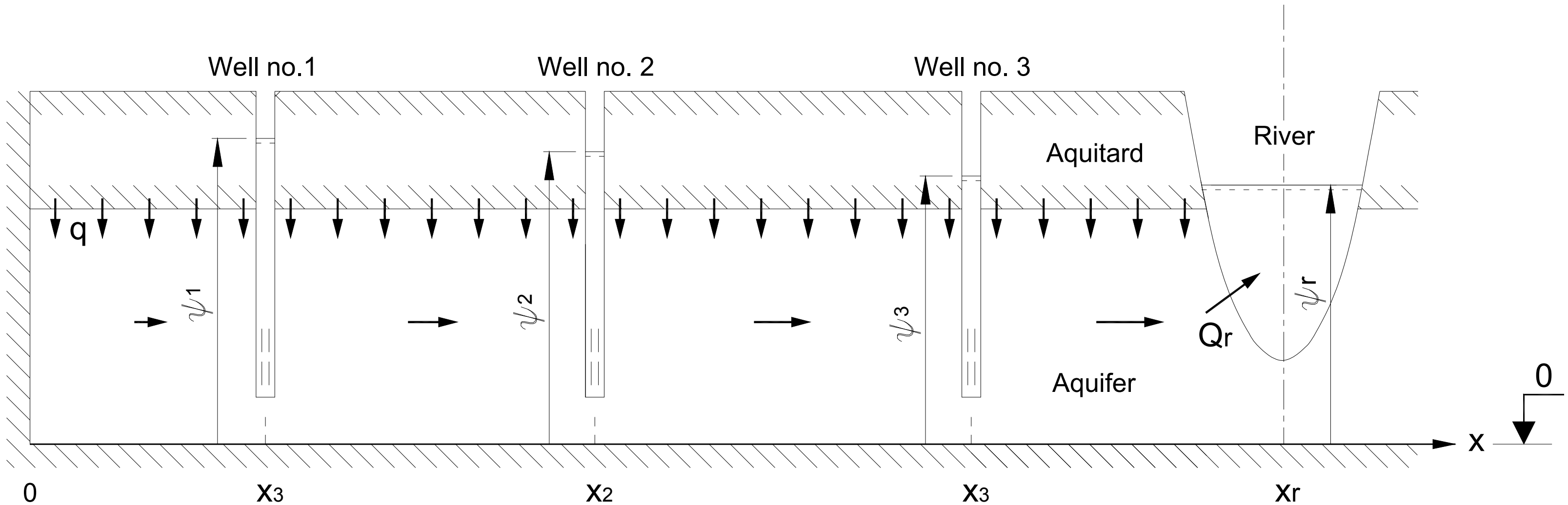
	Obs. error	Scale errors				non stationarity	Total error
		Vertical	Interpolation	Terrain	Heterogeneity		
Esbjerg	0.1	0.1	0.5	0.1	1	0.5	1.2
Fyn	0.1	0.1	1.5	0.2	2.1	0.5	2.6

(Ståbi i grundvandsmodellering, 2000

Expected errors on simulated groundwater potential:

	Error contribution	Standard deviation [m]
Observation error	Measuring equipment	0.03
	Reading and bookkeeping	0.05
	Reference level	0.05 - 2.0
	Atmospheric pressure	0.0 - 0.15
Scale error	Horizontal discretisation	0.5 *Dx J*
	Vertical discretisation	0.5 J_V *Dz* – 2.0
	Topographical variations	s_{topo}/d
	Heterogeneity	$\sqrt{\frac{1}{3}J^2\sigma_{\ln K}\alpha_l^2}$
Time effects	Non-stationarity	D*H*/2
Total error		$\sqrt{\sum \sigma^2}$

Uniqueness



Uknown parameters:
q: Infiltration
T: Transmissivity

Governing equation:

$$\psi(x) = \frac{q}{2T}\left(x_r^2 - x^2\right) + \psi_r$$

Observations:
Case 1: potential, ψ_1, ψ_2, ψ_3
Case 2: potential, ψ_1, ψ_2, ψ_3
Stream discharge, Q_r

Case 1: Non-unique determination of q and T
Case 2: Unique determination of q and T

Requirements for inverse modelling (automatic calibration)

- Unique solution
  - Only one solution can be found
    - Many observation (evenly distributed in the model)
    - Few parameters
    - Different types of observations (head, discharge, etc.)
- Identifiable solution
  - A solution can be found
- Stable solution
  - Small error in an observed state variable leads to small changes in the parameter estimate

Regression based methods

- Search after one optimal parameter set
- Converges to locale minima
- Uniqueness, identifiability and stability is required!
- Parameter uncertainty estimates can be estimated from a gradient analyses near parameter optimum.
- Prediction uncertainty on state variables (head, stream flow, etc.)

Linear model with Gaussian distributed errors

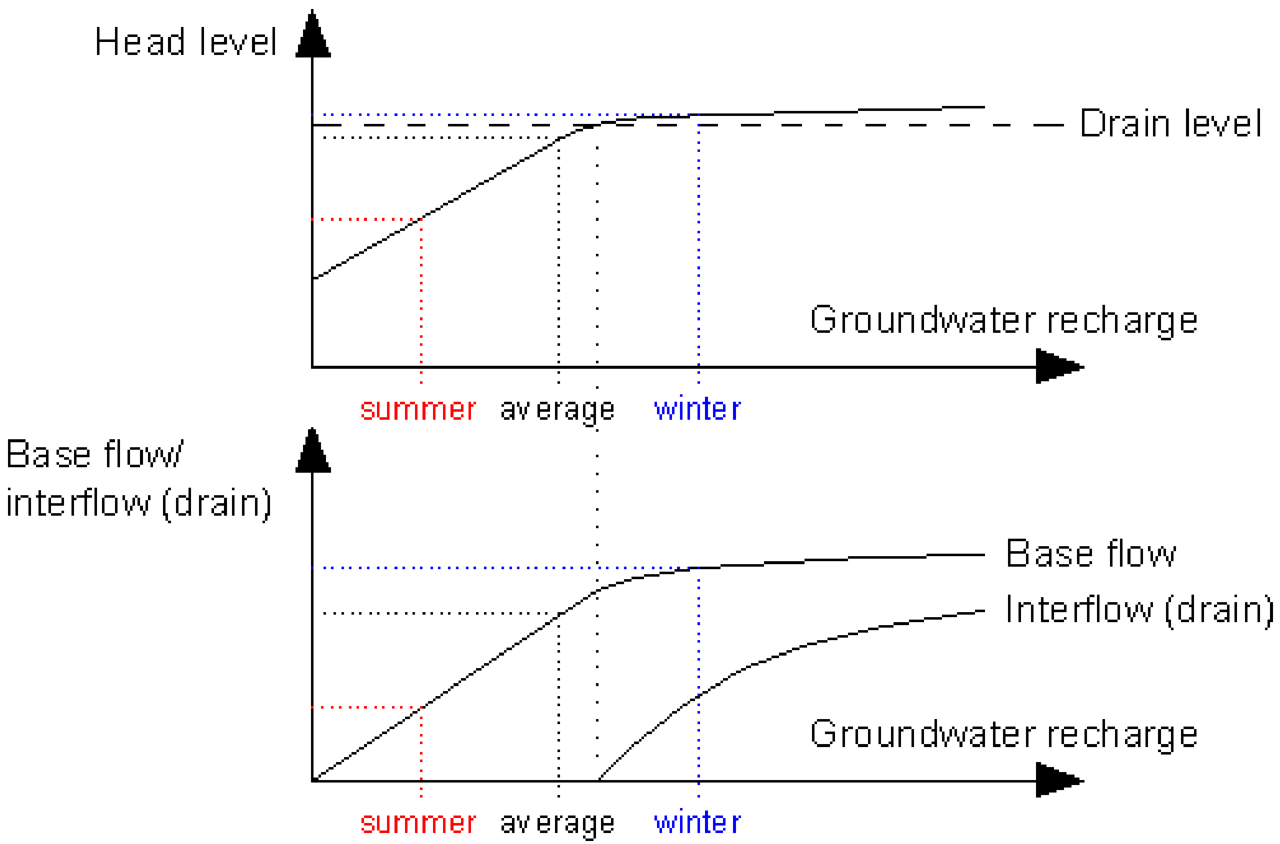
In high dimensional parameter space we have:

- Locale minima, valleys and plateaus in the objective function

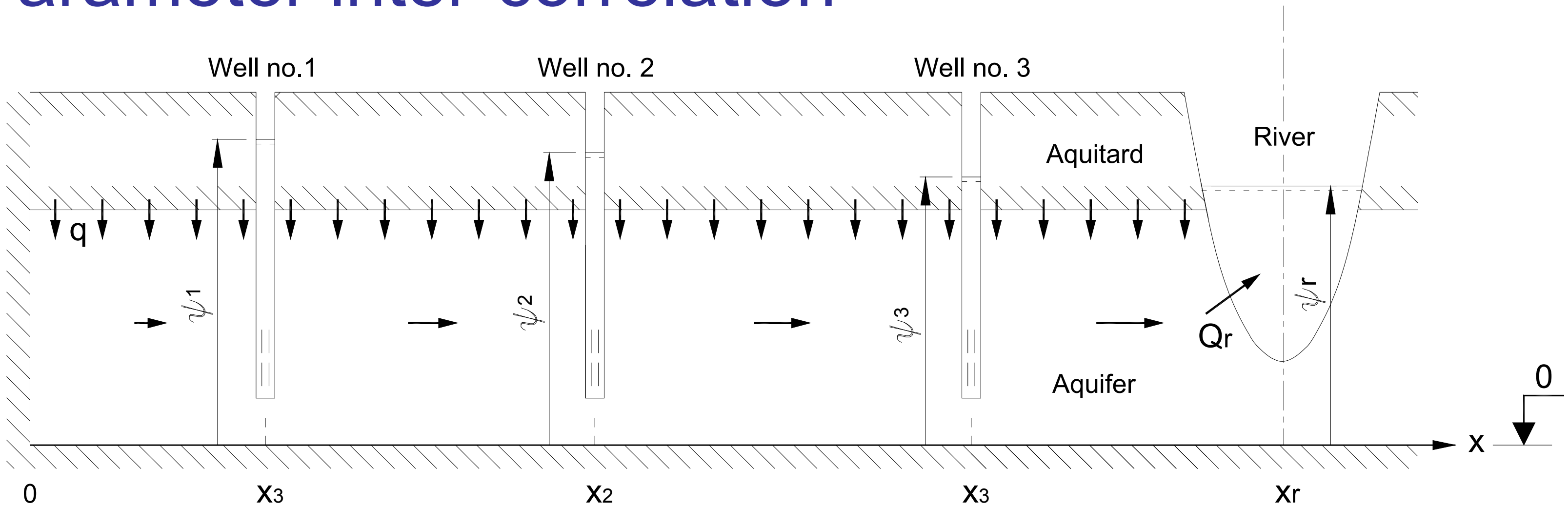
Why?:

- Insensitive parameters (e.g. hydraulic conductivity in a secondary aquifer.
- Treshold processes
- Parameter inter-correlation

- Treshold processes



Parameter inter-correlation



Unknown parameters:
q: Infiltration
T: Transmissivity

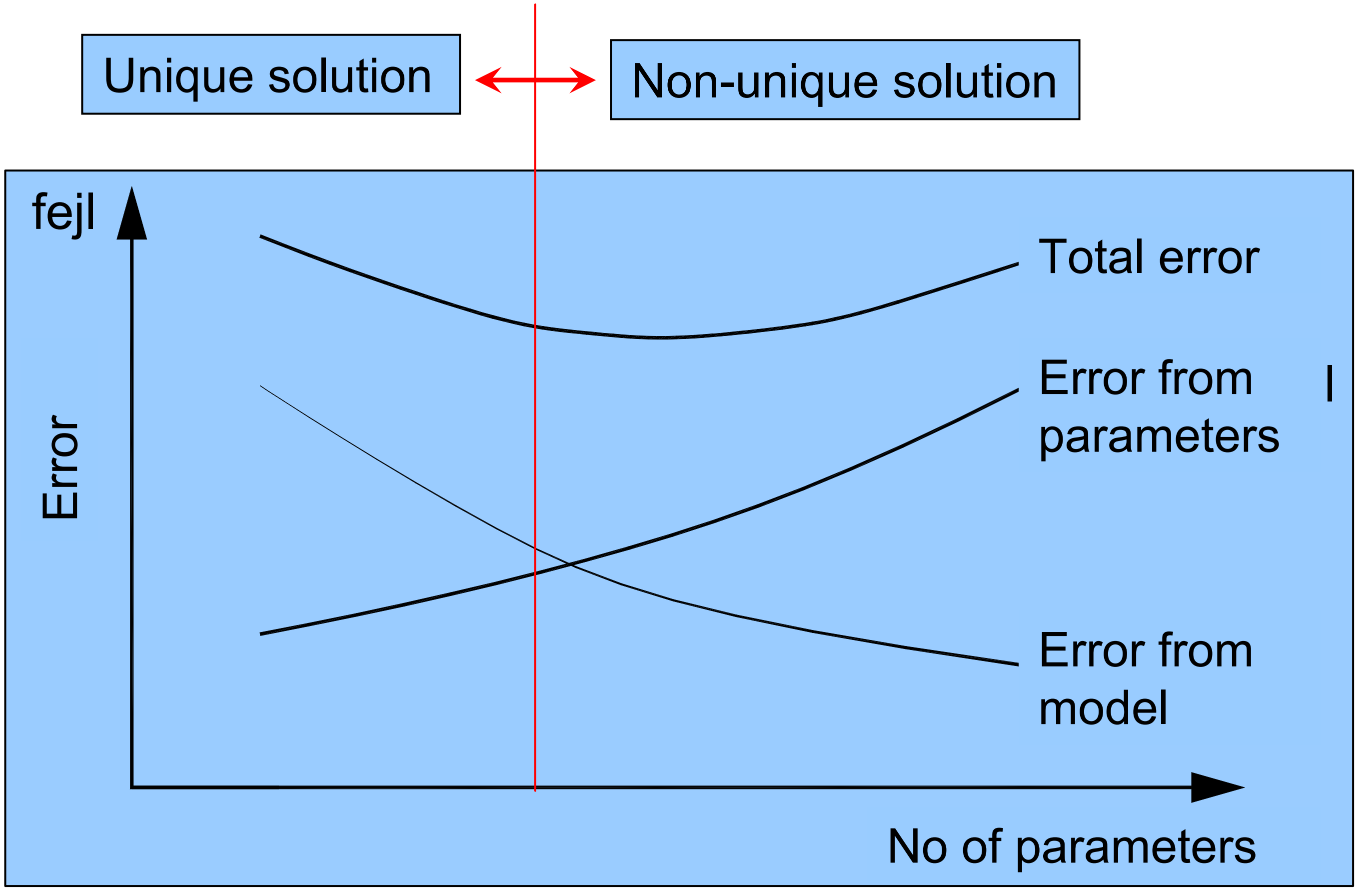
Governing equation:

$$\psi(x) = \frac{q}{2T}\left(x_r^2 - x^2\right) + \psi_r$$

q ↑ ➔T ↓

The equifinality problem

- *A large number of models, parameters and variables may acceptable for reproduction of the considered system*


Unique solution
Non-unique solution
fejl
Error
Total error
Error from
parameters
Error from
model
No of parameters

What is GLUE?

Stochastic model:

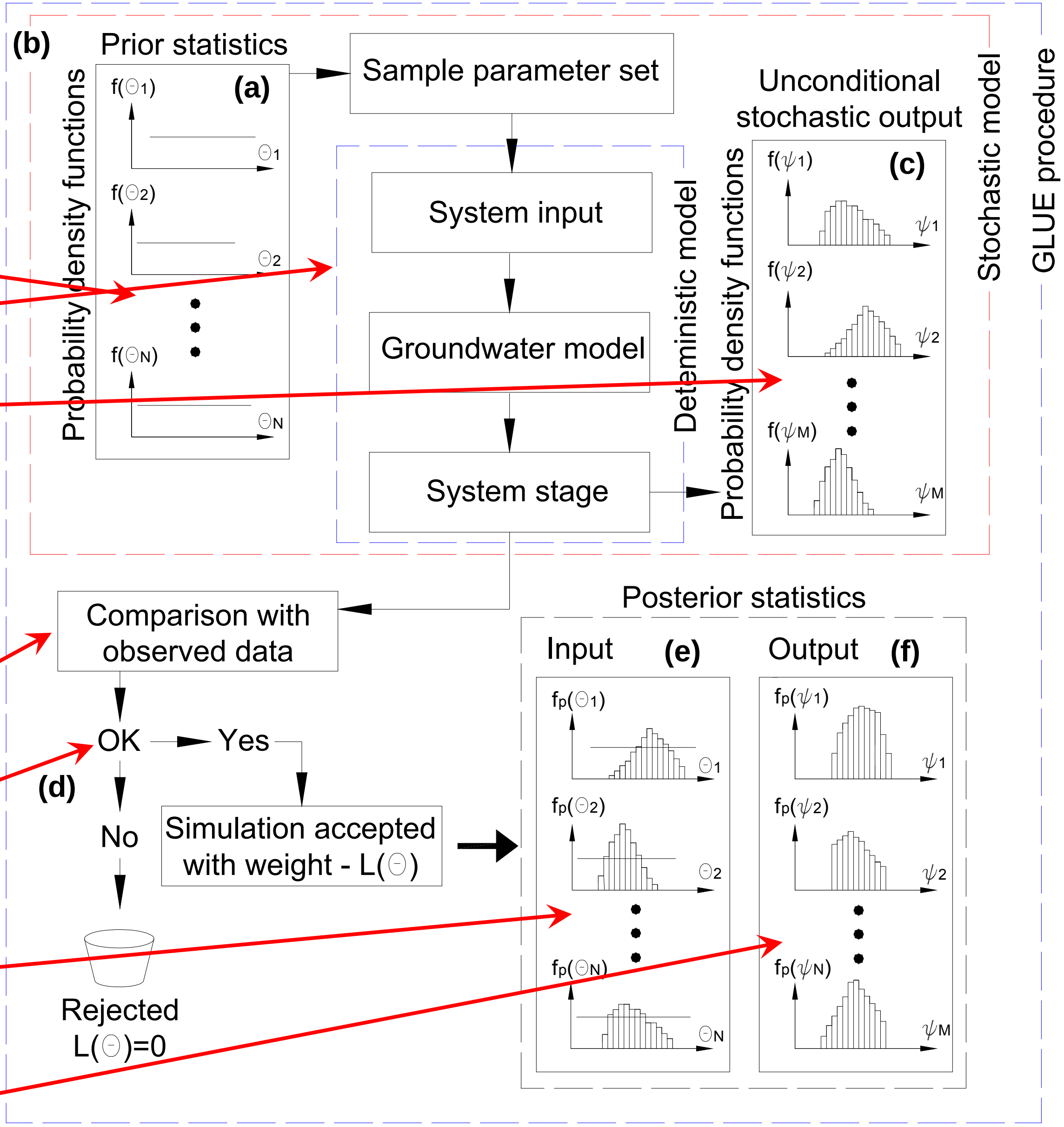
- stochastic input
- deterministic model
- stochastic output

Parameter estimation model:

- compare results from each deterministic simulation with observations
- reject or accept the simulation

➔ posterior parameter distribution

➔ density functions for output

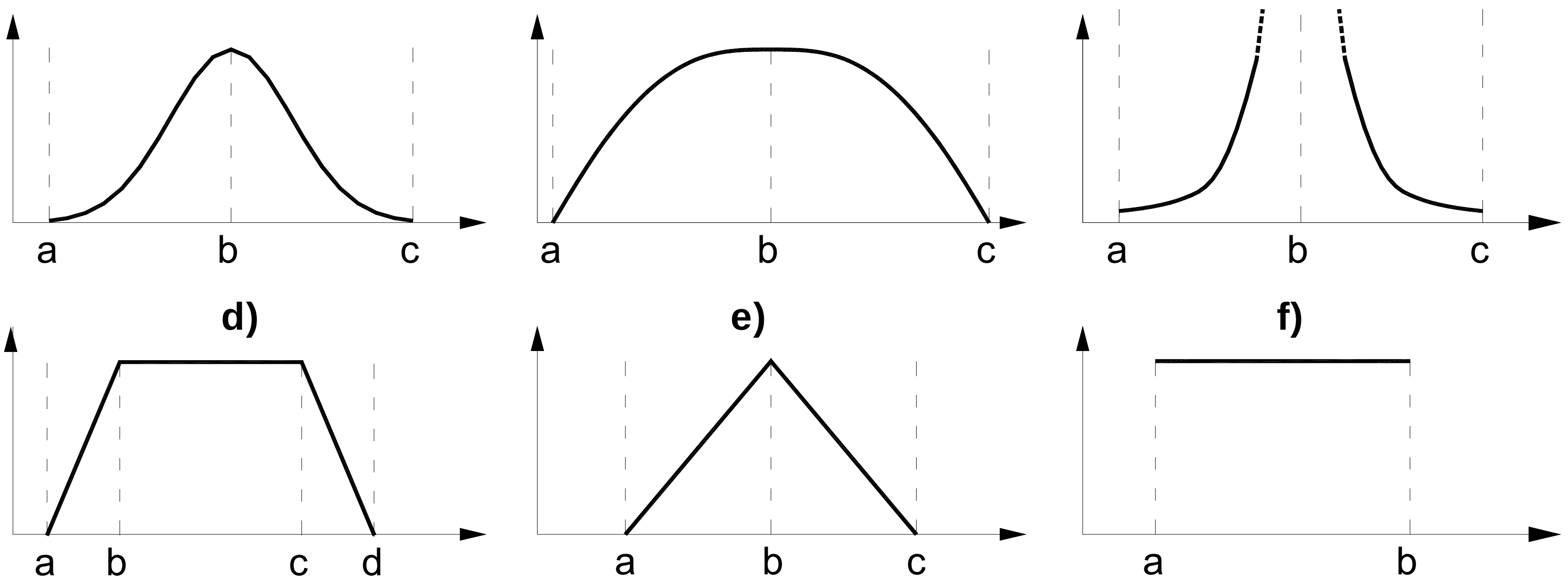


GLUE

Generalized Likelihood Uncertainty Estimation methodology

Calculate the conditional likelihood $L(\theta_i|\mathbf{y}_j^*)$

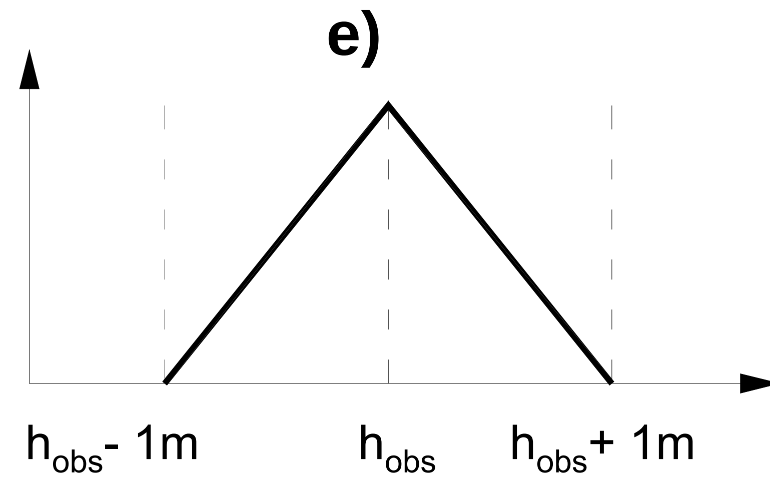
Point likelihood measure:



Likelihood measures

Observed and simulated heads:

Well no.	Sim. head	Obs. head	Point Likelihood
1	29	28.1	0.1
2	28	27.5	0.5
3	26	25.25	0.25



"Global" likelihood:

Geometric inference function

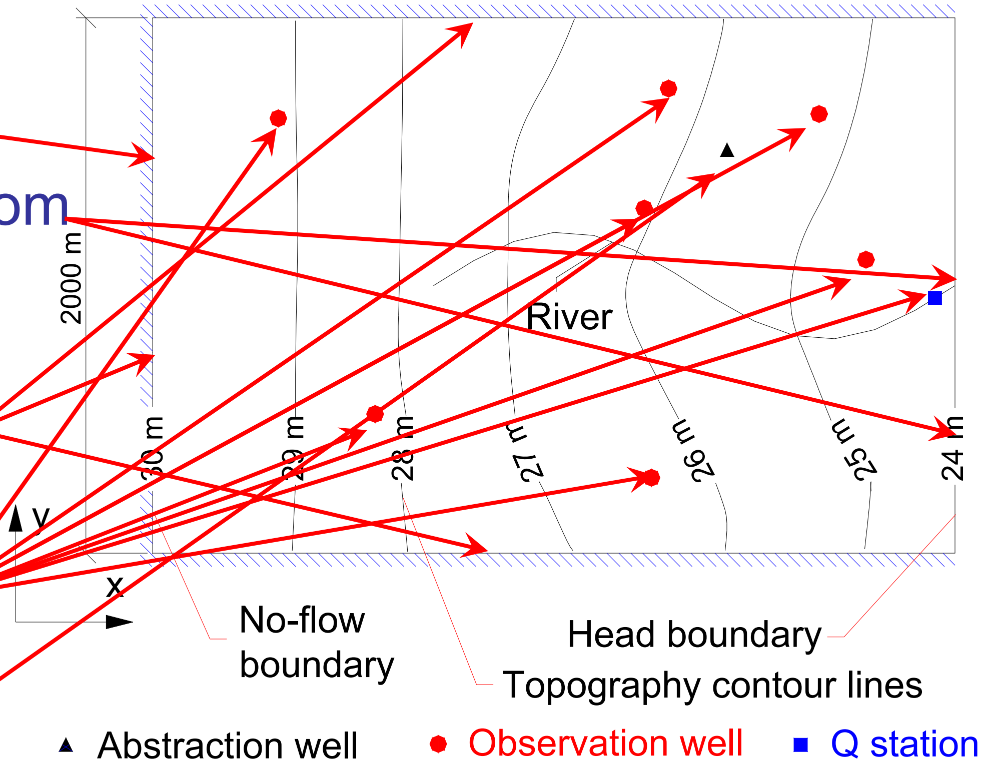
$L(\theta_i|\mathbf{y}^*) = (L(\theta_i|\mathbf{y}_1^*)\ L(\theta_i|\mathbf{y}_2^*)\ L(\theta_i|\mathbf{y}_3^*))^{1/3}$

$L(\theta_i|\mathbf{y}^*) = (0.1*0.5*0.25)^{1/3} = 0.232$

Case study – synthetic setup

Conceptual model

- River catchment
- Base flow and river outlet from catchment in East
- No-flux boundary at South, West and North
- Head and river discharge gauging points
- Groundwater abstraction



Objective of the case study: **Capture zone estimation**

Case study – synthetic setup

Conceptual model – geological model

Two alternative geological models:

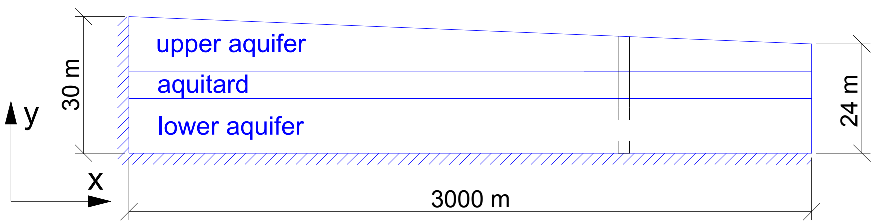
Model A:

- three continuous layers
- constant parameters within each layer

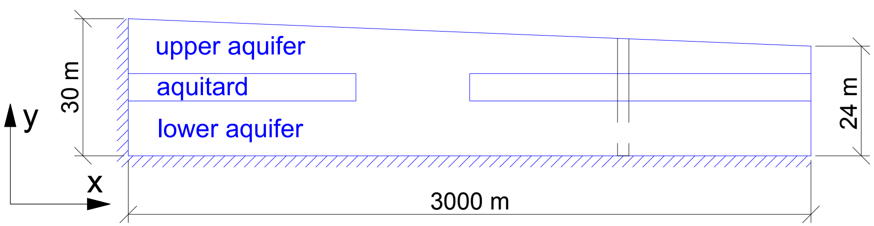
Model B:

- continuous upper and lower aquifer
- sandy window in aquitard
- constant parameters within each layer

Model A



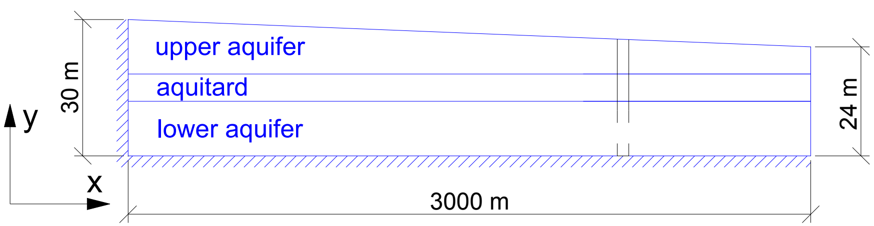
Model B

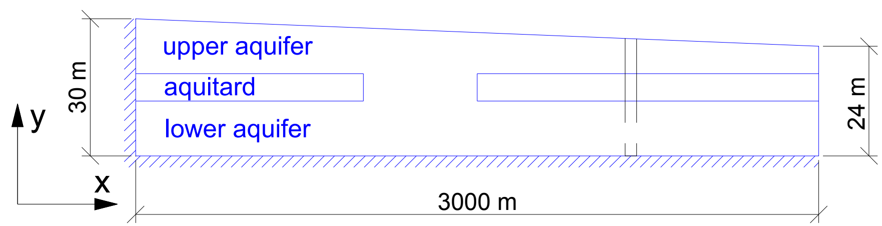


Case study – synthetic setup

Conceptual model – key parameters

1. Geological model
2. Net precipitation [mm/year]
3. Horizontal conductivity in upper aquifer
4. Horizontal conductivity in aquitard
5. Vertical conductivity in aquitard
6. Horizontal conductivity in lower aquifer
7. Vertical conductivity in lower aquifer





Case study – synthetic setup

Numerical model

Flow model:

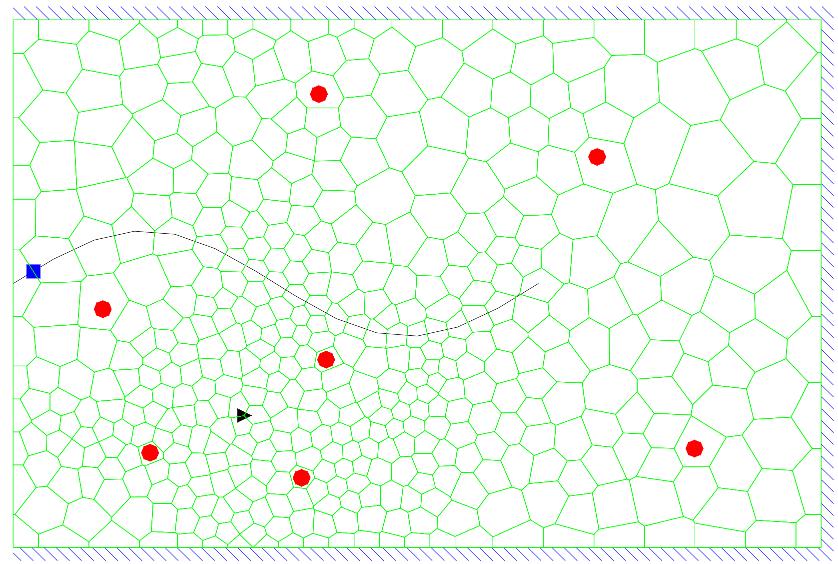
- Unstructured finite difference grid
- Steady state simulation
- River flow: 1D diffusive wave approximation.
- Overland flow: 2D diffusive wave approximation.
- Saturated zone: 3D flow

Fully integrated

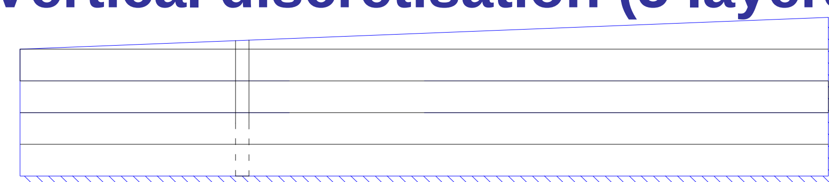
Capture zone determination

- Particle tracking (advective transport)
- Particle transport in all components

Horizontal discretisation (470 elements)



Vertical discretisation (5 layers)



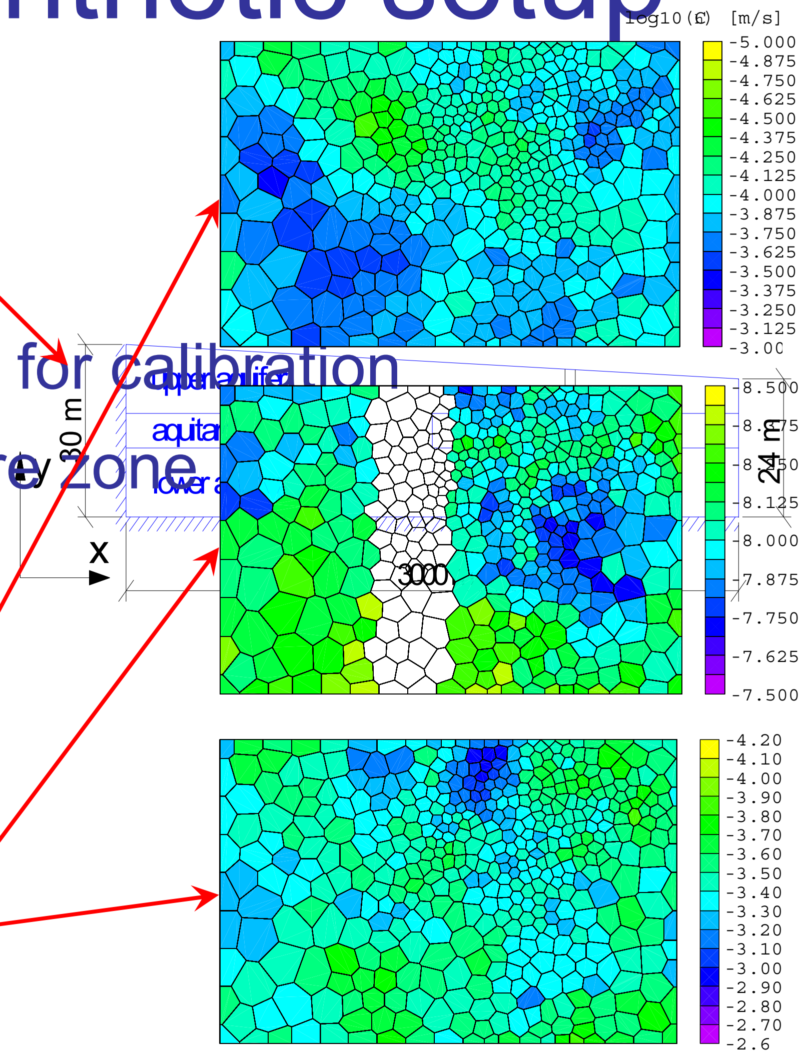
Case study – synthetic setup

Reference model

Why?

- Generation of “observed” data for calibration
- Generation of the “true” capture zone

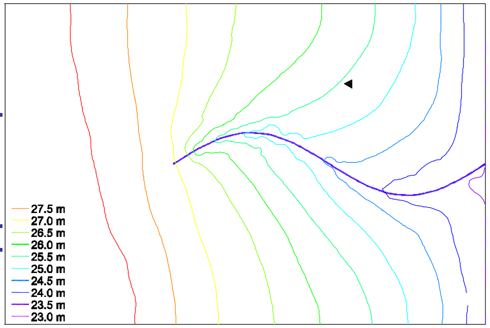
		Dist.	Range
Geological model		D	B
Net precipitation [mm/year]	p	D	315
Abstraction [mm/year]	Q	D	50
Upper aquifer [m/s]	C_h	D	random field
	C_z	D	1.e-7
Aquitard [m/s]	C_h	D	1.e-8
	C_z	D	random field
Lower aquifer [m/s]	C_h	D	random field
	C_z	D	1.e-6



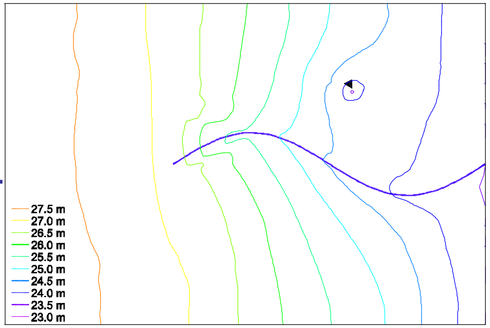
Case study – synthetic setup

Groundwater potential

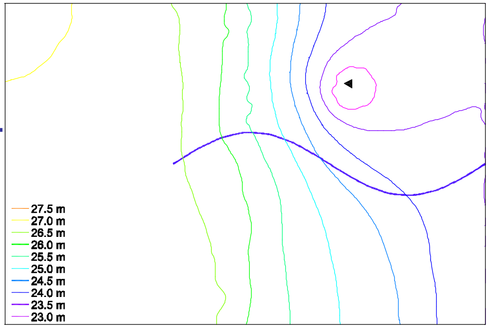
upper aquifer



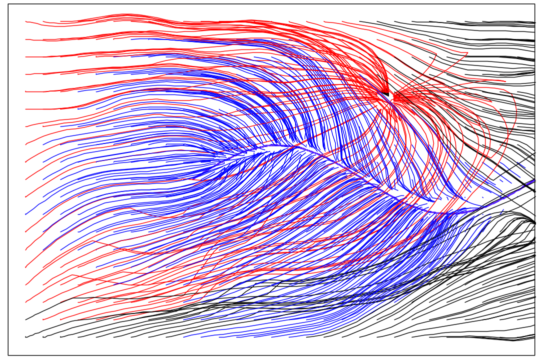
aquitard



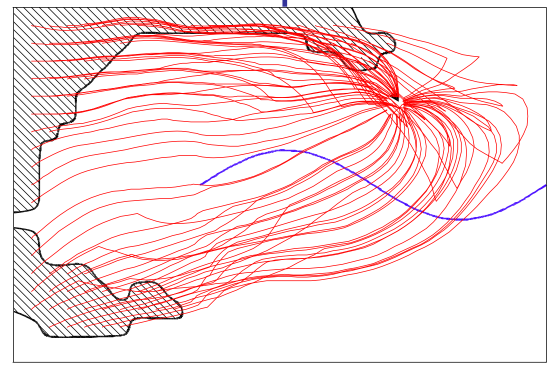
lower aquifer



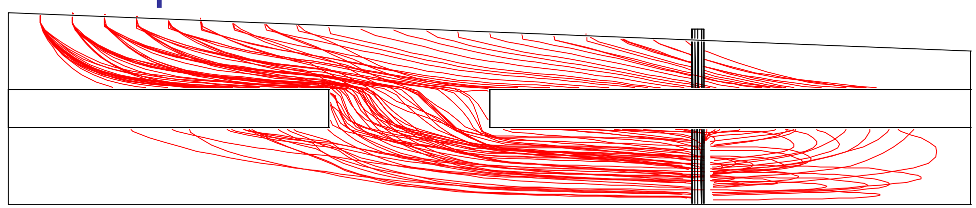
Flow paths



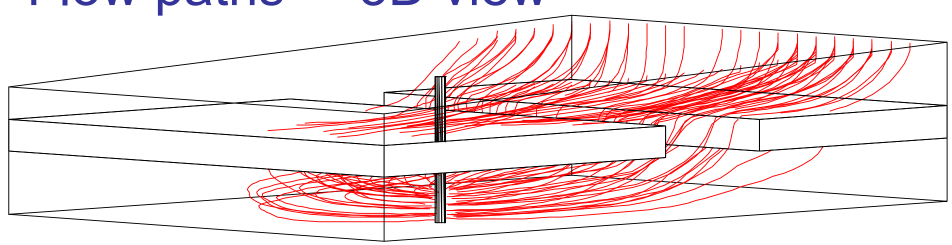
Capture zone



Flow paths – vertical view



Flow paths – 3D view



Case study – synthetic setup

What have we got?

- two conceptual m[illegible]els
- conceptual m[illegible]el error
- many pa[illegible]meters
- few o[illegible]ervations (lower aquifer)
- [illegible]n water balance

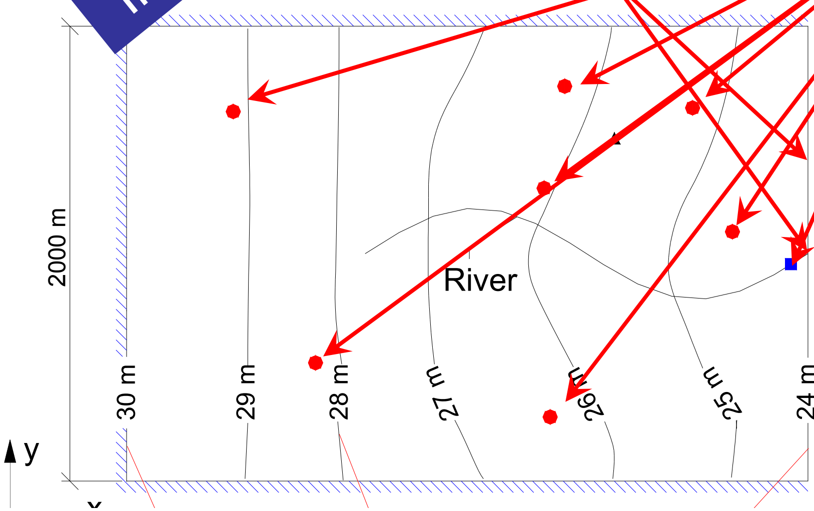
Ill-posed calibration problem

		Dist.	Range
Geological model		U	A;B
Net precipitation [mm/year]	p	U	270 – 330
Abstraction [mm/year]	Q	D	50
Upper aquifer [m/s]	C_h	$L_{10}U$	1.E-5 – 5.E-3
	C_z	D	1.0E-7
[illegible]	[illegible]	[illegible]	5.E-9 – 5.E-7
[m/s]	C_z	$L_{10}U$	5.E-9 – 5.E-7
[illegible]	[illegible]	[illegible]U	1.E-5 – 5.E-3
[m/s]	C_z	$L_{10}U$	1.E-6 – 1.E-4

Net precipitation unknown

Boundary base flow unknown

River discharge uncertain



Case study – synthetic setup

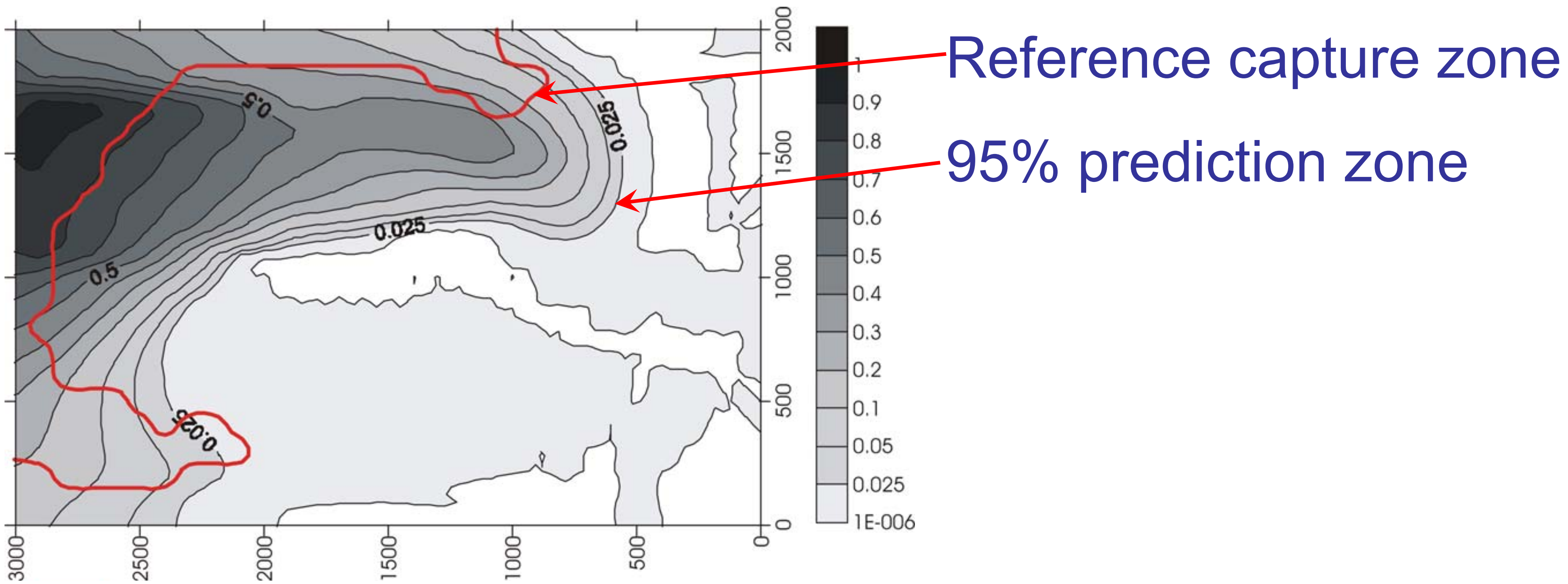
GLUE analysis

Monte Carlo simulation

- 200,000 flow and particle simulations
- ~ 4 weeks on a 4 GHz PC cluster (six PCs)

Case study – synthetic setup

Capture zone results – Monte Carlo



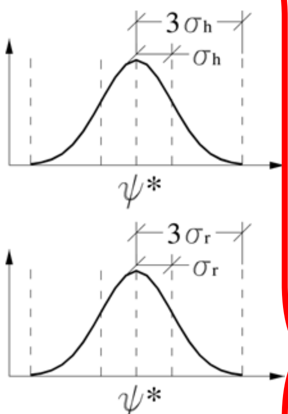
Case study – synthetic setup

Capture zone results – GLUE results

Point likelihood function:

Head:
Gaussian, s_h=0.2m

River flow:
Gaussian, s_r=10%

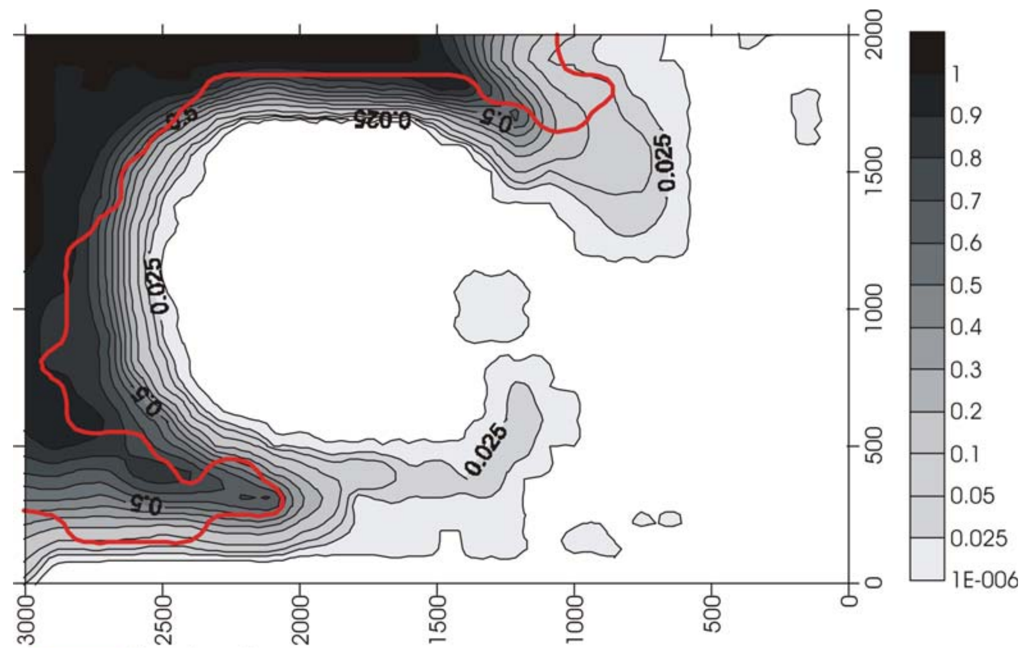


Rejection level:

Head and river flow: 3s

Inference function:

Geometric mean

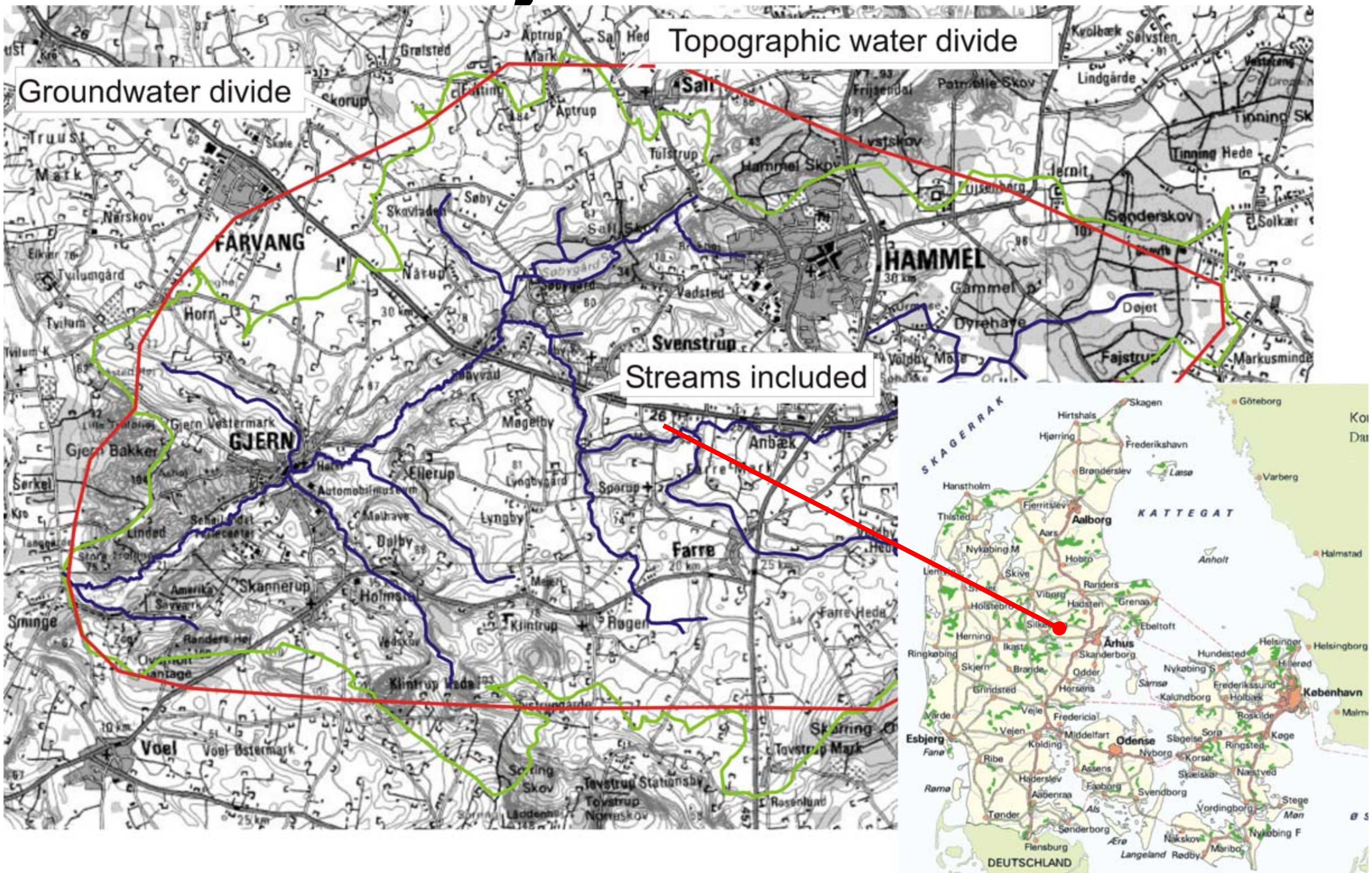


Case study – synthetic setup

The “optimal” solution (highest likelihood)

Parameter		Reference model	Best fit
		Value/range	Value
Geological model		B	A
Net precipitation [mm/year]	p	315	309
Abstraction [mm/year]	Q	50	-
Upper aquifer [m/s]	C_h	$\log_{10}$(1.5E-04,0.75E-04,500)	1.88e-4
	C_z	1.e-7	-
Aquitard [m/s]	C_h	1.e-8	3.72e-7
	C_z	$\log_{10}$(1.E-08,0.5E-08,500)	5.08e-9
Lower aquifer [m/s]	C_h	$\log_{10}$(5.E-04,2.5E-04,500)	2.62e-4
	C_z	1.e-6	1.36e-6

Gjern model

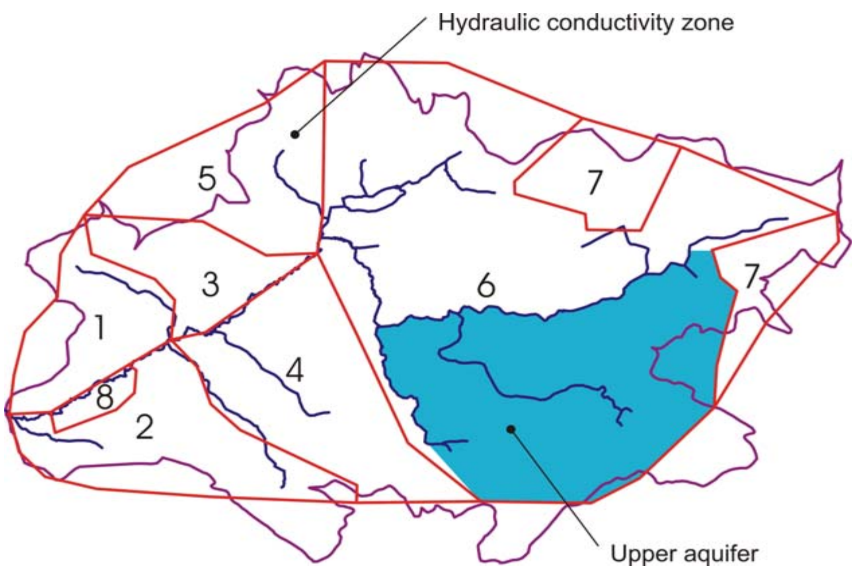


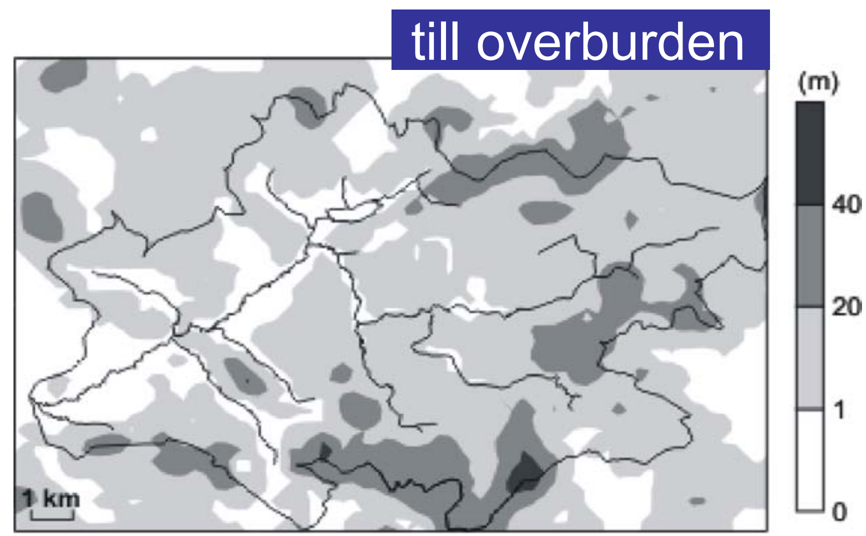
Topographic water divide
Groundwater divide
Streams included

Gjern model

Geology

- Main aquifer: sand and gravel – eight conductivity zones
- Aquitard - Till overburden > 1 m
- Secondary upper aquifer





Gjern model

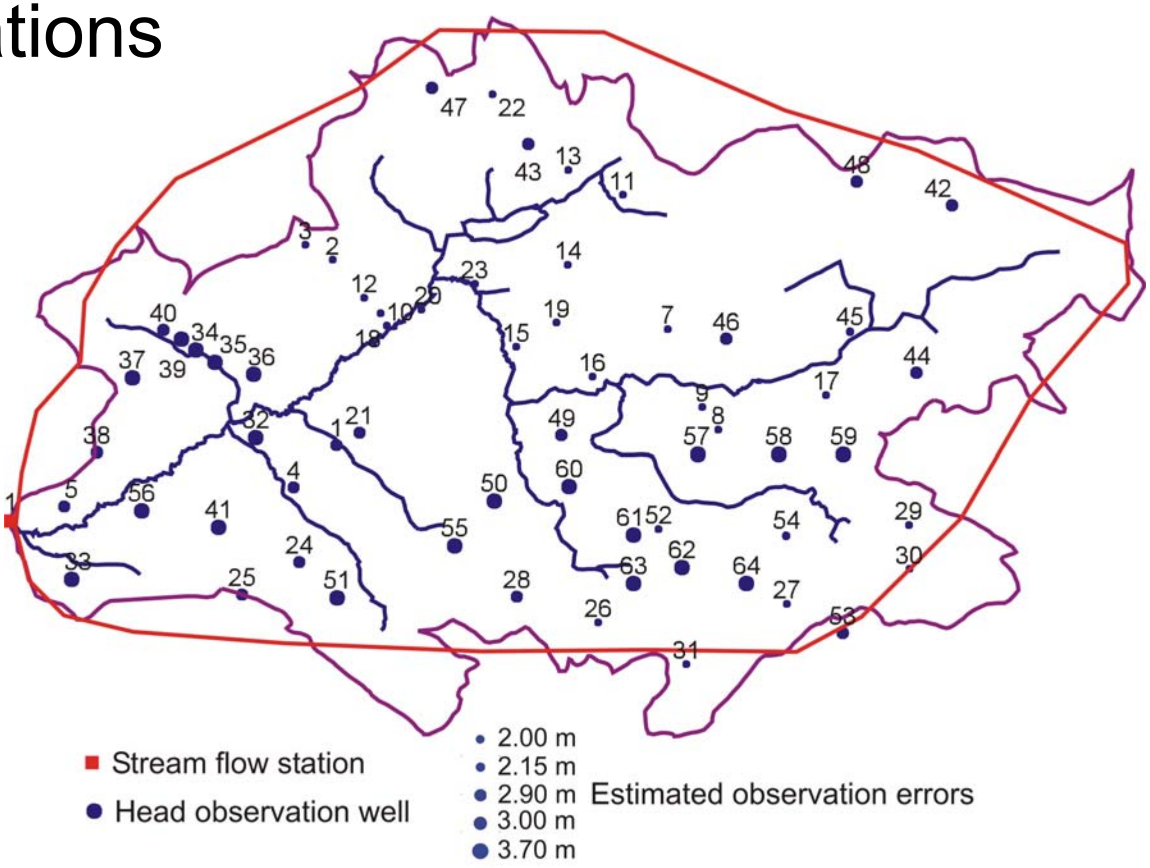
Recharge

1. Recharge directly to the lower main aquifer
2. Recharge to the upper secondary aquifer
3. Leakage from the aquitard to the lower main aquifer

Gjern model

Observation data – calibration

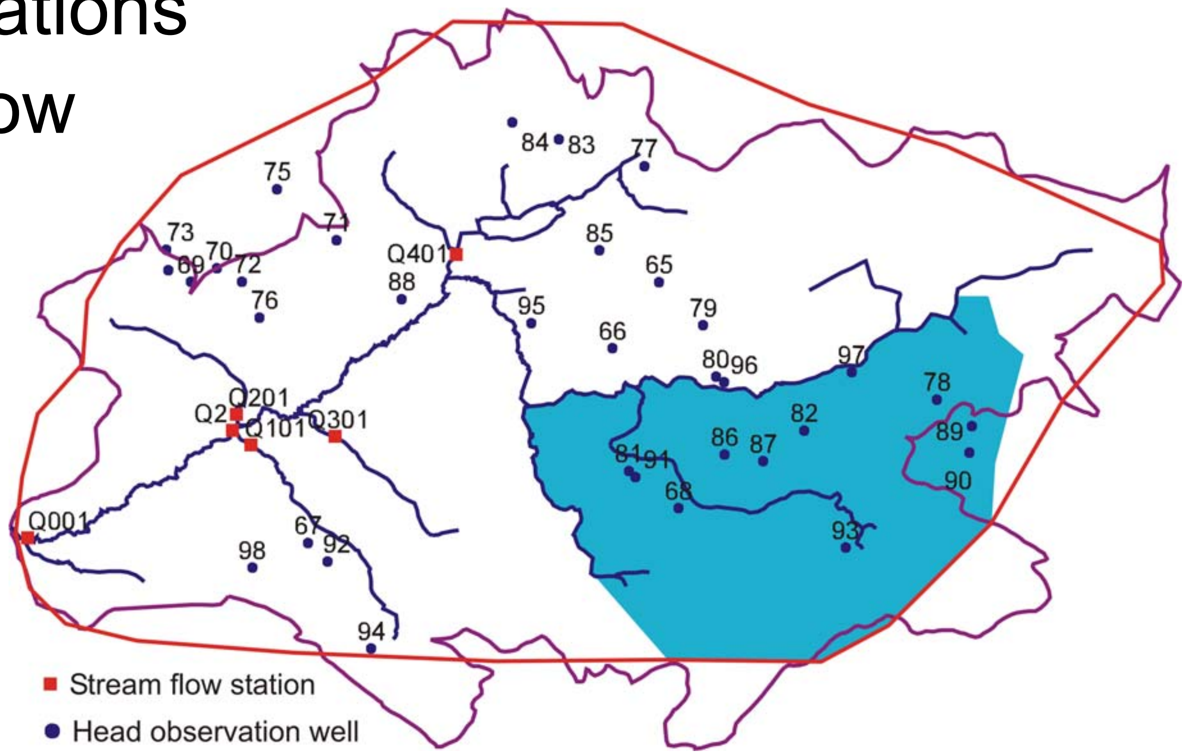
- 64 head observations
- one stream flow observation



Gjern model

Observation data – validation

- 34 head observations
- seven stream flow observations



Gjern model

Unknown parameters

- Recharge: RCH1, RCH2
- Horizontal hydraulic conductivity, C1–C7 (main aquifer)
- Vertical hydraulic conductivity, Cv (aquitard)
- Transmissivity, Tu (secondary aquifer)

➔ In a total of eleven parameters

Gjern model

GLUE analysis

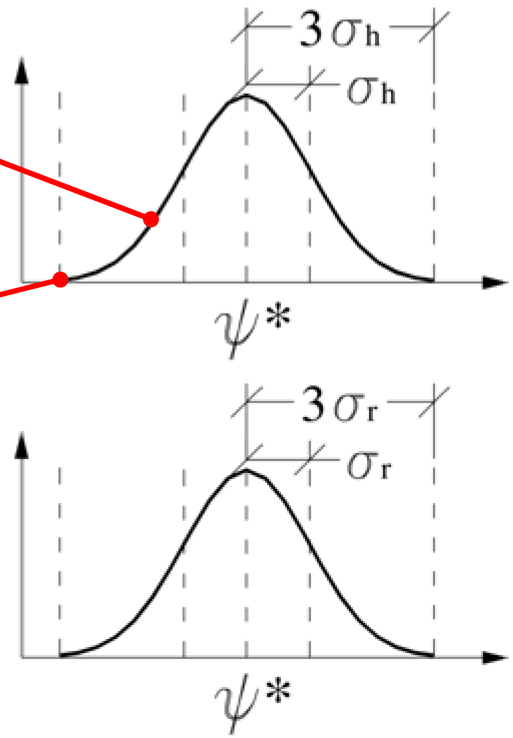
Point likelihood function:

Head:

Gaussian, s_h=2.0 – 3.7m

River flow:

Gaussian, s_r=10%



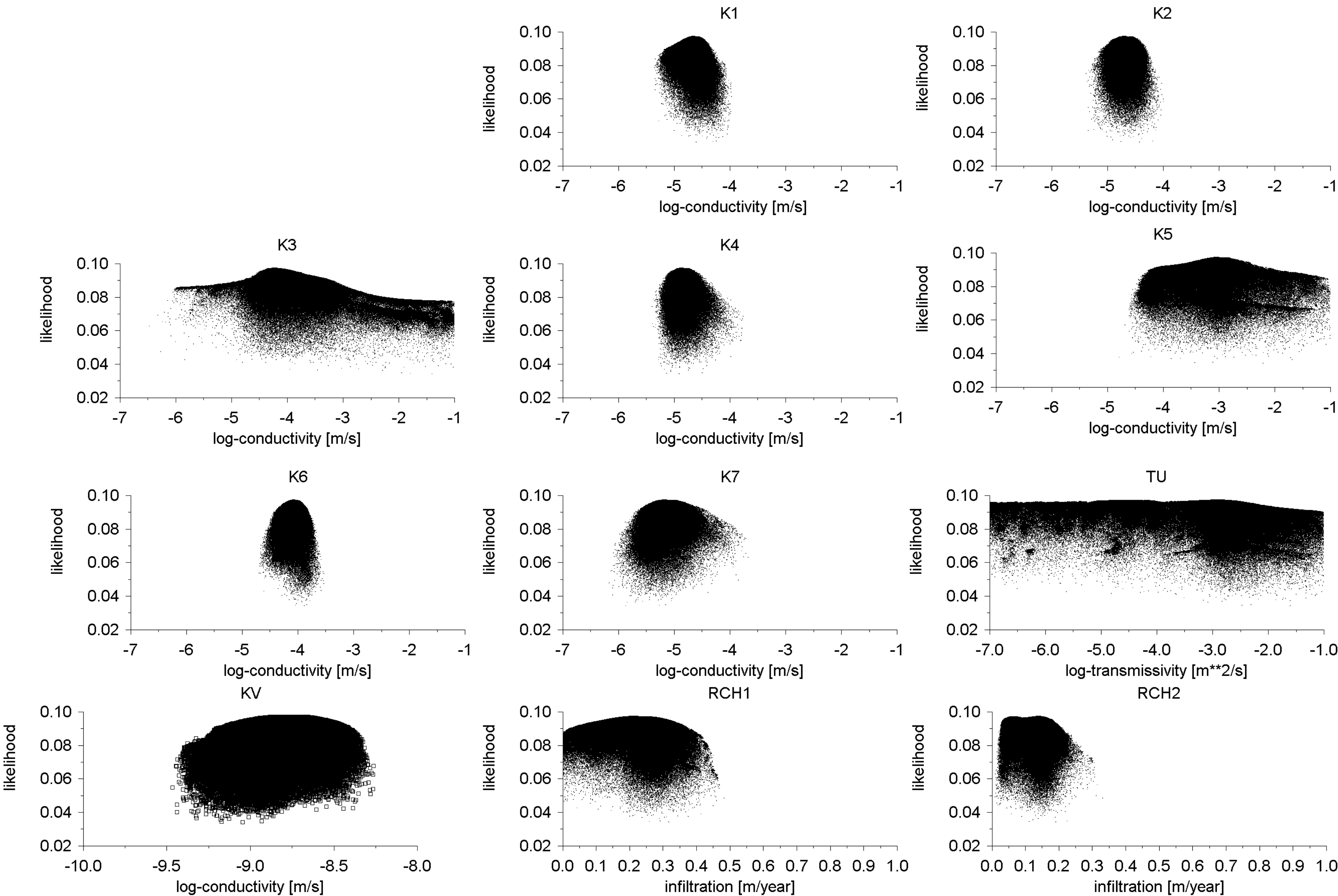
Rejection level:

Head and river flow: 3s

Inference function:

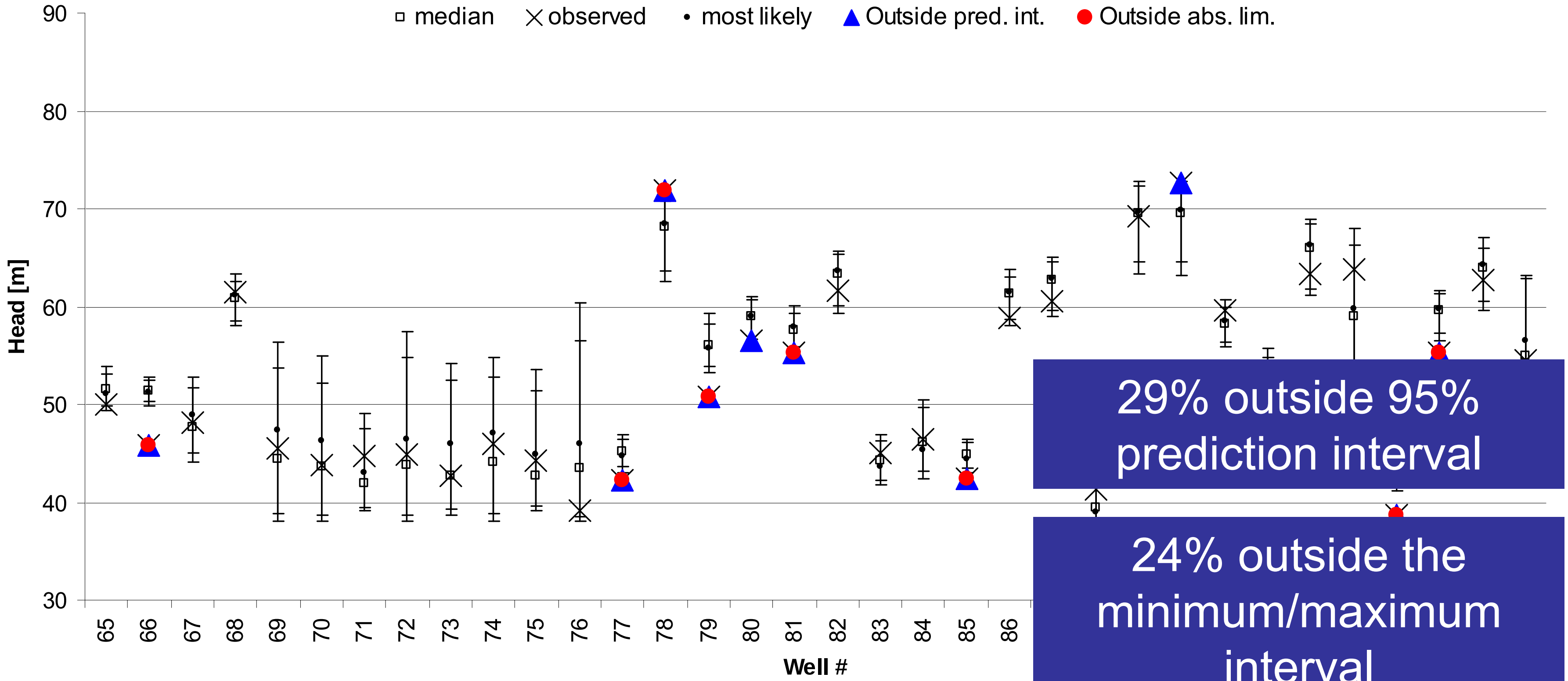
Geometric mean

Parameter scatter plots



Gjern model

Validation – 34 head obs. (validation data)



29% outside 95% prediction interval

24% outside the minimum/maximum interval

Gjern model

Validation – 98 head observations