Effective approaches for Assessing the Predicted Environmental COncentrations of Pesticides

A project supporting the harmonised registration of pesticides in Europe

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EU-FP5- Quality of Life programme

Who?

- Université catholique de Louvain (M. Vanclooster et al.)
- Alterra (J. Boesten et al.)
- Swedish university of agricultural sciences (N. Jarvis et al.)
- Forschungszentrum Jülich GmbH (P. Burauel et al.)
- Instituto de Recurso Naturales y Agrobiologica de Sevilla (E. Fernandez et al.)
- Universita Cattolica de Sacro Cuore (M. Trevisan et al.)
- Fraunhofer Institut für Umweltchemie und Okotoxikologie (M. Klein et al.)
- Rijksinstituut voor volksgezondheid en milieu (A. Tiktak et al.)
- Joint Research Centre (G. Bidoglio et al.)

Research context

Directive 91/414/EU: ‘ Uniform principles ’ for registration of crop protection products

> “...Use validated simulation models for PEC to groundwater, surface water and air…”

EU/DG-SANCO: FOCUS (Forum for the co-ordination of the pesticide fate models and their use) working groups

- Develop guidelines on the selection and use of pesticide emission models
- Define scenarios for the use of pesticide emission models in the process of registration

Objectives

To evaluate the validation status of PEC groundwater models

To evaluate the validation status of PEC groundwater scenarios (i.e. FOCUS scenario's)

To propose new effective approaches considering

- preferential flow
- volatilization

Valid?

Pan-European agri-environmental data

i.e. FOCUS Groundwater Scenario

↓

Fate and transport model for the soil crop continuum

- PEARL
- MACRO
- PELMO

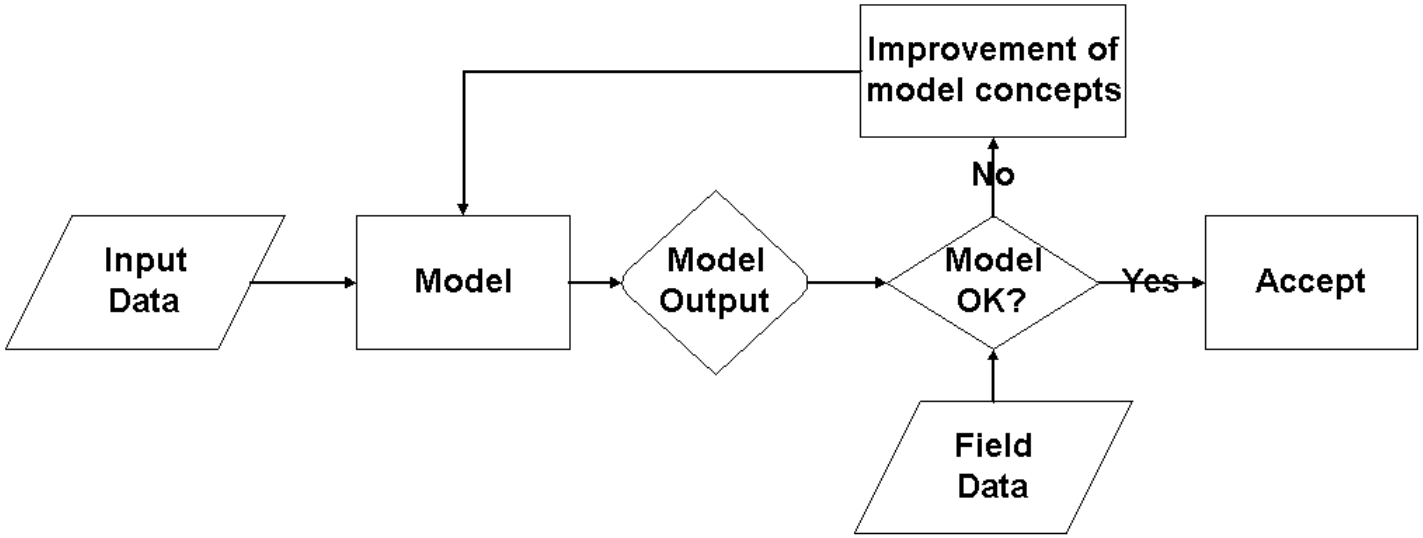
↓

Pan-European PEC

Valid?

Validating local scale PEC groundwater models

Research method



Local PEC model

Local scale agro-environmental data

↓

Fate and transport model for the soil-crop continuum

- PEARL
- MACRO
- PELMO

↓

Local PEC

Local PEC model test sites

Local PEC model test sites

Lanna	Sweden	Cold humid	Silty clay over clay	Larsson and Jarvis, 1999
Brimstone	United Kingdom	Moderate sea climate	Cracking heavy clay	Bromilow et al., 1998; Harris and Catt, 1999; Armstrong et al., 2000.
Andelst	the Netherlands	Moderate sea climate	Medium clay	In press.
Vredepeel	the Netherlands	Moderate sea climate	Sand	Boesten and van der Pas, 1999, 2000
Lebrija	Spain	Mediterranean	Silty (drained marshland)	Andreu et al., 1996, Rieu et al, 1998;
Coria	Spain	Mediterranean	Silty clay loam	In press.
Bologna	Italy	Mediterranean	Loam	Araldi, 1997, Scarabello, 1999

Evaluation protocol for the local scale PEC model

- Blind validation (neither laboratory or field data)
  - Evaluate generic parameter identification procedures (pedo-transfer functions, environmental fate data base, …)
- Calibration using laboratory data
  - Evaluate local scale parameter identification approach
- Calibration using field data
  - Evaluate inverse modelling approach
- Blind prediction

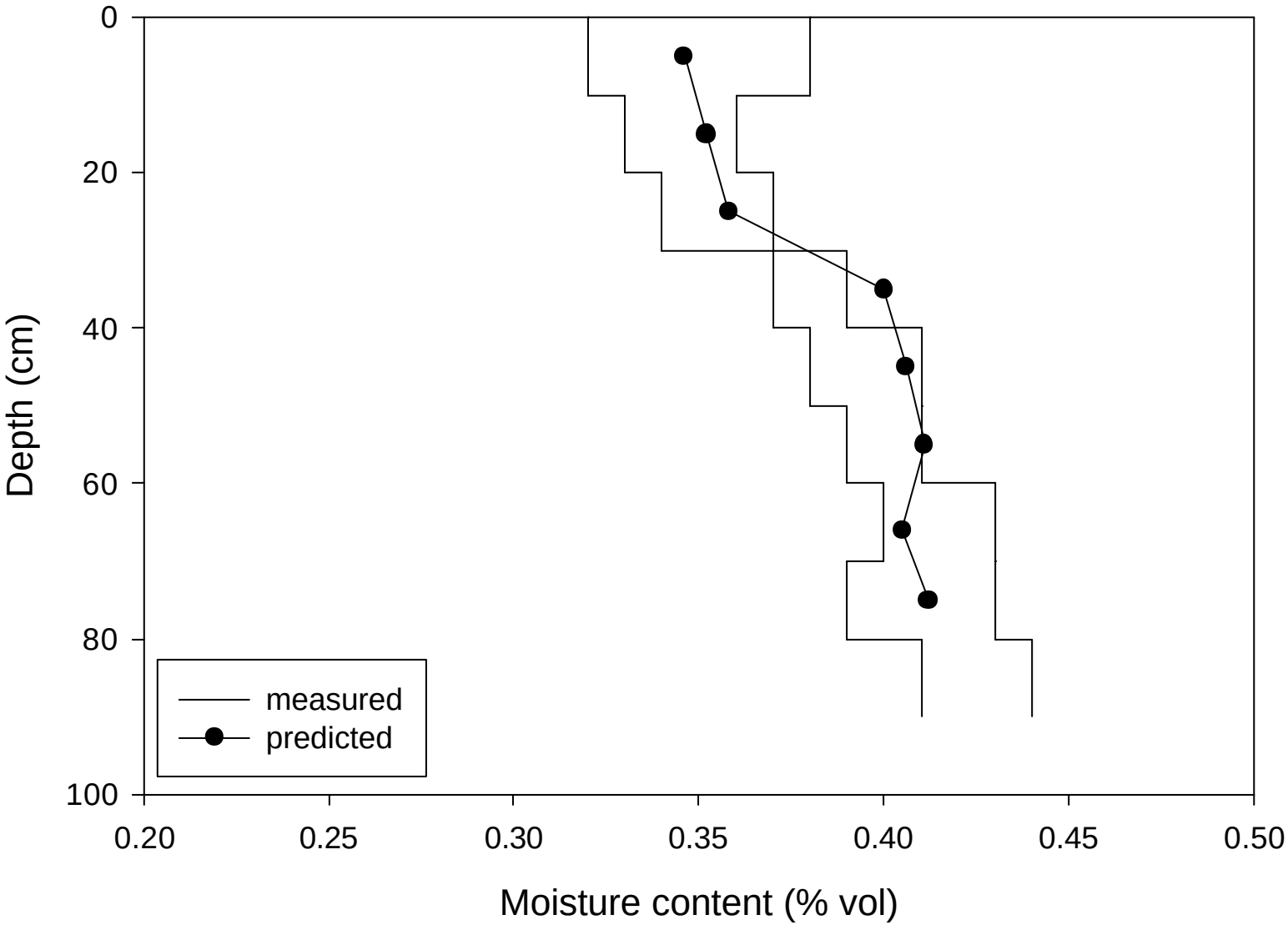
Evaluation protocol for the local scale PEC model

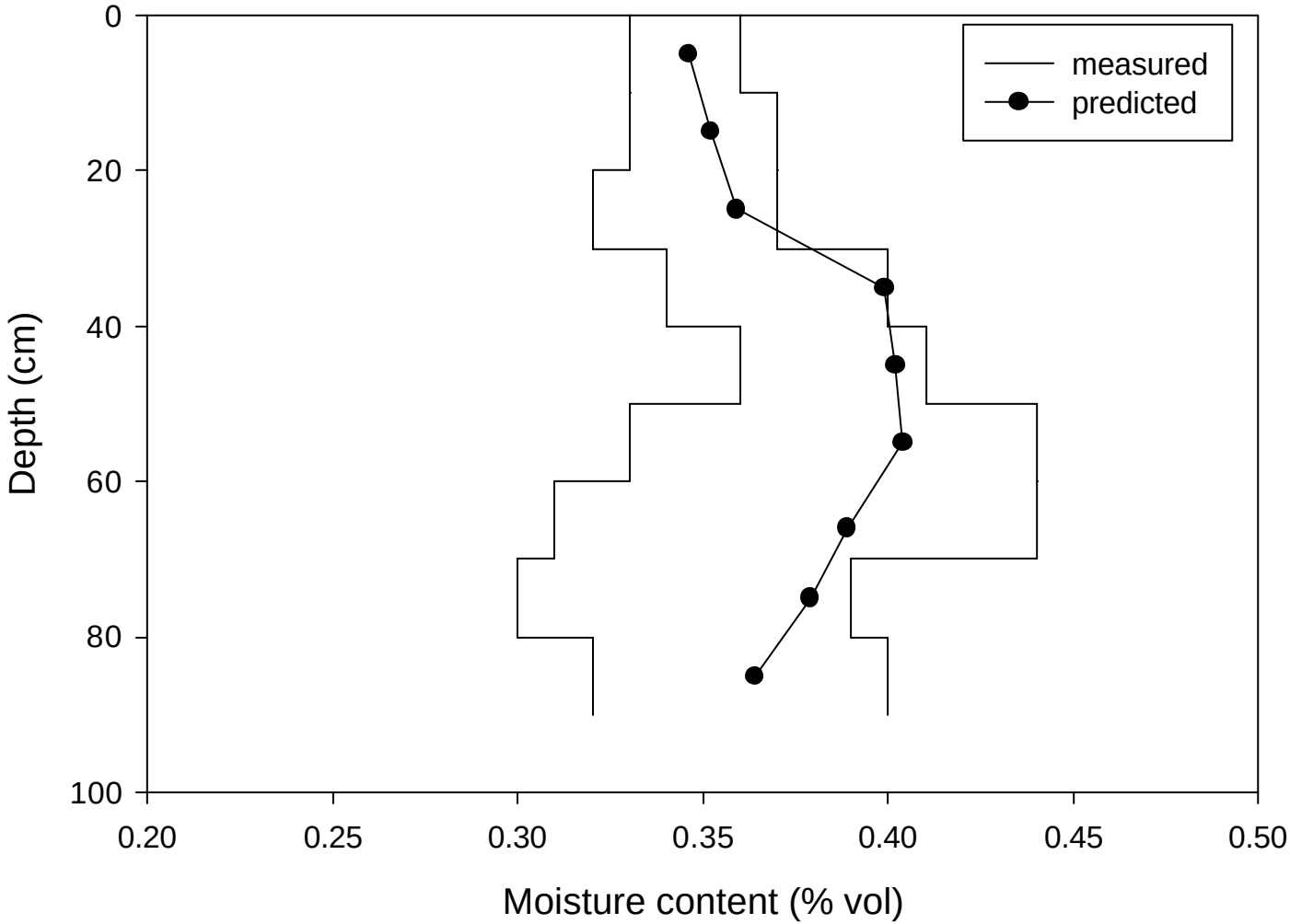
- Phased approach
  - Water, solute, heat and pesticide fate evaluated separately
- Use of standardised evaluation criteria
  - Graphical and numerical criteria

Target objective

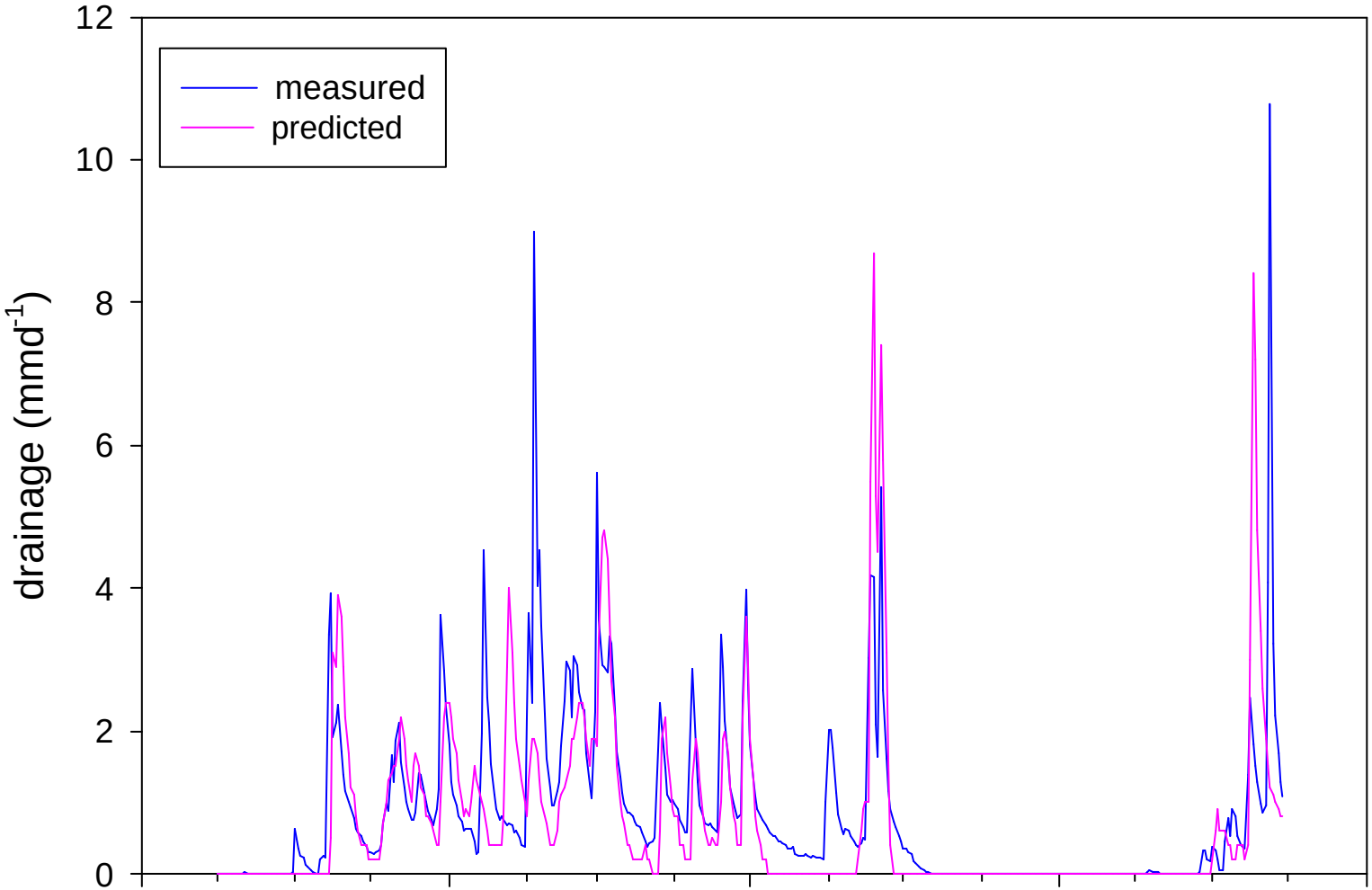
- Soil moisture in the profile
- Soil temperature
- Soil water drainage
- Groundwater position
- Bromide in profile, drainage water and groundwater
- Active substance in profile, drainage water and groundwater
- Products: bentazone, ethoprophos, imidacloprid, aclonifen, isporoturon, chloridazon

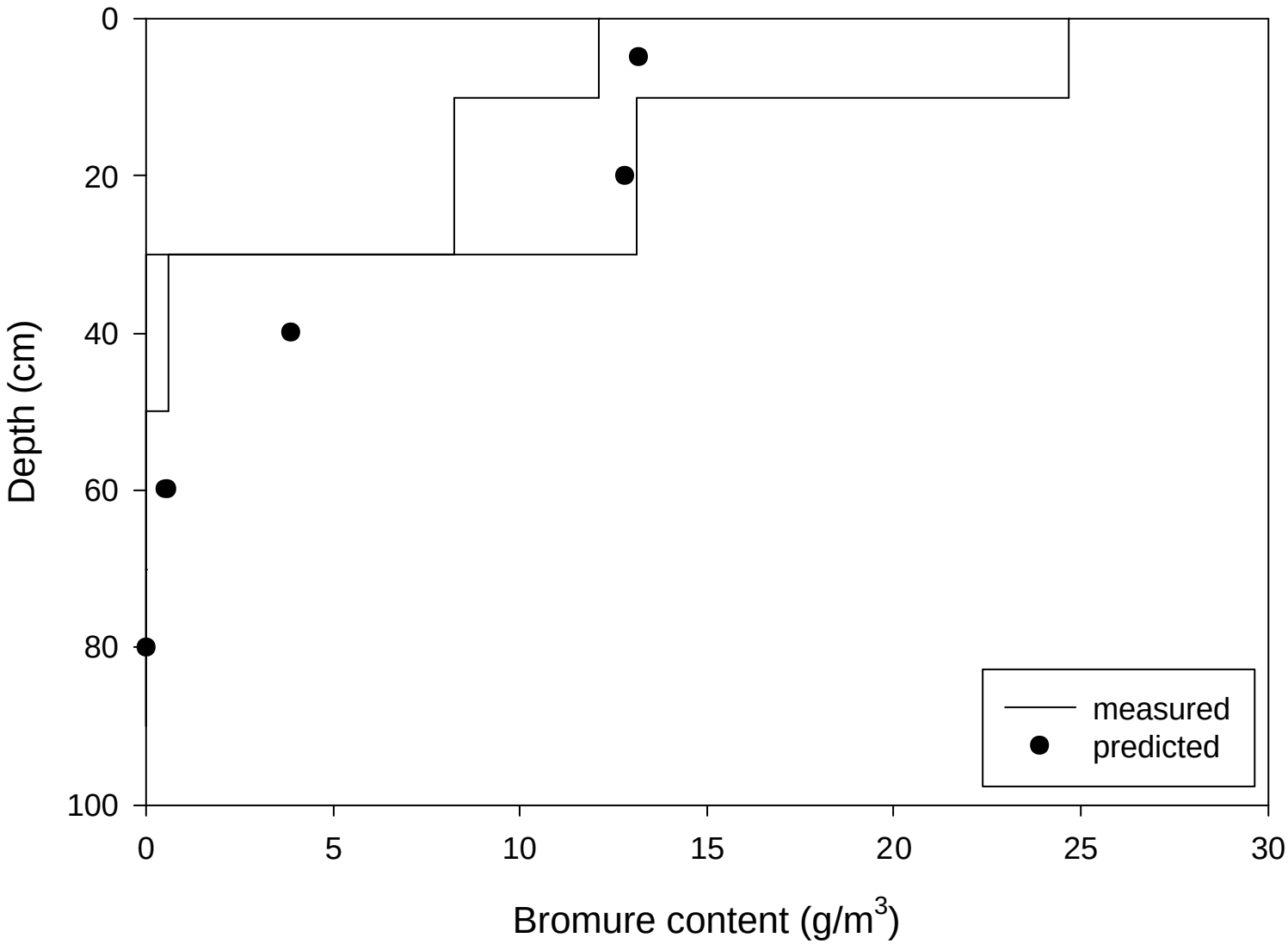
Exemple

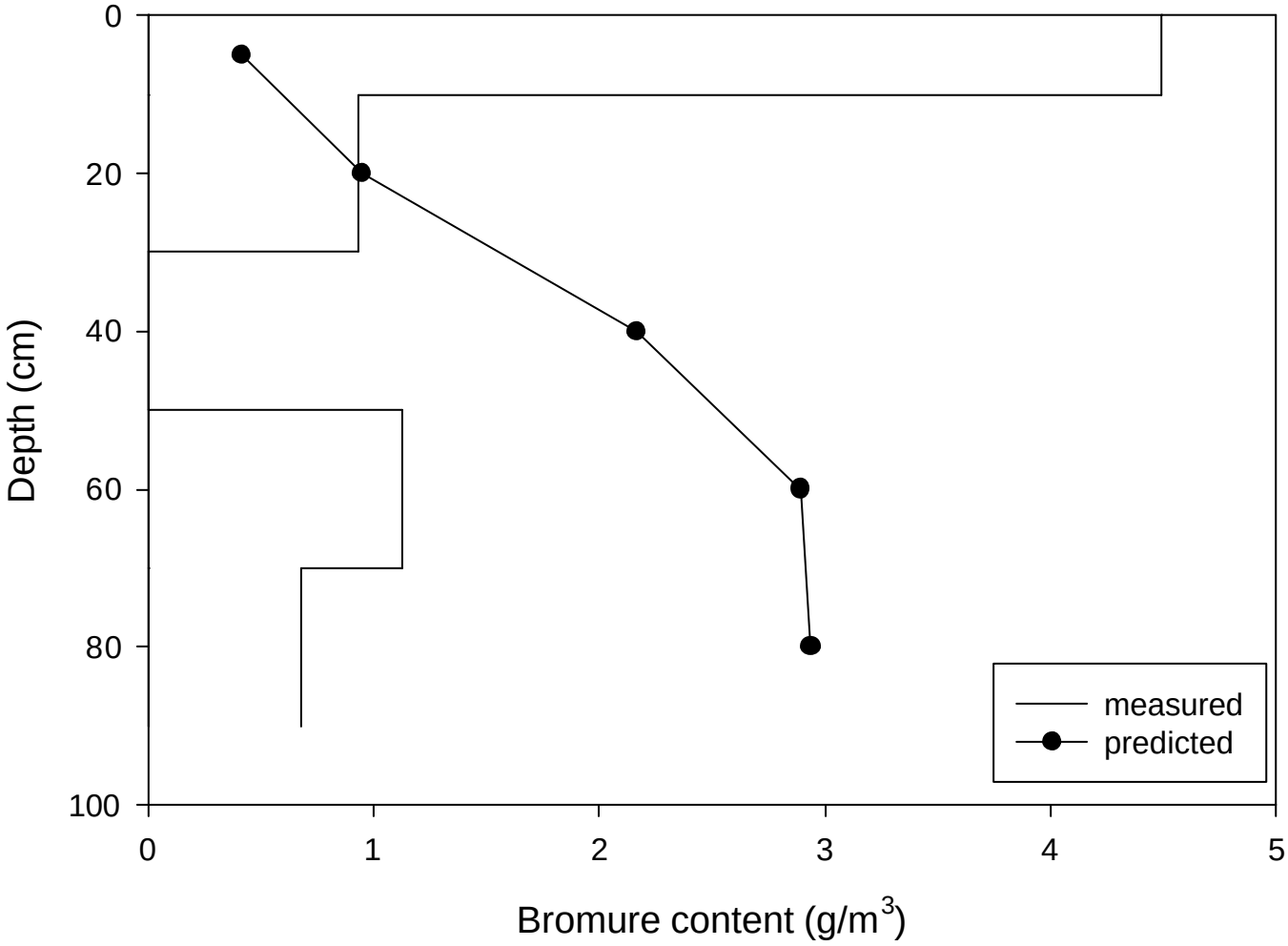

0
20
40
60
80
100
Depth (cm)
0.20
0.25
0.30
0.35
0.40
0.45
0.50
Moisture content (% vol)
measured
predicted


measured
predicted
Depth (cm)
0
20
40
60
80
100
0.20
0.25
0.30
0.35
0.40
0.45
0.50
Moisture content (% vol)

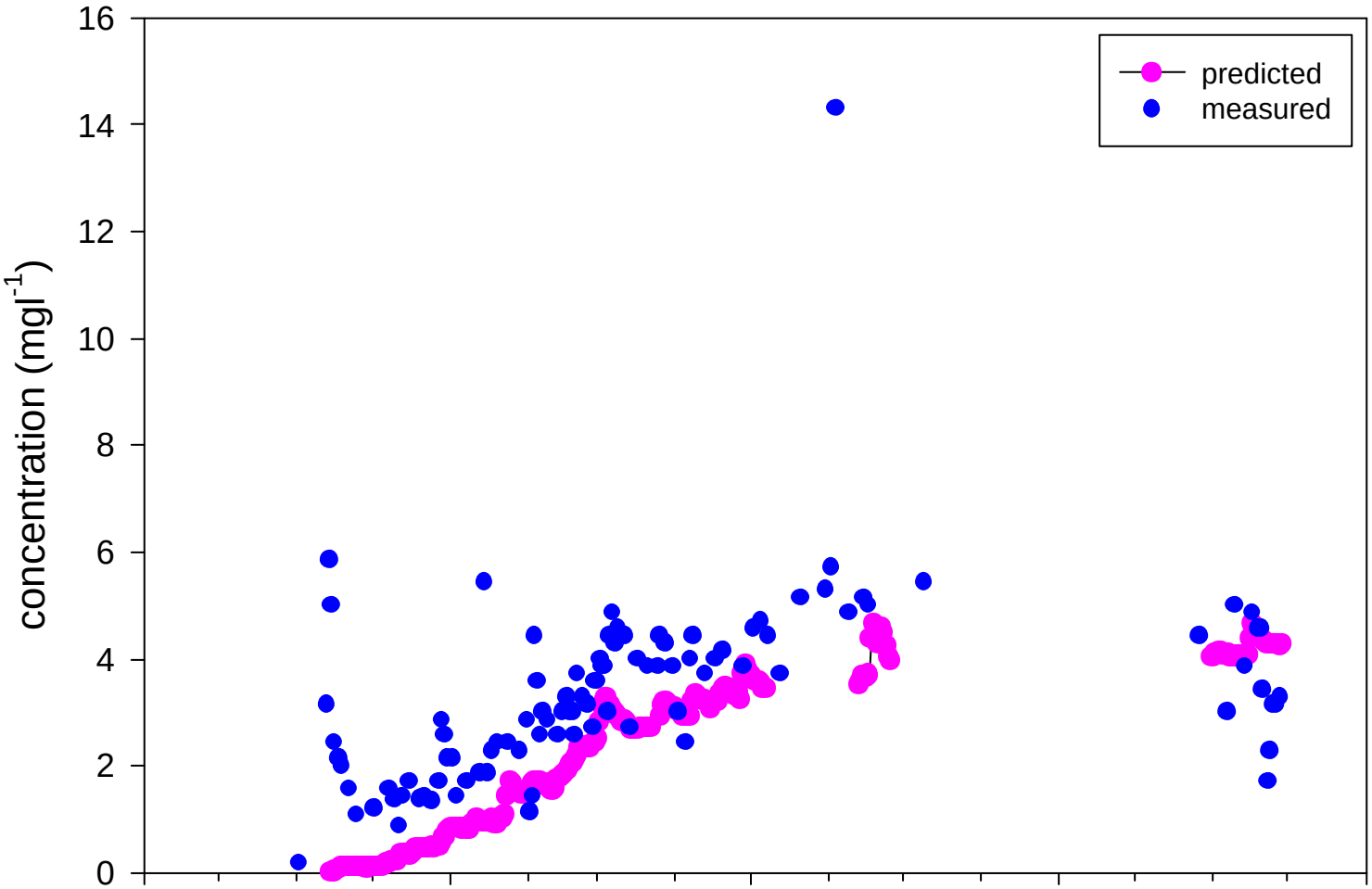
measured and predicted drainage

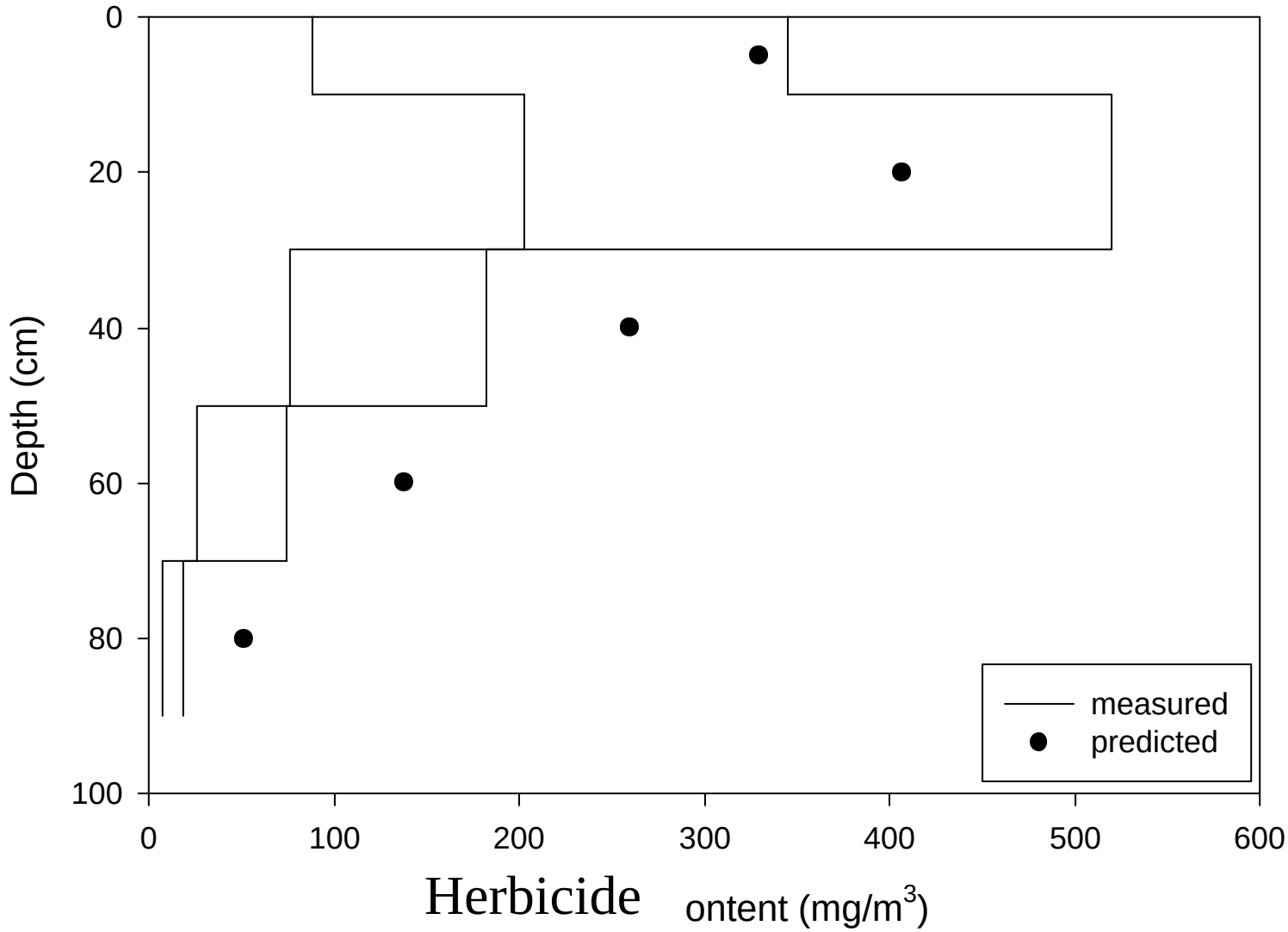


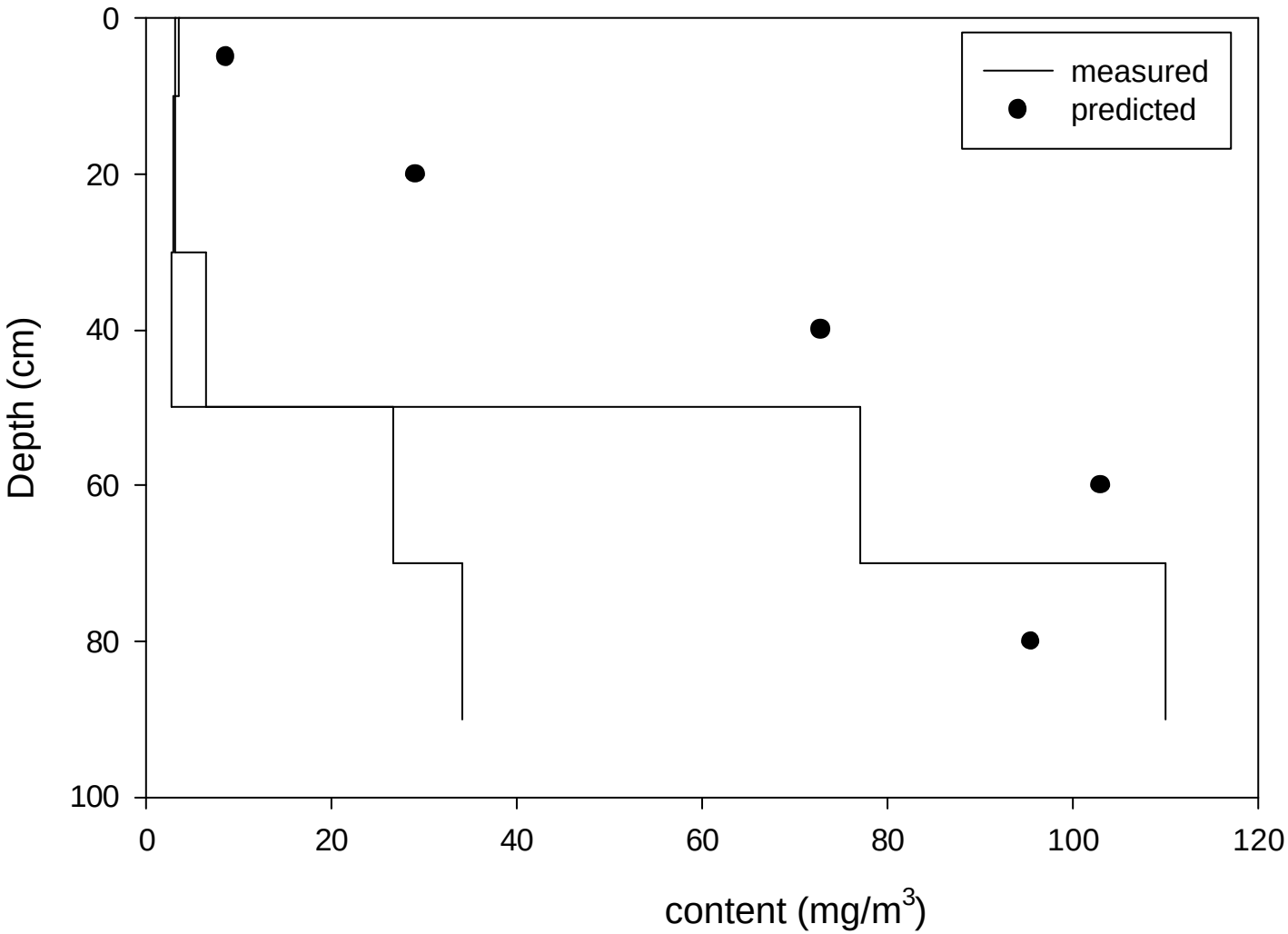

0
20
40
60
80
100
Depth (cm)
0
5
10
15
20
25
30
Bromure content (g/m3)
measured
predicted


0
20
40
60
80
100
Depth (cm)
0
1
2
3
4
5
Bromure content (g/m3)
measured
predicted

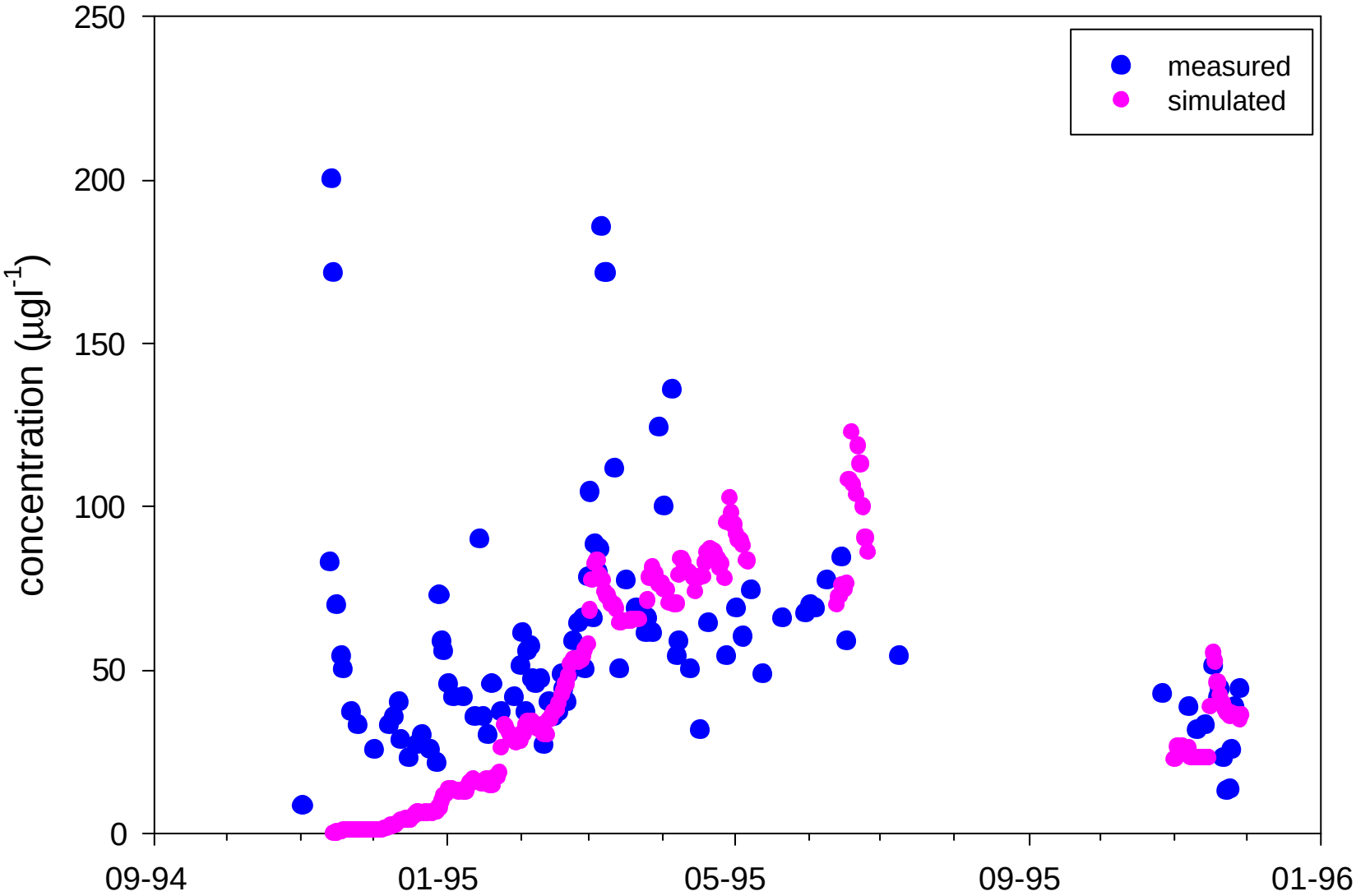
bromide concentration in drainage




0
20
40
60
80
100
Depth (cm)
0
100
200
300
400
500
600
Herbicide ontent (mg/m3)
measured
predicted


measured
predicted
Depth (cm)
content (mg/m3)
0
20
40
60
80
100
0
20
40
60
80
100
120

Herbcide concentration in drainage water



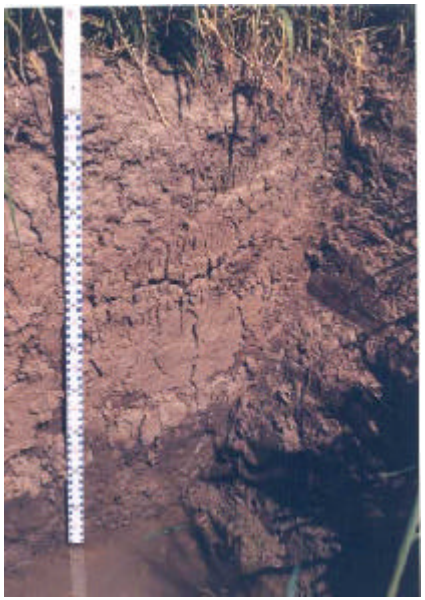
Some remarks: weak points on the procedure

- No benchmarking on analytical solutions
- No stochastic validation approach (No ‘statistical’ validation test is done since uncertainty propagation is not considered explicitly in the validation approach)

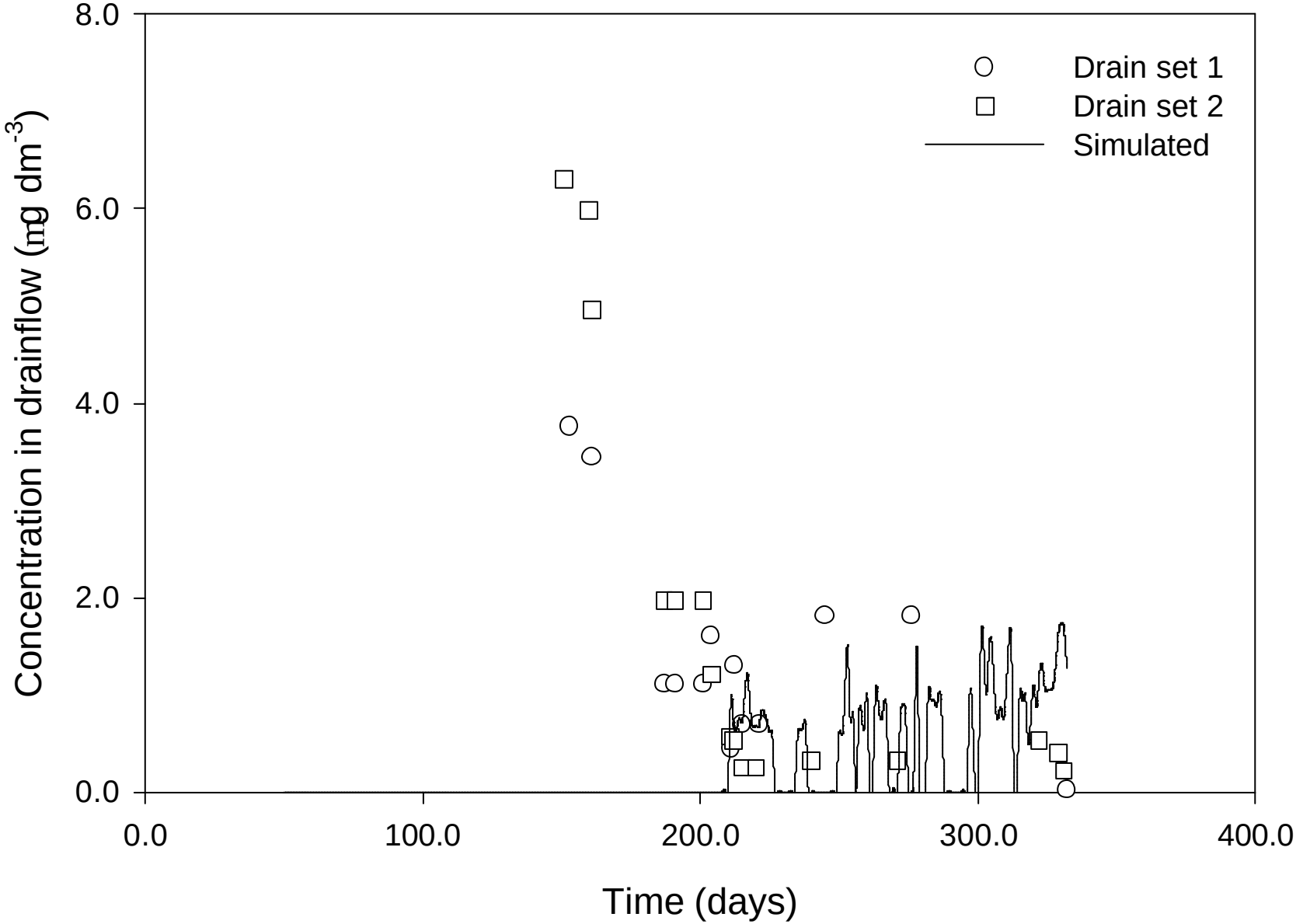
New modelling approaches for preferential flow and volatilization

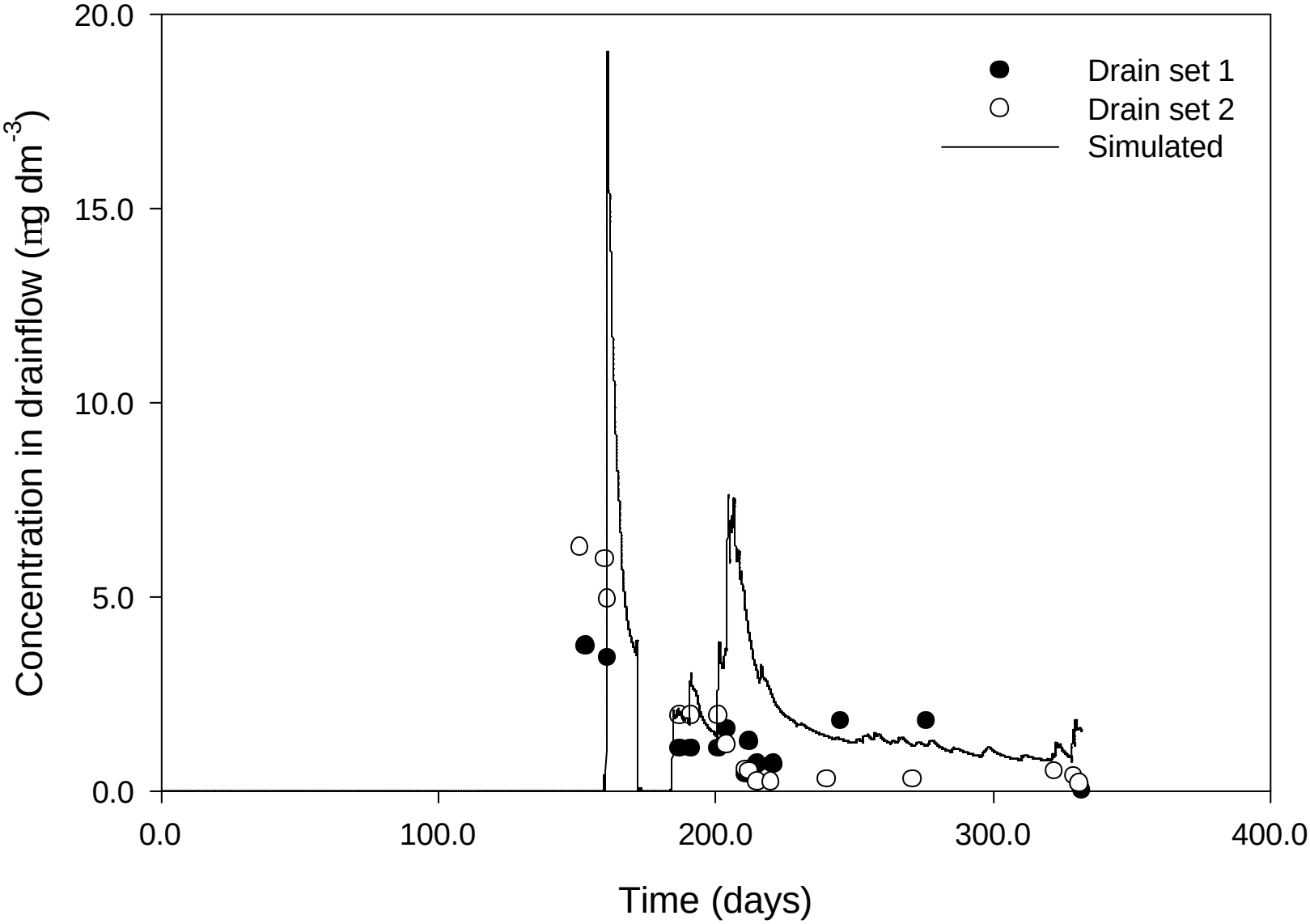
Local scale PEC model improvement

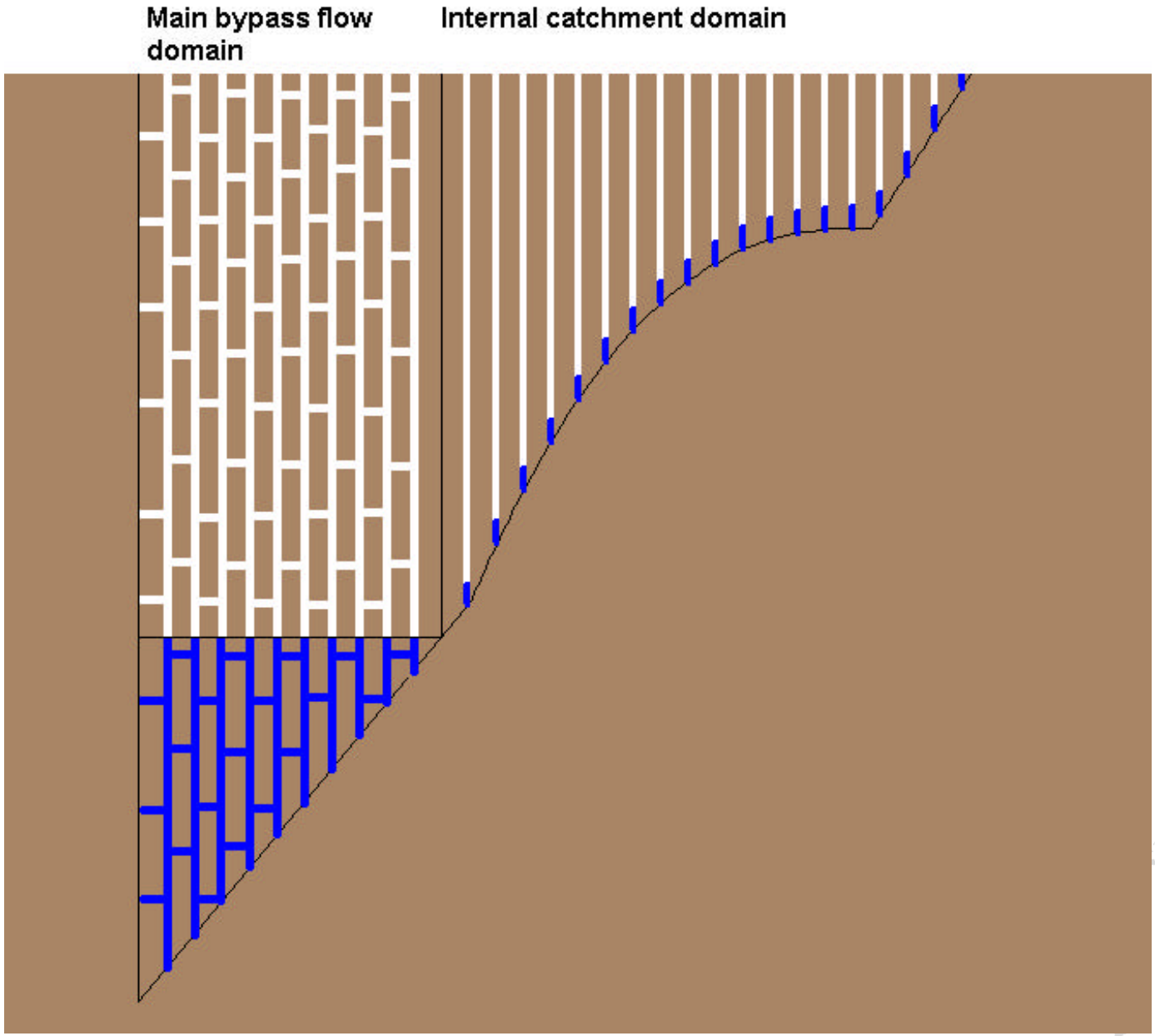
Preferential flow



Exemple


8.0
6.0
4.0
2.0
0.0
Concentration in drainflow (mg dm-3)
0.0
100.0
200.0
300.0
400.0
Time (days)
Drain set 1
Drain set 2
Simulated


Drain set 1
Drain set 2
Simulated
Concentration in drainflow (mg dm-3)
20.0
15.0
10.0
5.0
0.0
0.0
100.0
200.0
300.0
400.0
Time (days)


Main bypass flow domain
Internal catchment domain

Volatilization

Validating groundwater scenarios

Why scenario validation?

- The selection/definition of the “scenario”, which is a data model, is equally important than the selection/definition of the “leaching model”
- Bias in expert judgement cannot be excluded
- Prepare authorization procedures after 2012
- Prepare harmonized European higher tier assessment

Pan-European scale PEC model

Pan-European agri-environmental data

i.e. FOCUS Groundwater Scenario

↓

Fate and transport model for the soil crop continuum

- PEARL
- MACRO
- PELMO

↓

Pan-European PEC

Definition of FOCUS groundwater scenario

"A representative combination of crop, soil, climate and agronomic parameters to be used in modeling; representative means in this context that the selected scenarios should represent physical sites known to exist, i.e. the combination of crop, soil, climate and agronomic conditions should be realistic" (FOCUS, 1995).

A combination of parameter values selected in such a way that the leaching calculated with pesticide leaching models using these parameter values equals the 90th percentile of leaching inside the corresponding FOCUS area.

Evaluation/validation of a groundwater scenario?

Validation level 1 : *Are FOCUS scenarios combinations of parameter values selected in such a way that when used in pesticide PEC modeling the calculated leaching equals the 90th percentile of leaching inside the corresponding FOCUS area, as obtained from measurements?*

Validation level 2 : *Are FOCUS scenarios combinations of parameter values selected in such a way that when used in pesticide PEC modelling the calculated leaching equals the 90th percentile of leaching inside the corresponding FOCUS area, as obtained from detailed and spatially distributed modeling results ?*

Validation level 1

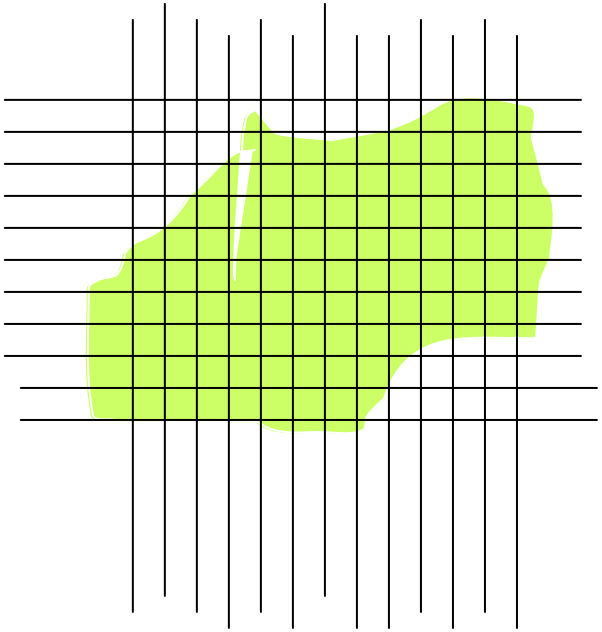
Not possible for the time being since pan European data on pesticide concentration in groundwater are not available.

Validation level 2: Summary of the protocol

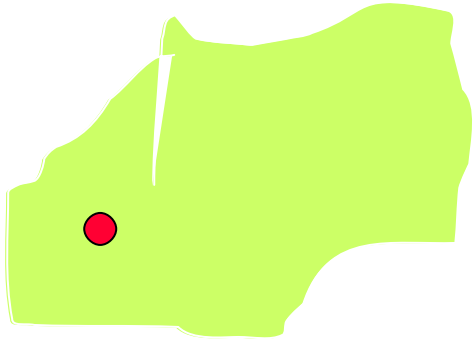
- Step 1: Identify the FOCUS area
- Step 2: Calculate probability of PEC groundwater with FOCUS scenario
  ➔(PEC_FOCUS)
- Step 3: Calculate probability of PEC groundwater with detailed and spatially distributed pan European assessmen model
  ➔(PEC_PE)
- Step 4: Test: 90^{-th} perc. (PEC_PE) <> 90^{-th} perc. (PEC_FOCUS)

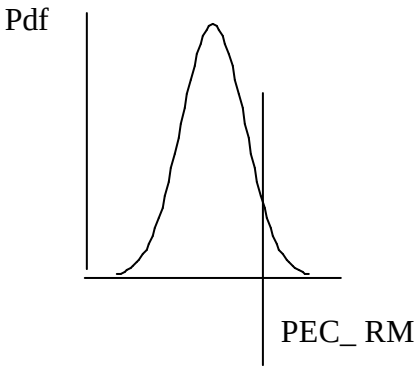
➔ Reject/accept

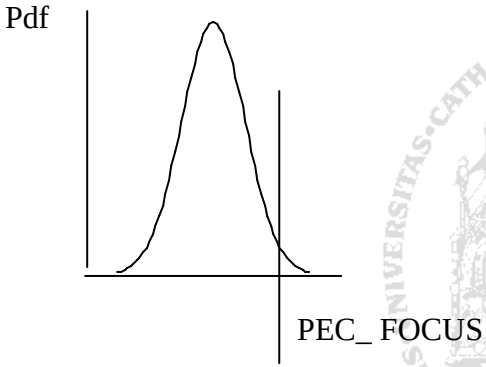
Spatially distributed approach



Actual FOCUS approach







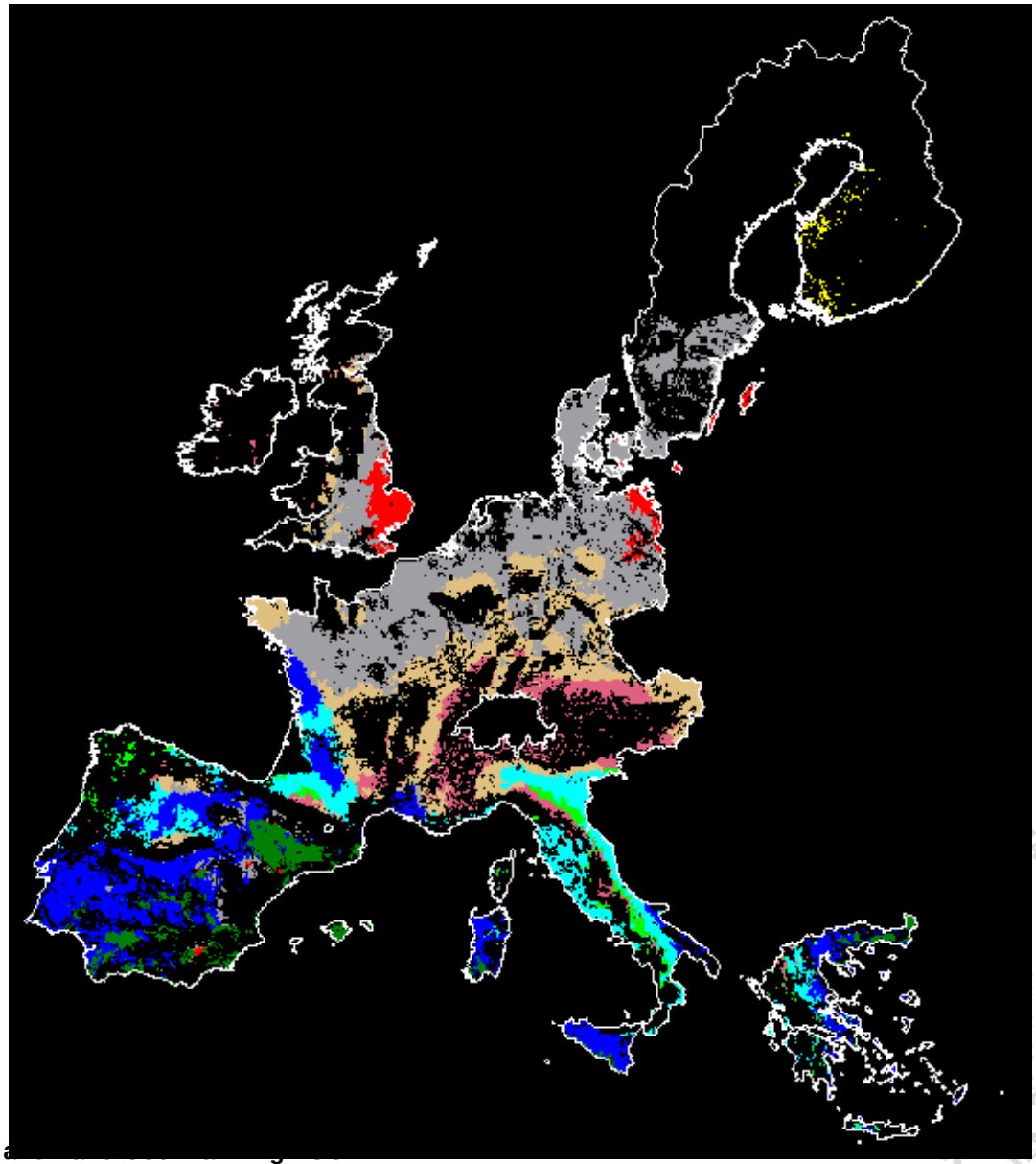
Step 1: Definition of the FOCUS area’s

Definition of the FOCUS groundwater areas

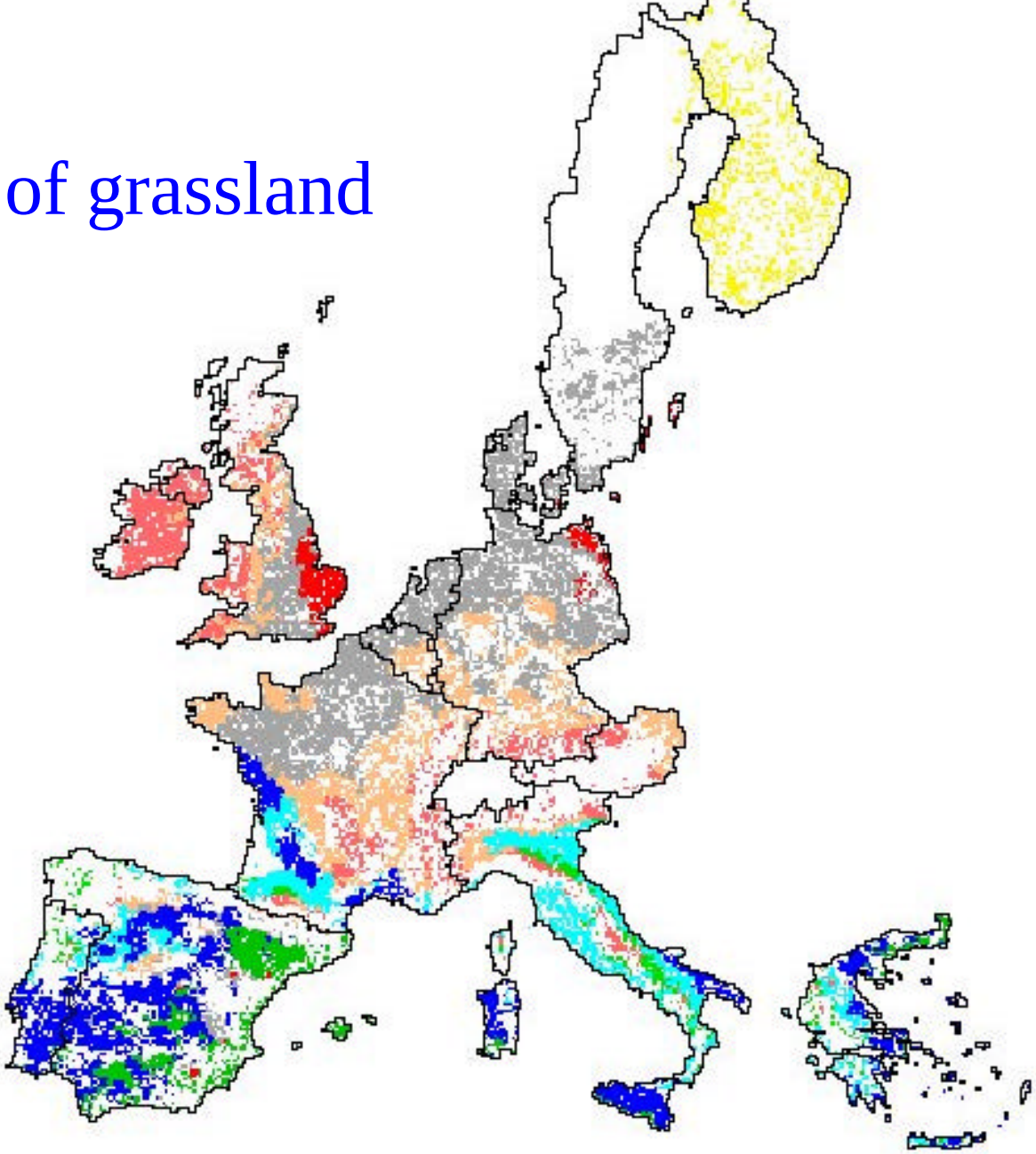
FOCUS AREA	mean annual rainfall	mean annual temperature	Corresponding scenario
1	<600	<5	Jokionen
2	<600	[5-12.5]	Chateaudun
3	[600-800]	[5-12.5]	Hamburg/Chateaudun(Irr)
4	]800-1000]	[5-12.5]	Kremsmunster
5	]1000-1400]	[5-12.5]	Okehampton
6	<600	>12.5	Thiva/Sevilla
7	[600-800]	>12.5	Thiva (Irr) /Sevilla (Irr)
8	]800-1000]	>12.5	Piacenza
9	]1000-1400]	>12.5	Porto

➔Define spatially

FOCUS area with arable land mask



The issue of grassland



Step 2: Definition of PEC_FOCUS: Trivial

Step 3: Definition of PEC_PE: Europearl

Approach in APECOP:

- **Step 1 (RIVM contribution: Tiktak and Denie):**
  Perform simulation with PEARL, using Pan European databases
  - PEARL is one of the FOCUS groundwater models;
  - Conceptual differences between FOCUS approach and regional scale model minimised;

- **Step 2 (UCL contribution: Pineros-Garcet and Vanclooster):**
  Substitute the rest of the data with a statistical (meta)model approach:
  - Gives 100% coverage
  - We use an interpolation method, to make sure that the original data points are retained.

Parameterisation of EuroPEARL

- **Step 1:** Derivation of the unique combinations, based on climate and soil mapping units;

- **Step 2a:** Parameterisation of the soil profiles (linkage between soil map and Soil Profile Analytical Database of Europe, SPADE);

- **Step 2b:** Parameterisation of weather conditions for each individual plot;

- **Step 3:** Translation into model parameters, using pedotransfer functions etc.

Step 1: Derivation of Unique Combinations (UC)

+

+

Country

- Based on the SMU soil map

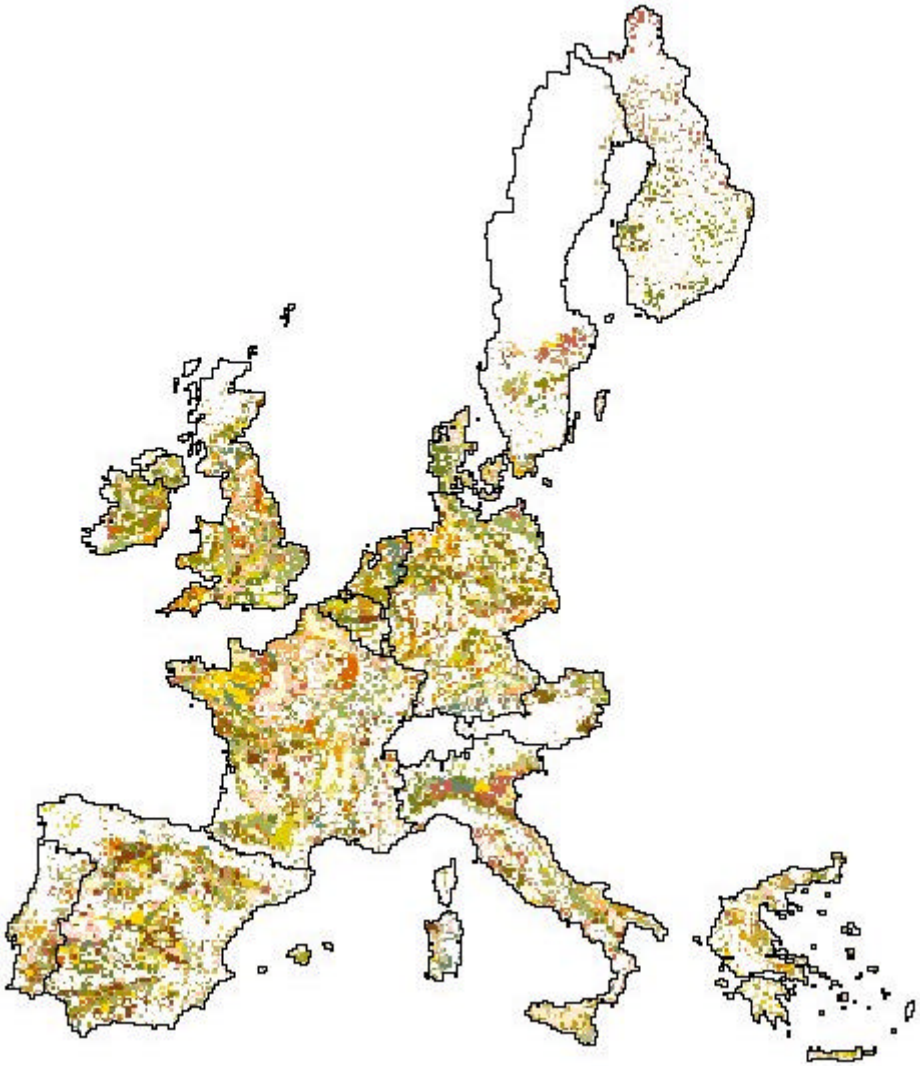
Soil Map (FAO)

- Created by JRC
- 1:1.000.000
- 'STU' info

FOCUS areas

- LU mask
- Precipitation and temperature maps

Step 1: Derivation of Unique Combinations (UC)

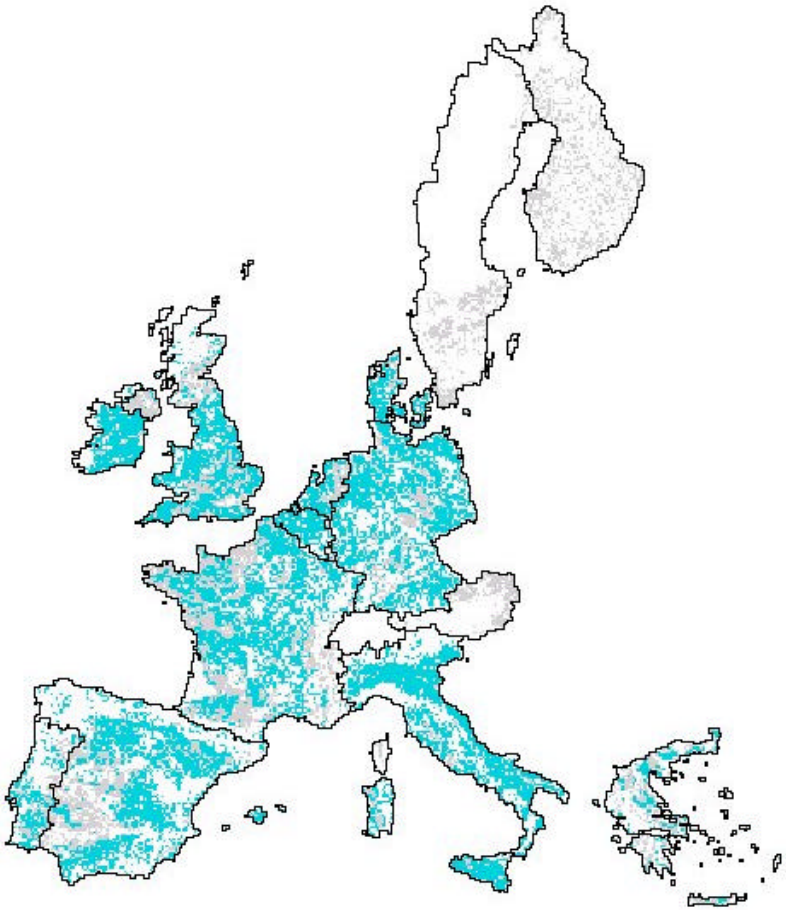


Unique combinations =>

- 1410 'calculation' plots
- each UC contains:

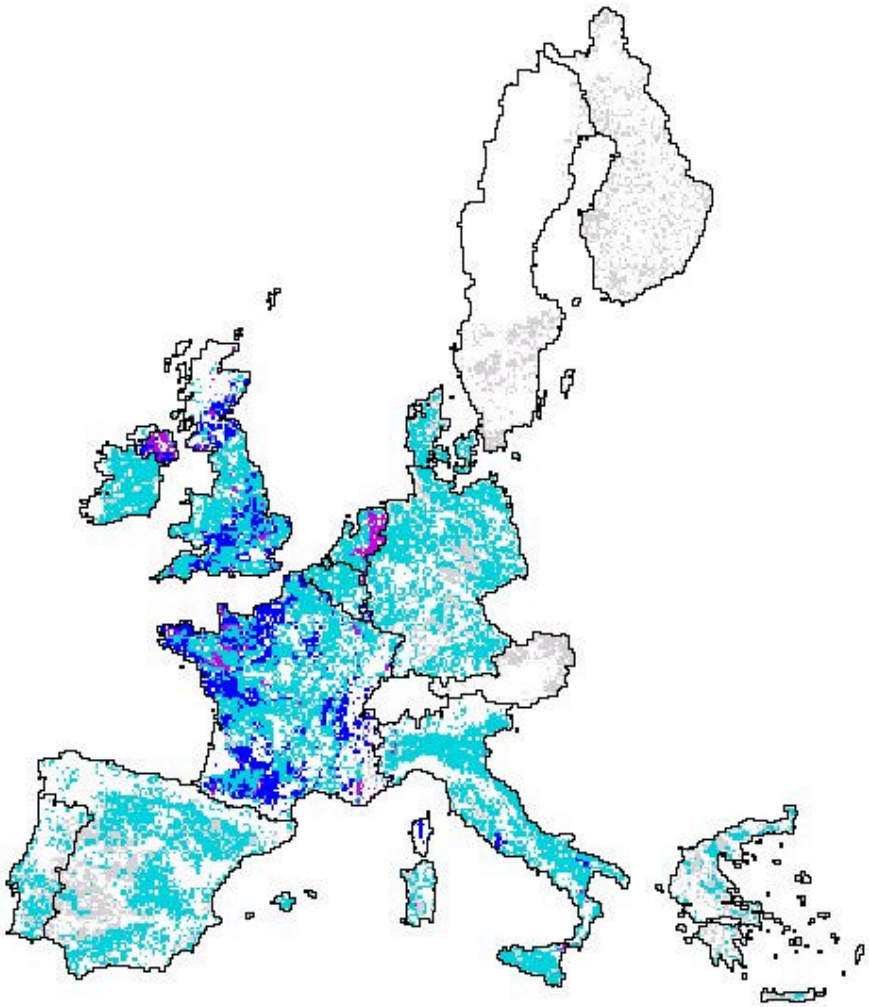
  - SMU
  - Country
  - FA

Step 2a: Combine SPADE & SMU's to PEARL profiles



Current status:

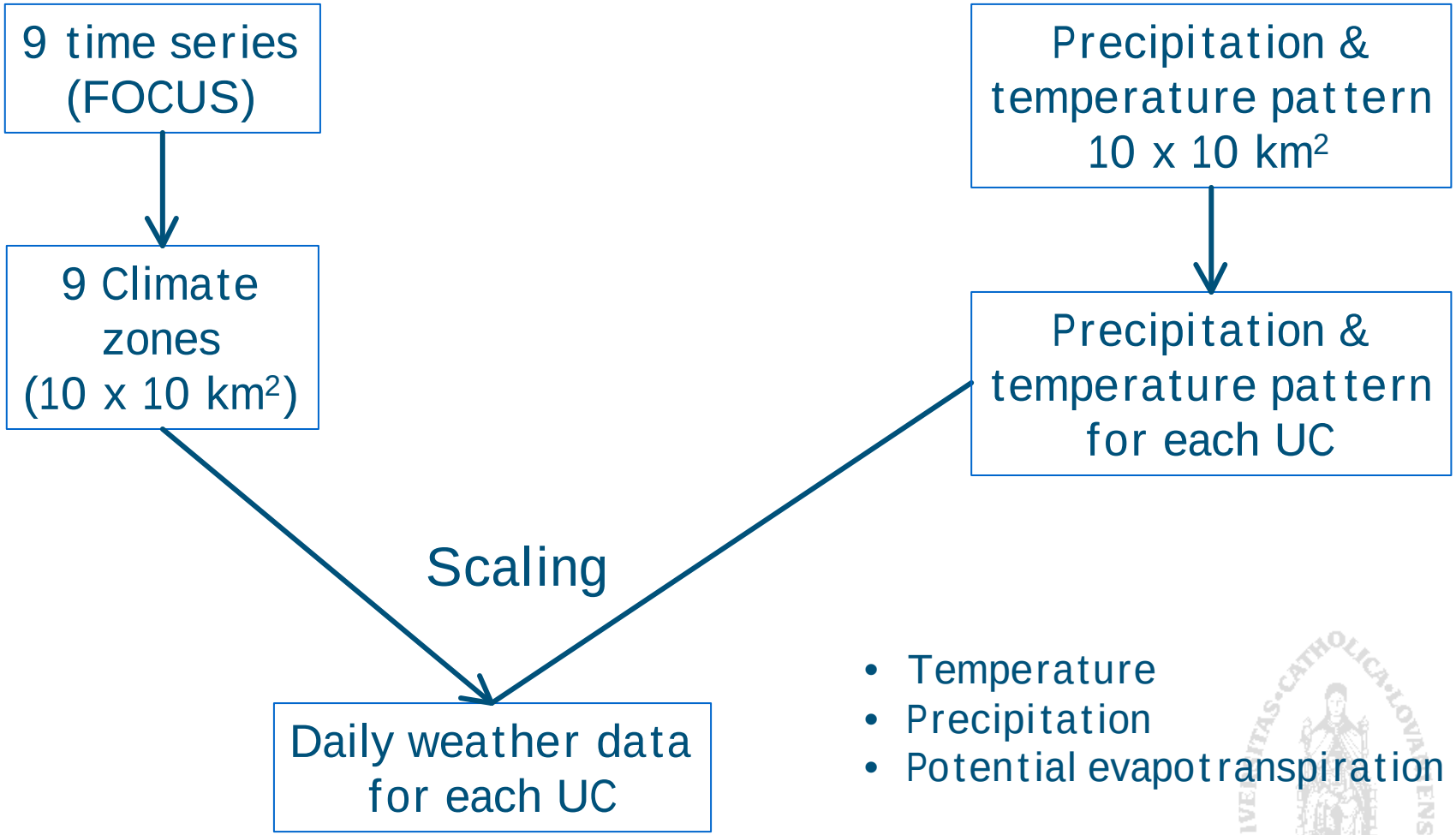
- SW and AUT not reperesented in SPADE
- 65 % of the UC area parameterised



Future possibilities:

- Expansion to 75% possible
- Linking 2nd dominant STU to UC ?
- Include more climatic parameters in construction UC's
- More detailed irrigation data

Step 2b: Combine daily weather & climate maps



- Temperature
- Precipitation
- Potential evapotranspiration

Step 3: specific model parameters

Substance
Substance properties, such as the half-live and the partitioning coefficient

Management
Application date
Application type
Application dosage

Run
Substance ID
Plot ID
Management ID
Start date
End date

Plot ID
Rainfall
Temperature
ETref
Irrigation switch

Plot
Plot ID
FOCUS Area ID
Land-use type ID
Soil profile ID
Groundwater depth group ID
Seepage flux and amplitude
Drainage characteristics

Soil profile
Soil layer ID

Soil layer
Soil physical unit ID
Layer thickness
Texture
Organic matter
pH

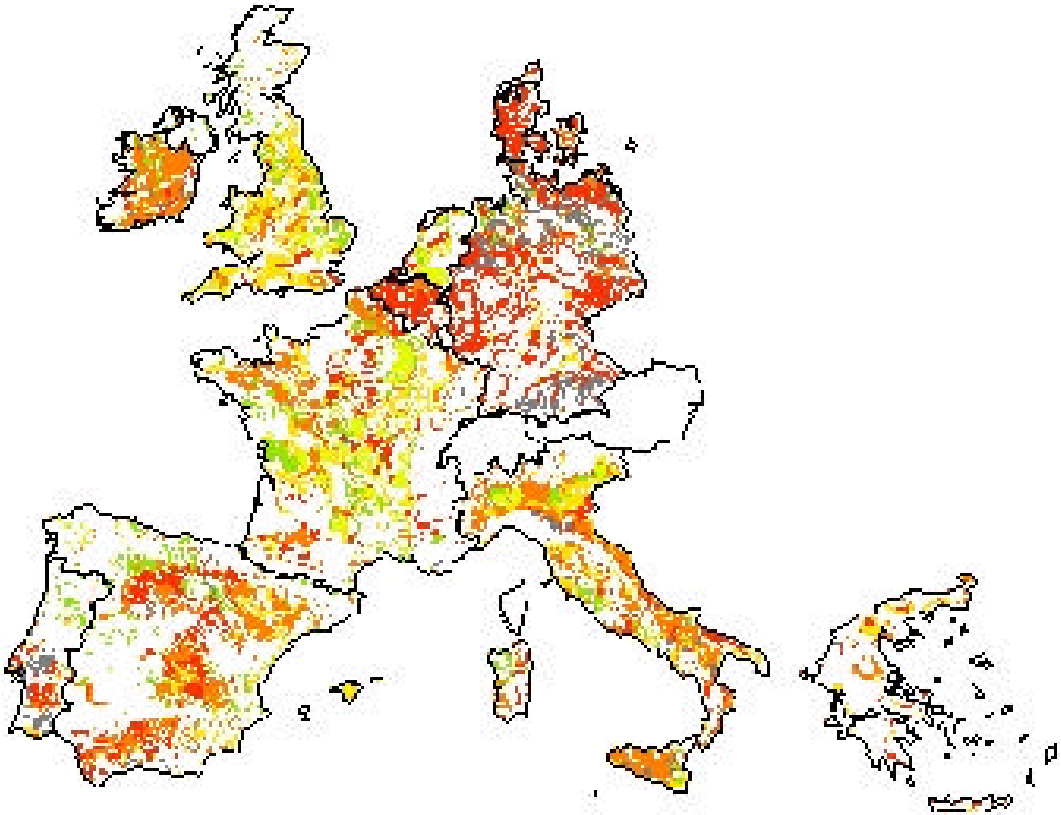
Soil physics
Parameters of the Mualem-van Genuchten functions
Dispersion length

FOCUS Area
Emergence date
Harvest date
Development stage ID
Critical pressure heads for drought stress and irrigation

Development stage
LAI
Crop factor
Rooting depth

Spatially distributed variables

Some preliminary results of EURO-PEARL

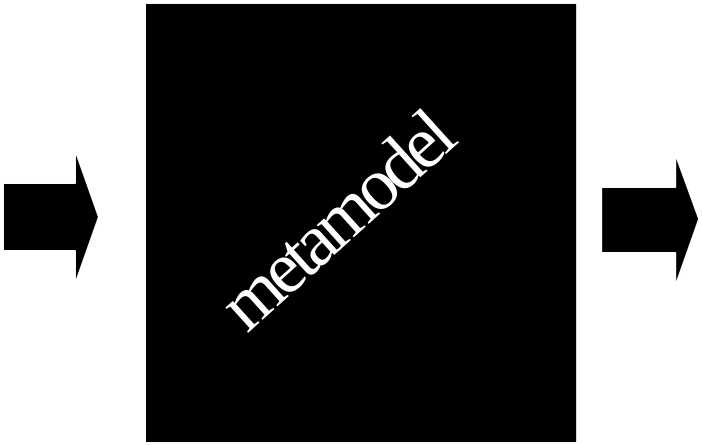


Fill out missing gaps: the EURO-PEARL meta-model ?

- statistical model
- similar to kriging,
- useful and efficient in multidimensional parameter spaces.

What are the inputs and outputs of the metamodel?

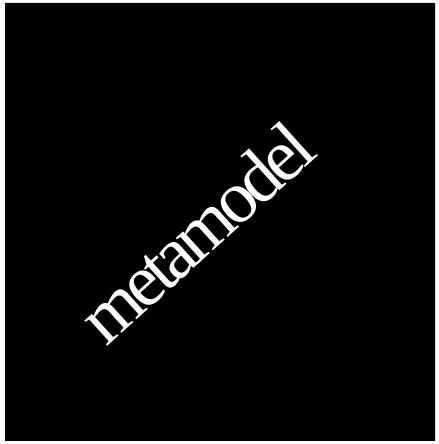
Sand
Silt
Clay
OM
pH
AveWat
Bulk density
Temp_yr
Prec_yr
Eva_yr
Temp_spring
Prec_spring
Eva_spring
Temp_spring
Prec_spring
Eva_spring
GWLevel



mean year
leaching concentration
(atrazine)

What do we use for calibration?

- 656 combinations of the input parameters



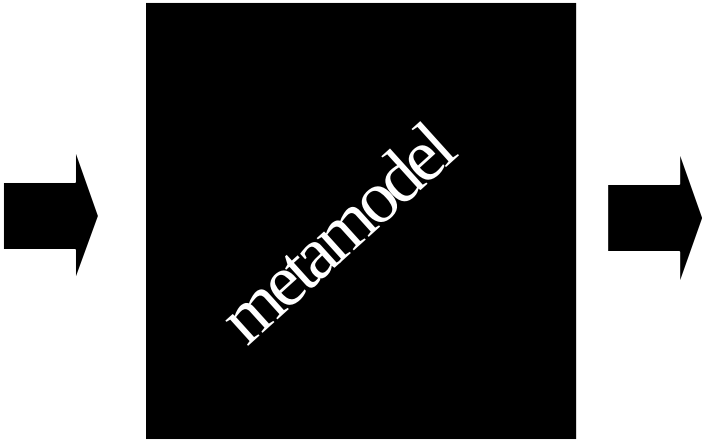
- 656 Pearl outputs

$$\mathbf{x_c} = \begin{array}{c} \begin{array}{ccc} P1 & P2 & P3 \end{array} \\ \begin{pmatrix} xc_{1,1} & xc_{1,2} & xc_{1,3} \\ xc_{2,1} & xc_{2,2} & xc_{2,3} \\ \dots & & \\ xc_{116,1} & xc_{116,2} & xc_{116,3} \end{pmatrix} \end{array}$$

$$\mathbf{y_c} = \begin{pmatrix} yc_1 \\ yc_2 \\ \dots \\ yc_{116} \end{pmatrix}$$

What do we use for validation?

- 72 combinations of the input parameters



- 72 Pearl outputs

How the calibration data where obtained ?

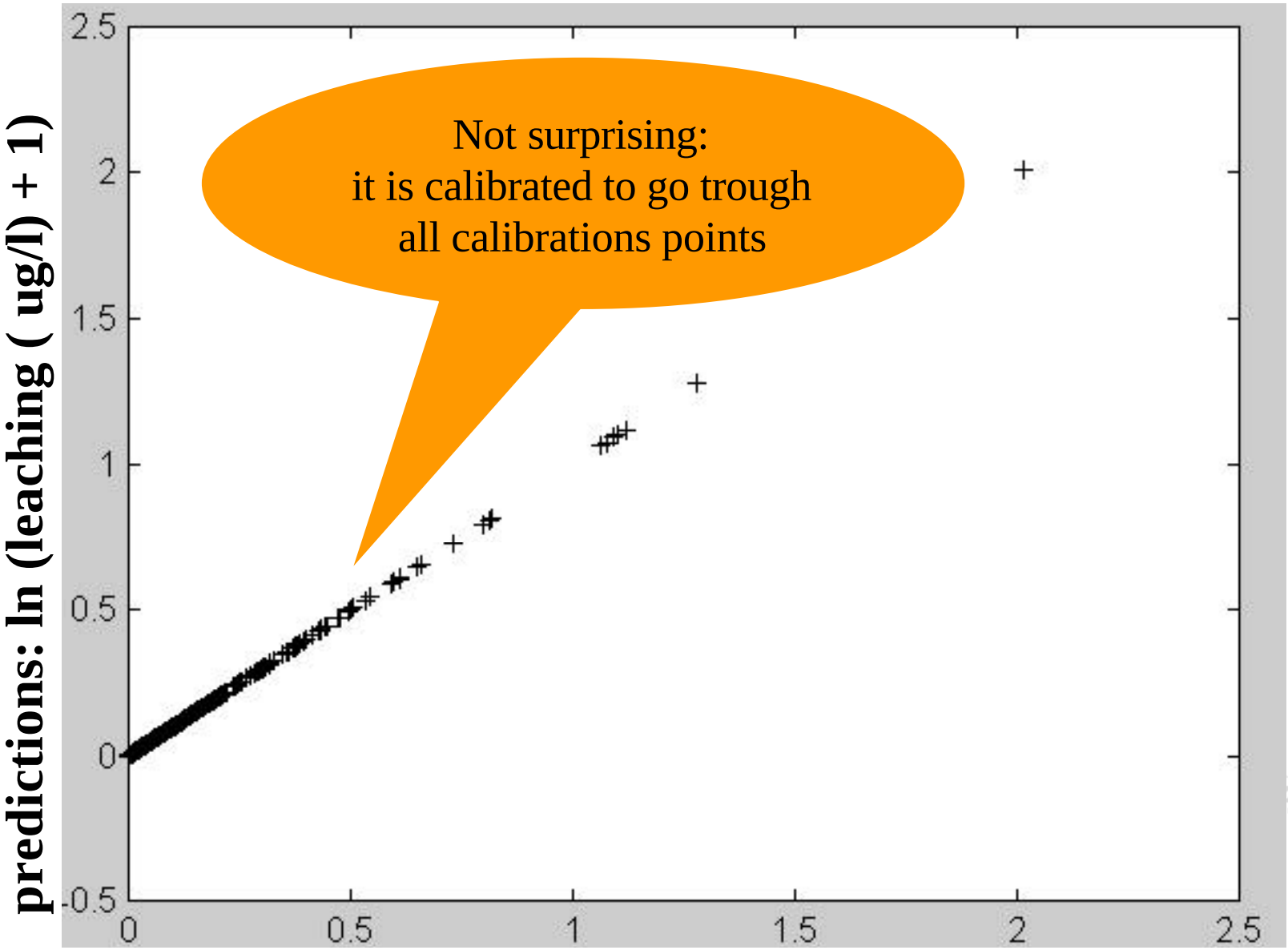
- **From +-5400 unique combinations** of soil and climate in the Netherlands, RIVM did Pearl simulations.

- From those simulations, **728 unique combinations where selected**, having the following characteristics:

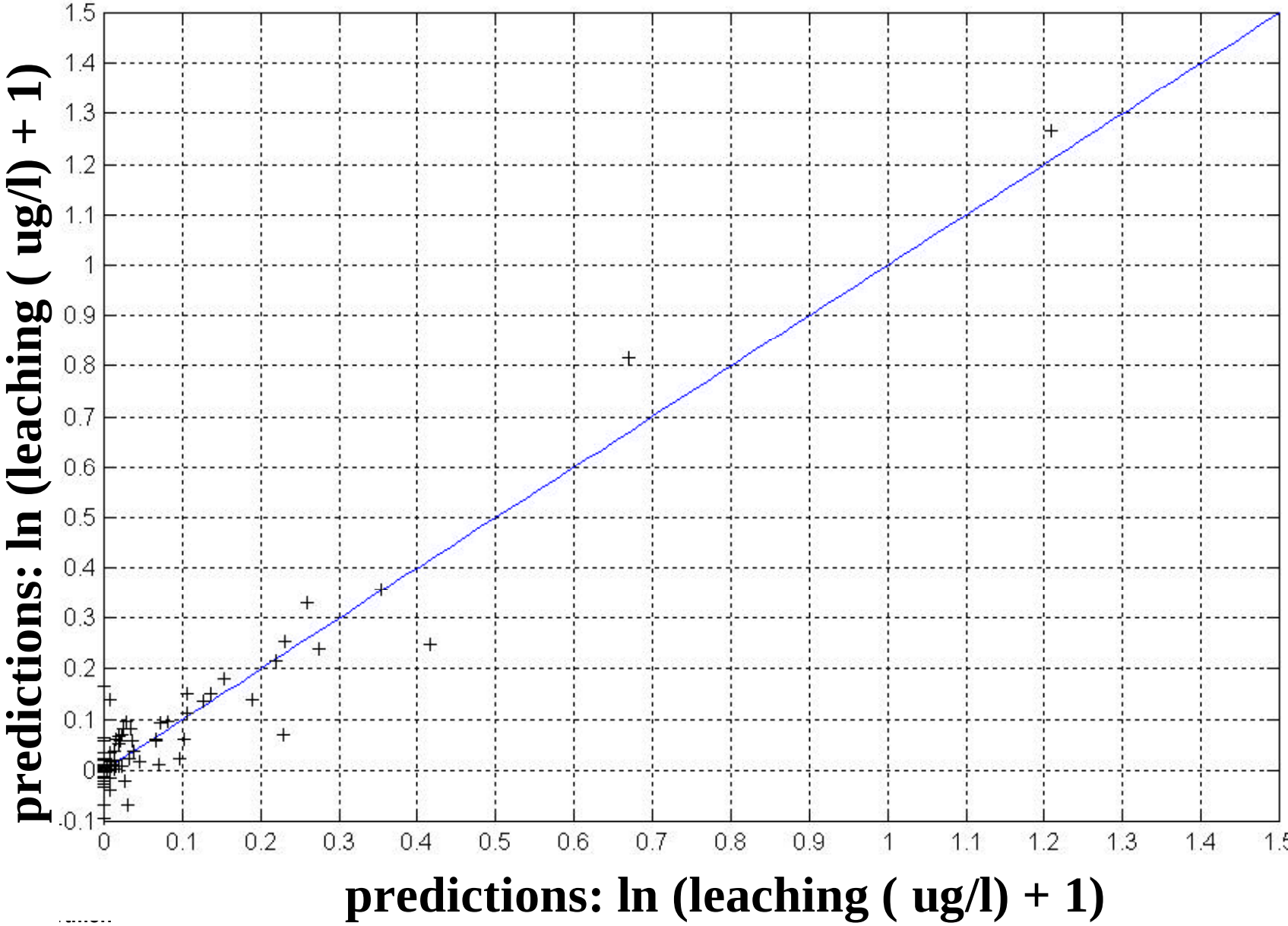
  - not irrigated
  - atrazine
  - non drained
  - maize

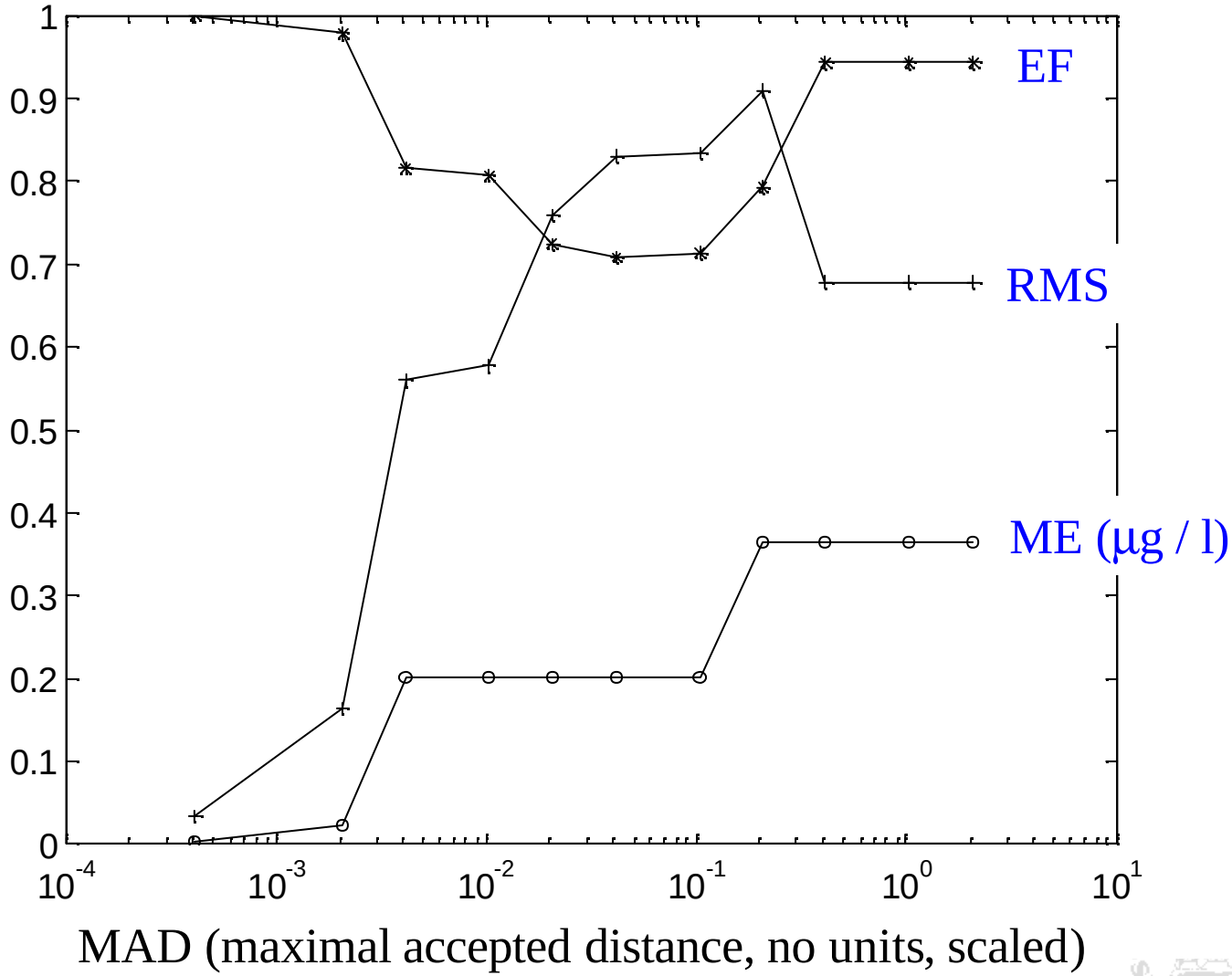
→ 72 pts (10%, random) for validation | 656 : calibration

Calibration results



Validation scatterplot




1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
EF
RMS
ME (µg / l)
MAD (maximal accepted distance, no units, scaled)

When and where will results be available

- Project deliverables available by march 2003
- Project results will be presented at the XII Pesticide chemistry symposium, Piacenza, Italy, May 2003
- Information

www.agro.ucl.ac.be/geru/recherche/projets/apecop-pub