Bernhard Gottesbüren (BASF)

Estimation of the key e-fate parameters of pesticides from field and lysimeter trials by inverse modelling

Principles of Inverse Modleling
Calibration
- lysimeter trials
- field trials
Validation
Extrapolation

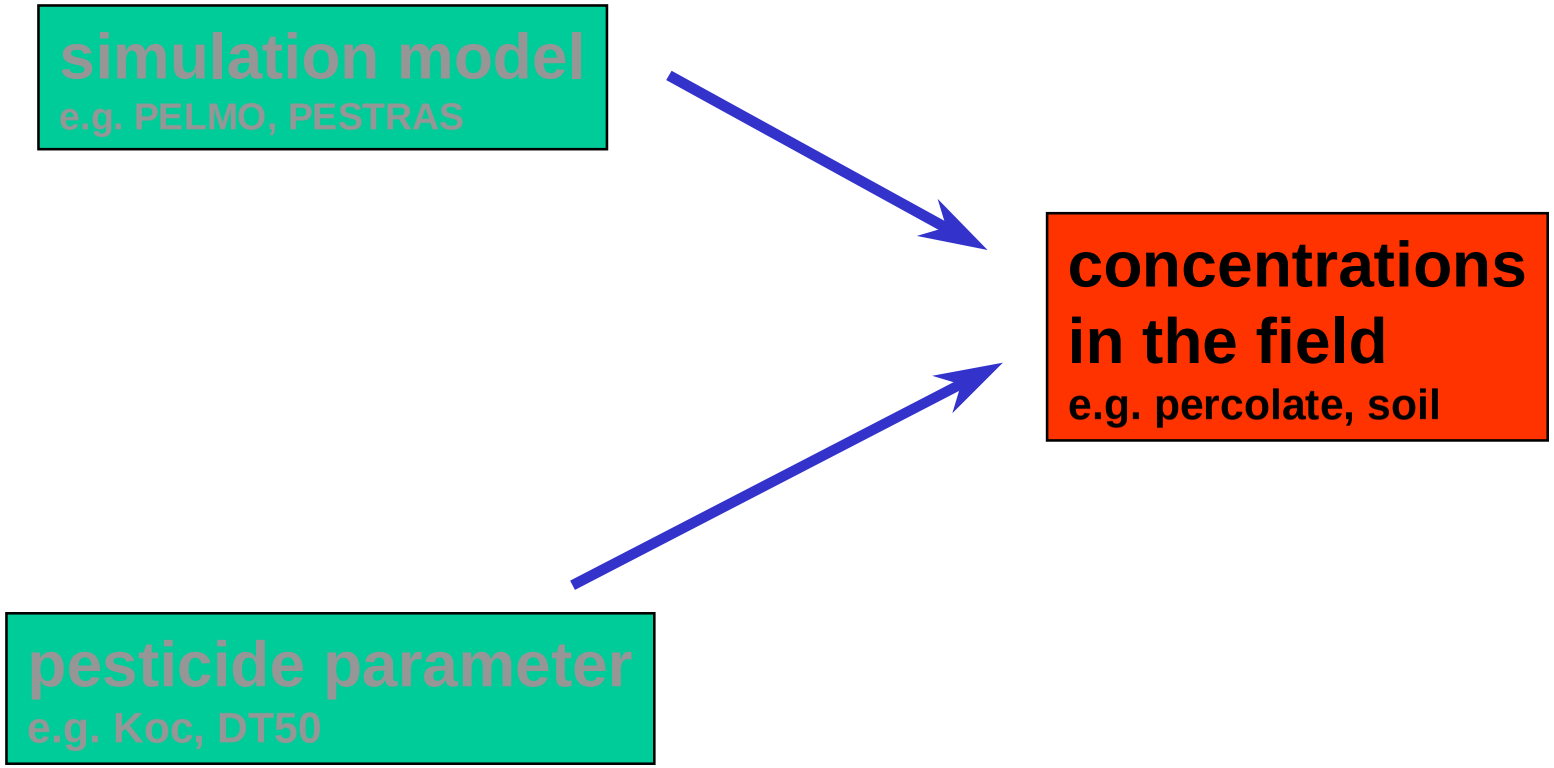
What is 'Inverse Modelling' ?

Inverse Modelling is a parameter estimation technique.

A simulation model is used to account for variable environmental conditions
and a special programme (shell) is implemented that compares simulated and measured values.

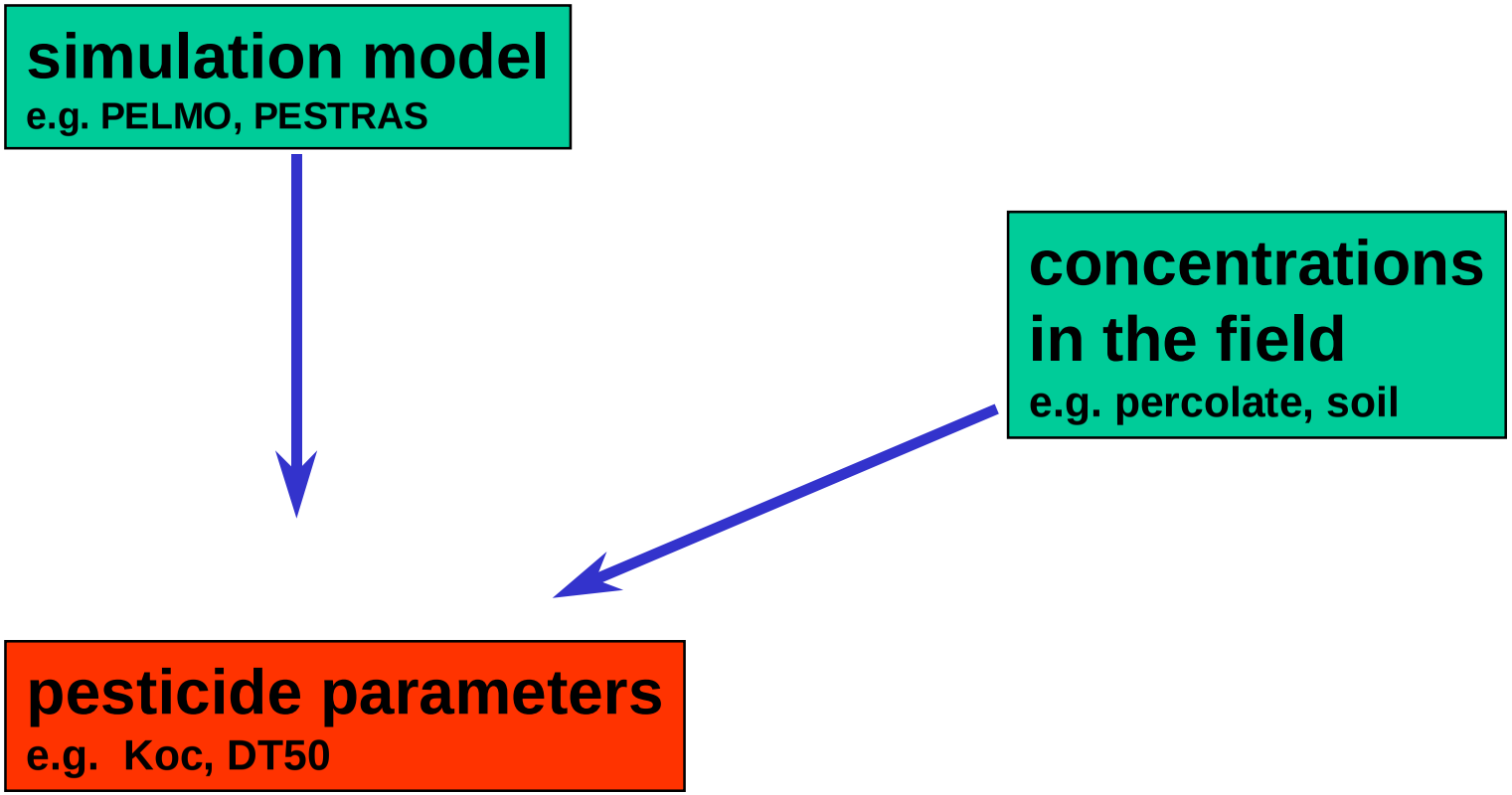
What is the difference between 'inverse' and 'usual' modelling?

1. 'Usual' Modelling:

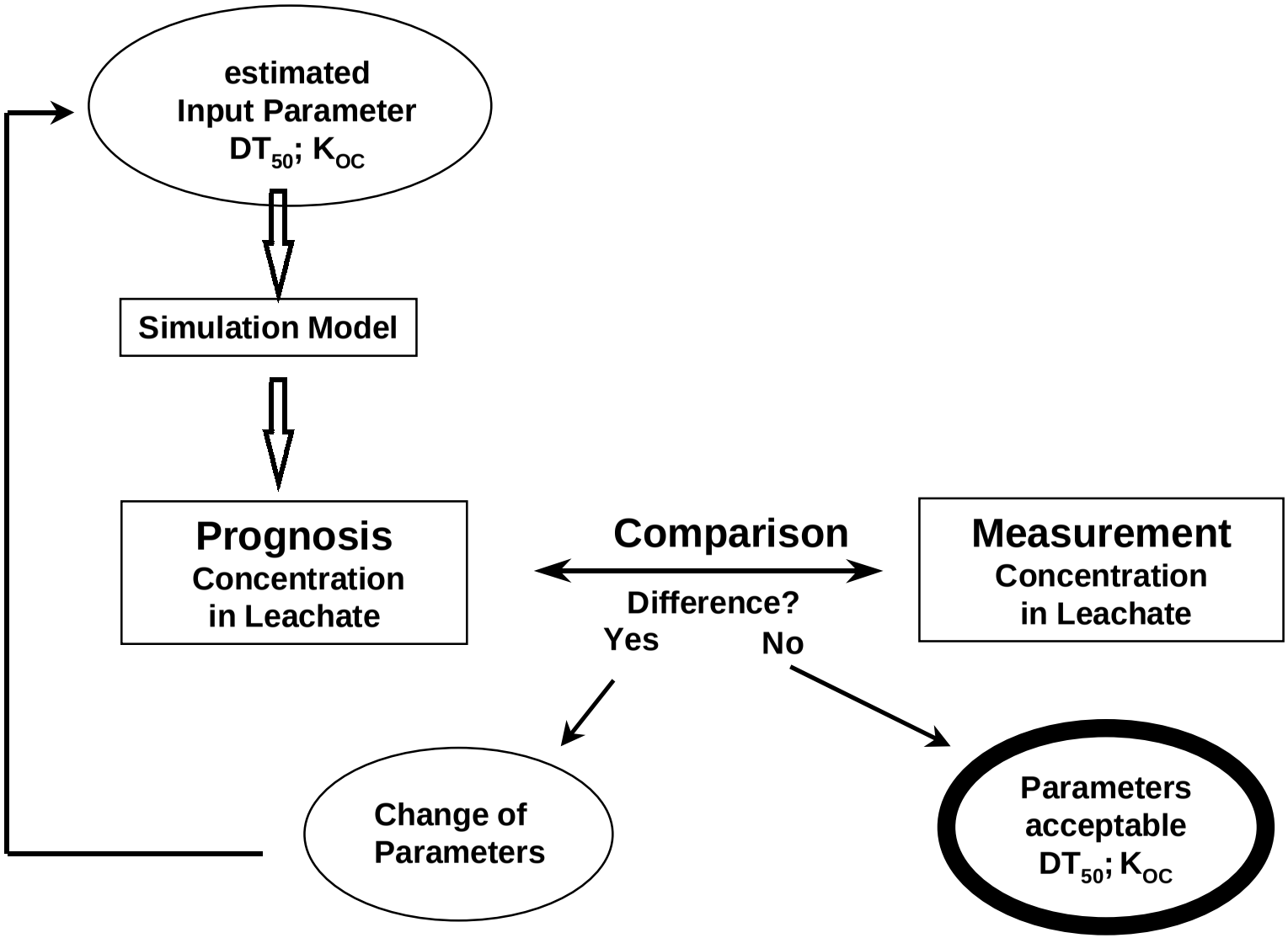


What is the difference between 'inverse' and 'usual' modelling?

-1. 'inverse' modelling:



The Principle of Inverse Modelling



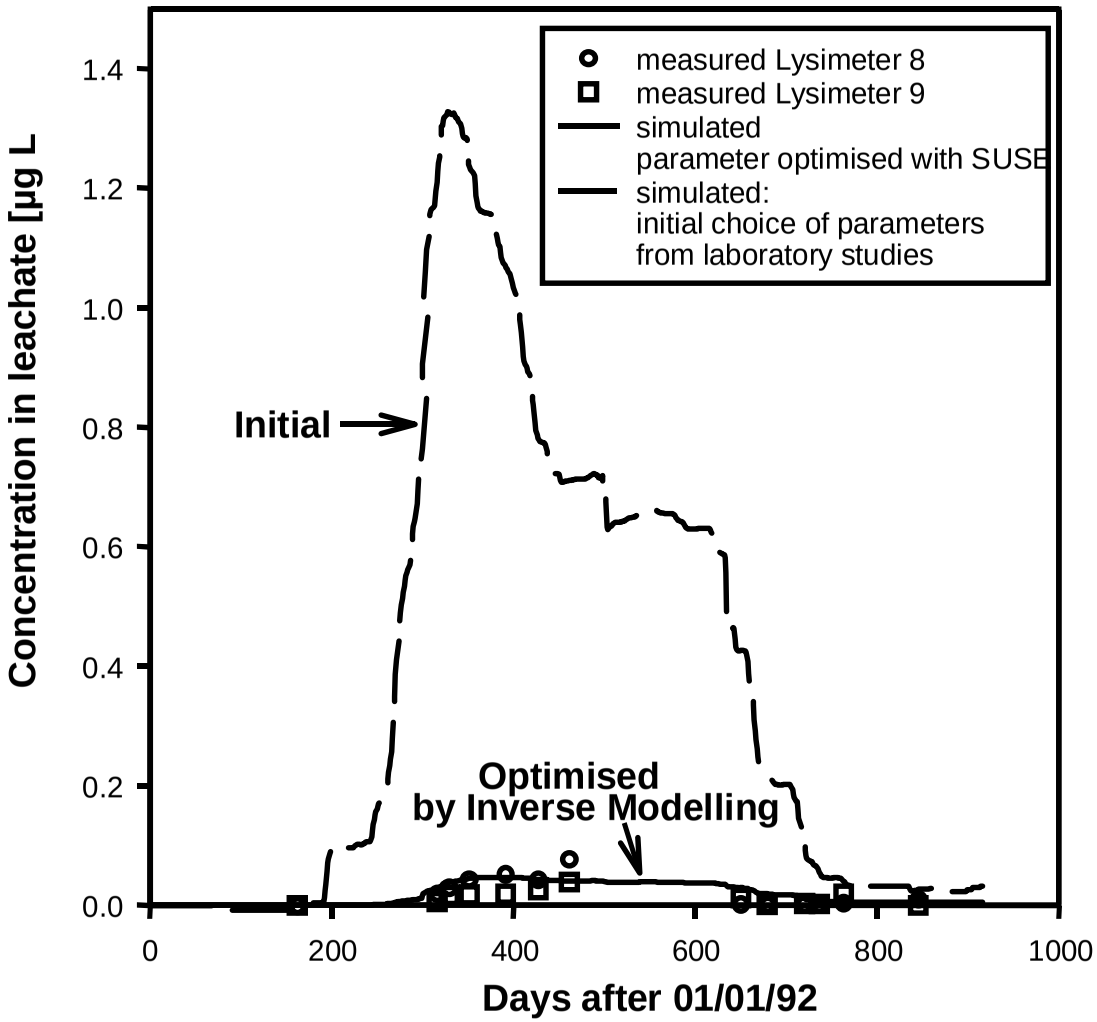
Estimation of Key E-fate Parameters

Sensitivity Analysis of Model Input Parameters

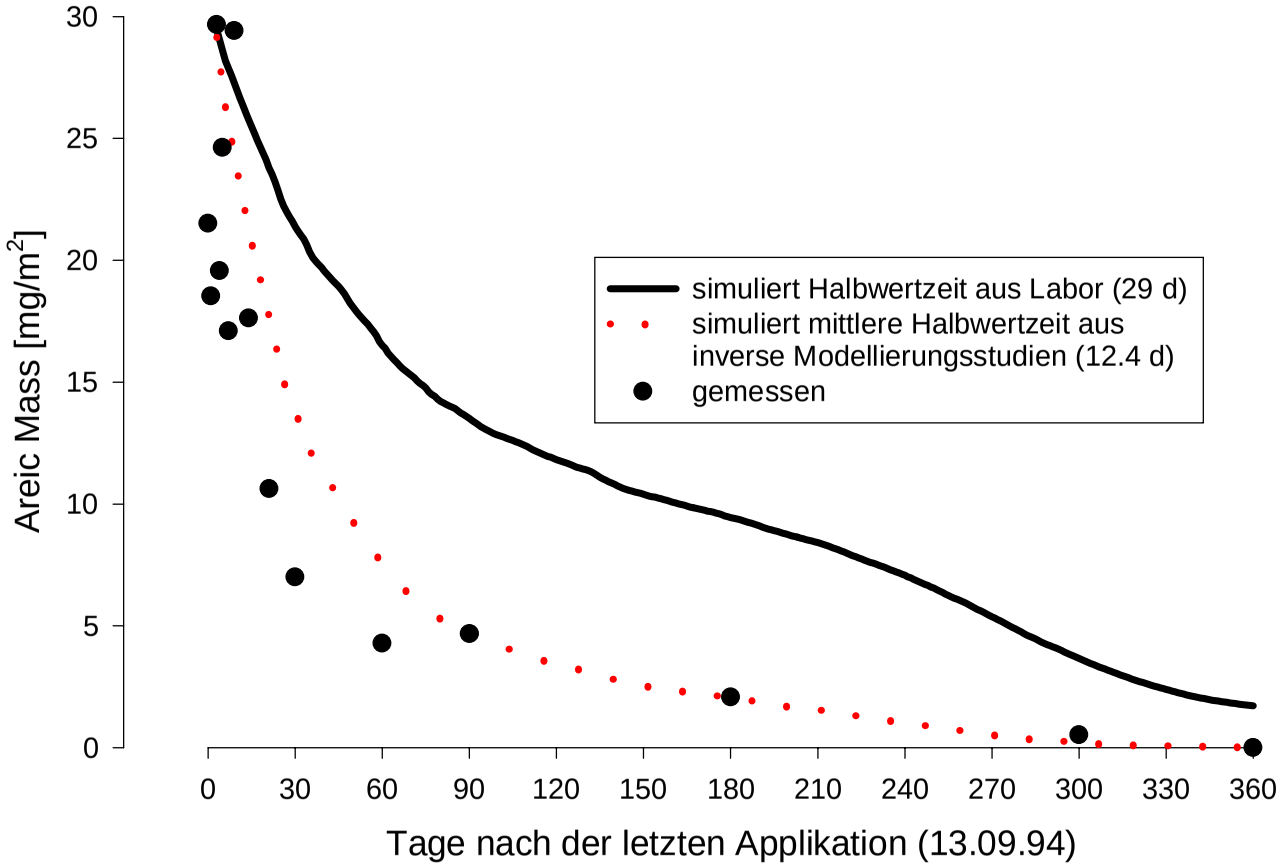
Parameter	Rank	# NRC
Freundlich Exponent	1	5 - 7
DT50	2	2 - 3
KOM	3	-1 - -3
TSCF	4	-2
Temp. factor	5	0 - -1
Moisture factor	6	0 – 0.5

1% change of input parameter has an effect of NRC% on the calculated model output

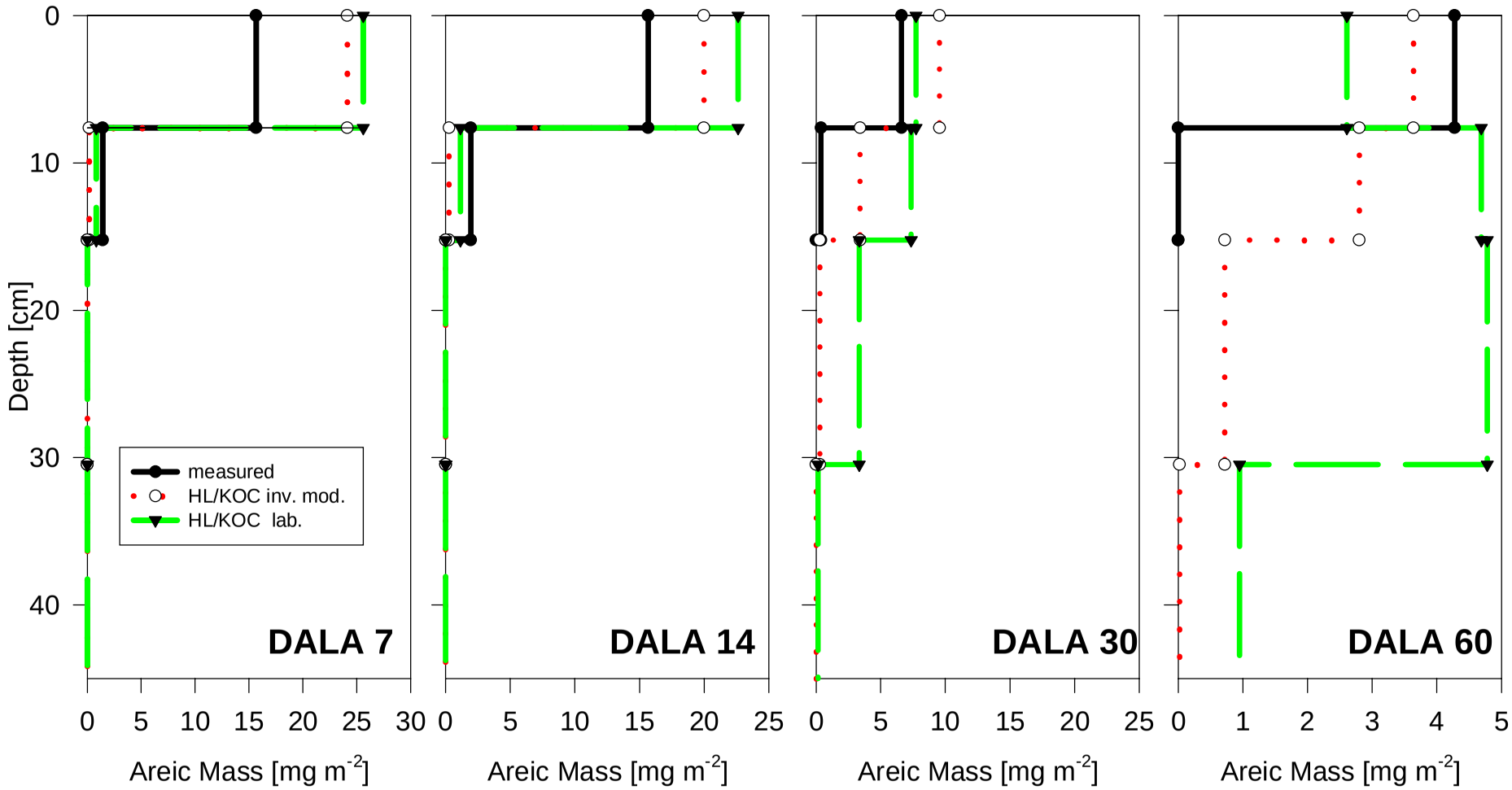
Inverse Modelling: Calibration Phase



Inverse Modelling: Validation Phase



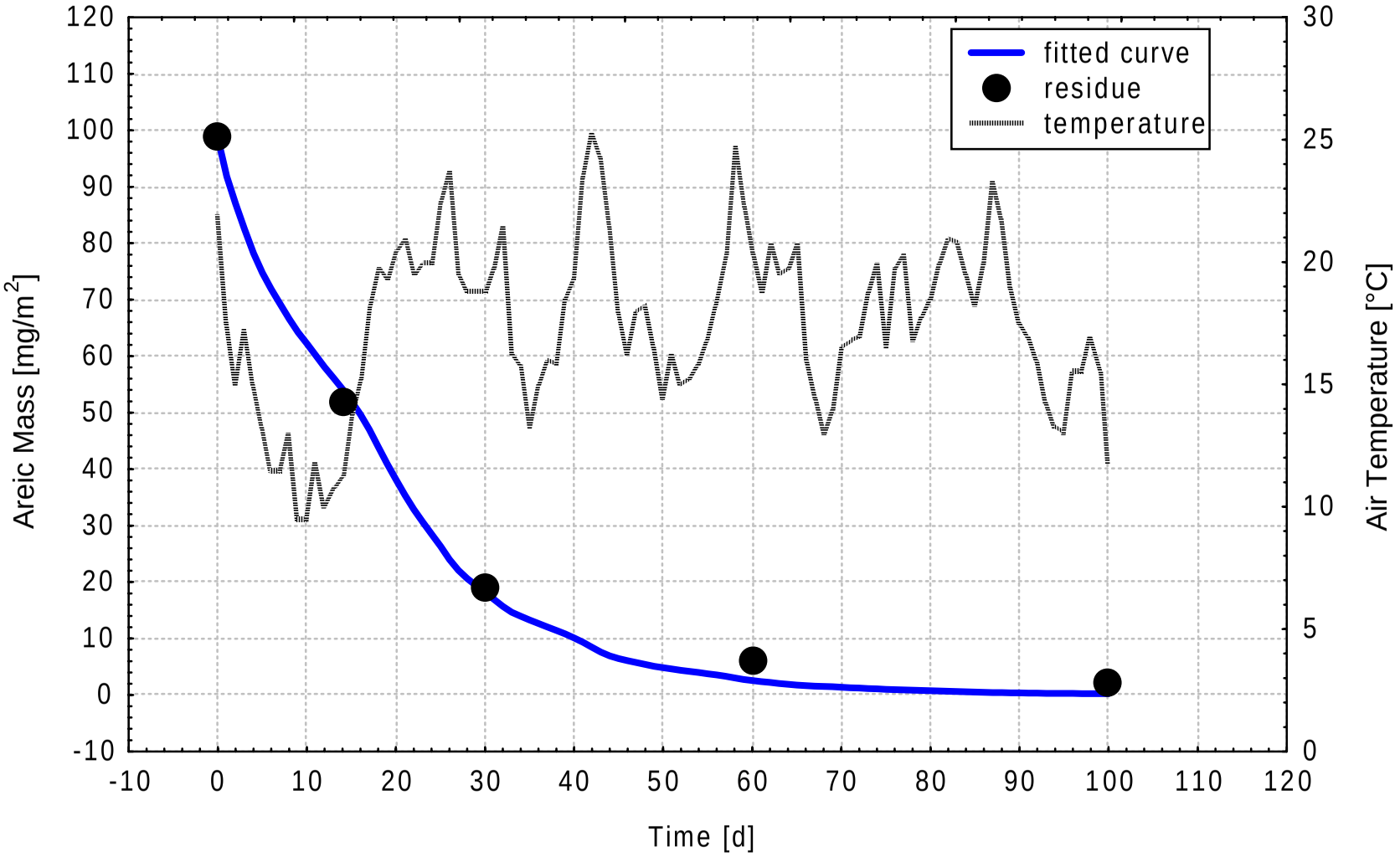
Validation Step of Inverse Modelled Parameters in an Independent Field Leaching Study



Estimation of Key E-fate Parameters

Inverse Modeling of Field DT50 at Reference Temperature

Goch/Nierswalde Half Life at 20 °C = 10 d

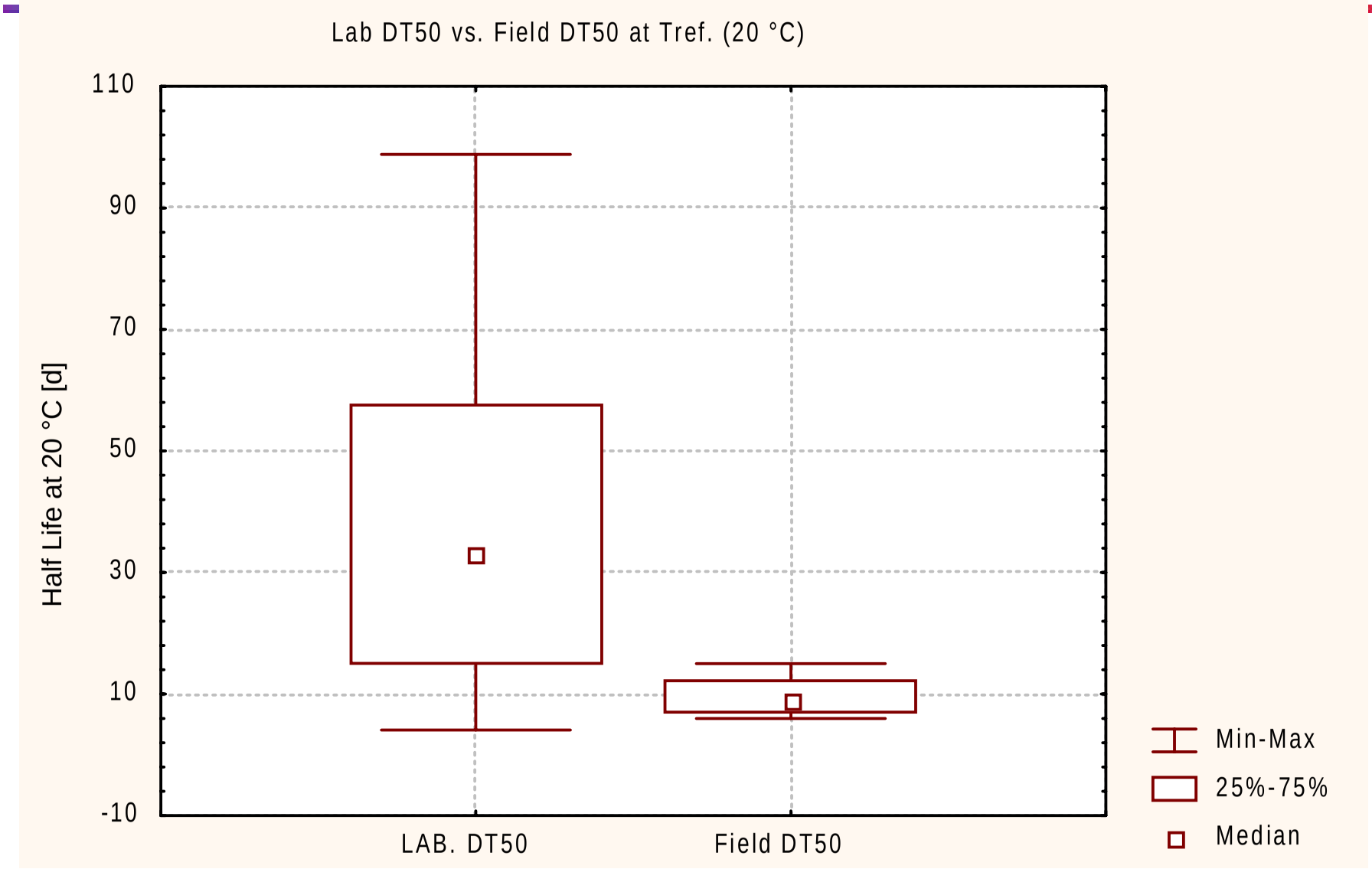


Standardisation of DT50field to Reference Temperature

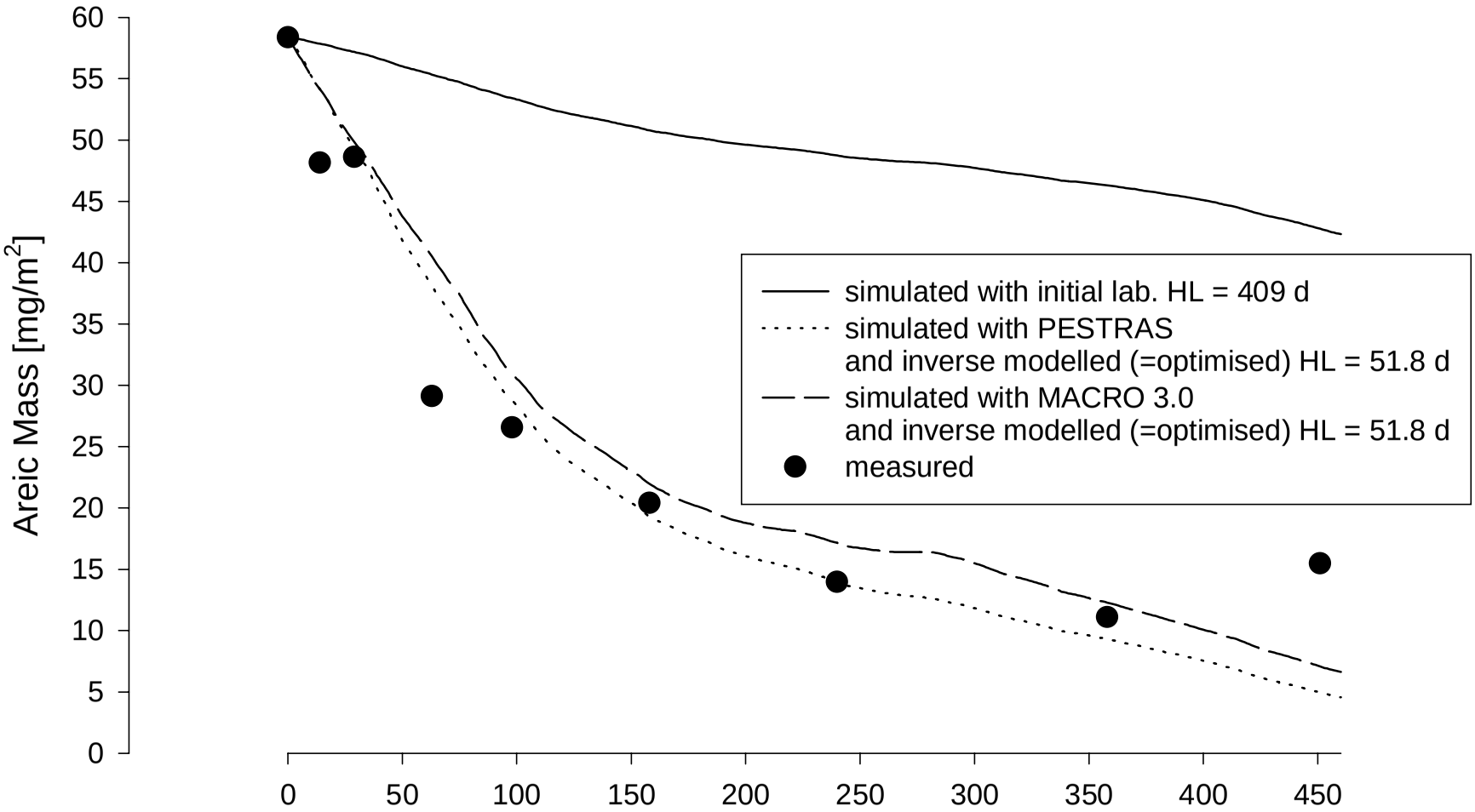
Site	average temperature [°C]	Half Life fitted 1st order [d]	Half Life 20°C daily temperature correction [d]
Goch/Nierswalde	17.5	14	10
Havixbeck	15.6	13	7
Limburgerhof	19.0	9	8
Holzen	15.2	22	15
Stetten	17.1	17	12

Estimation of Key E-fate Parameters

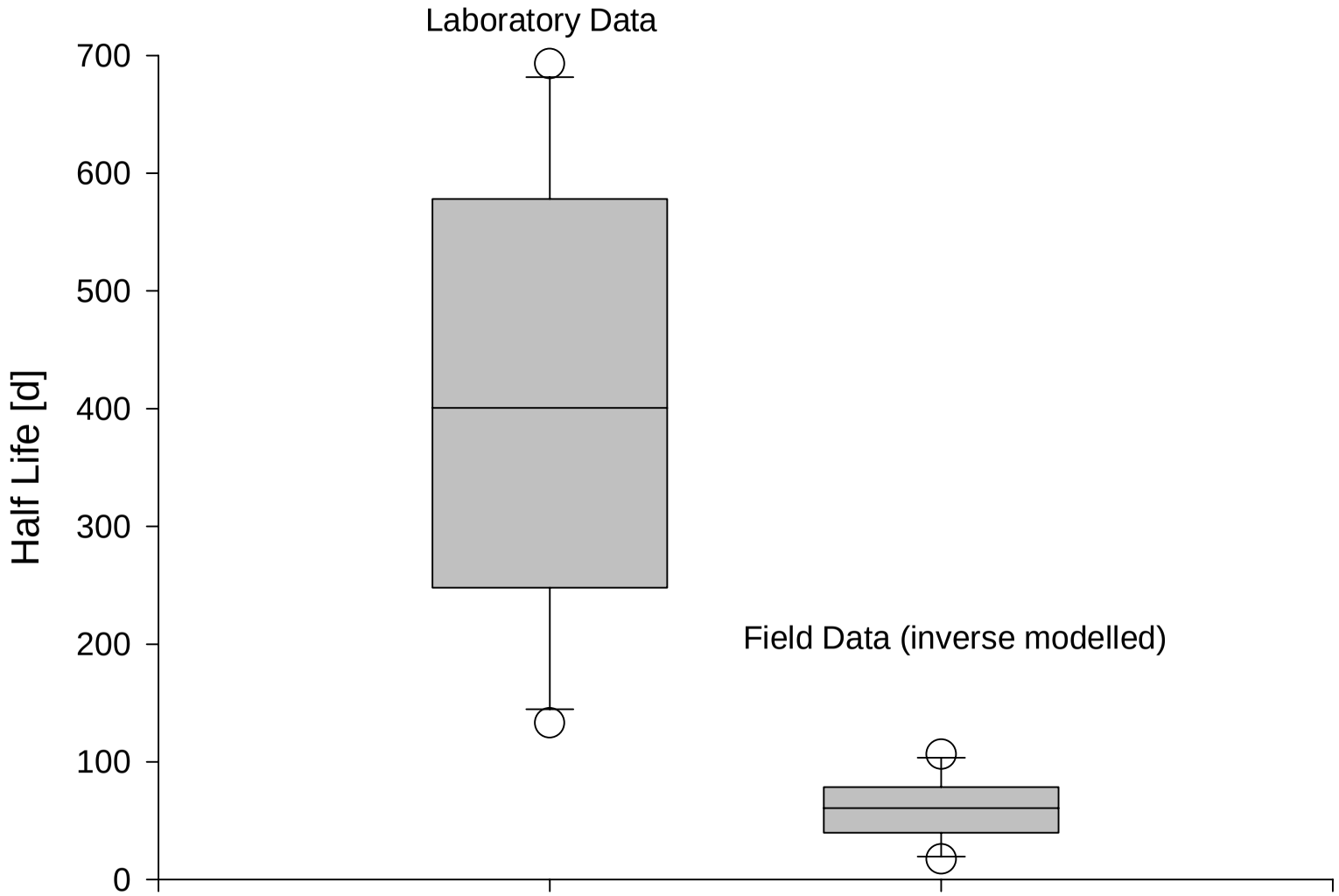
Lab. vs. Field DT50 at Reference Temperature



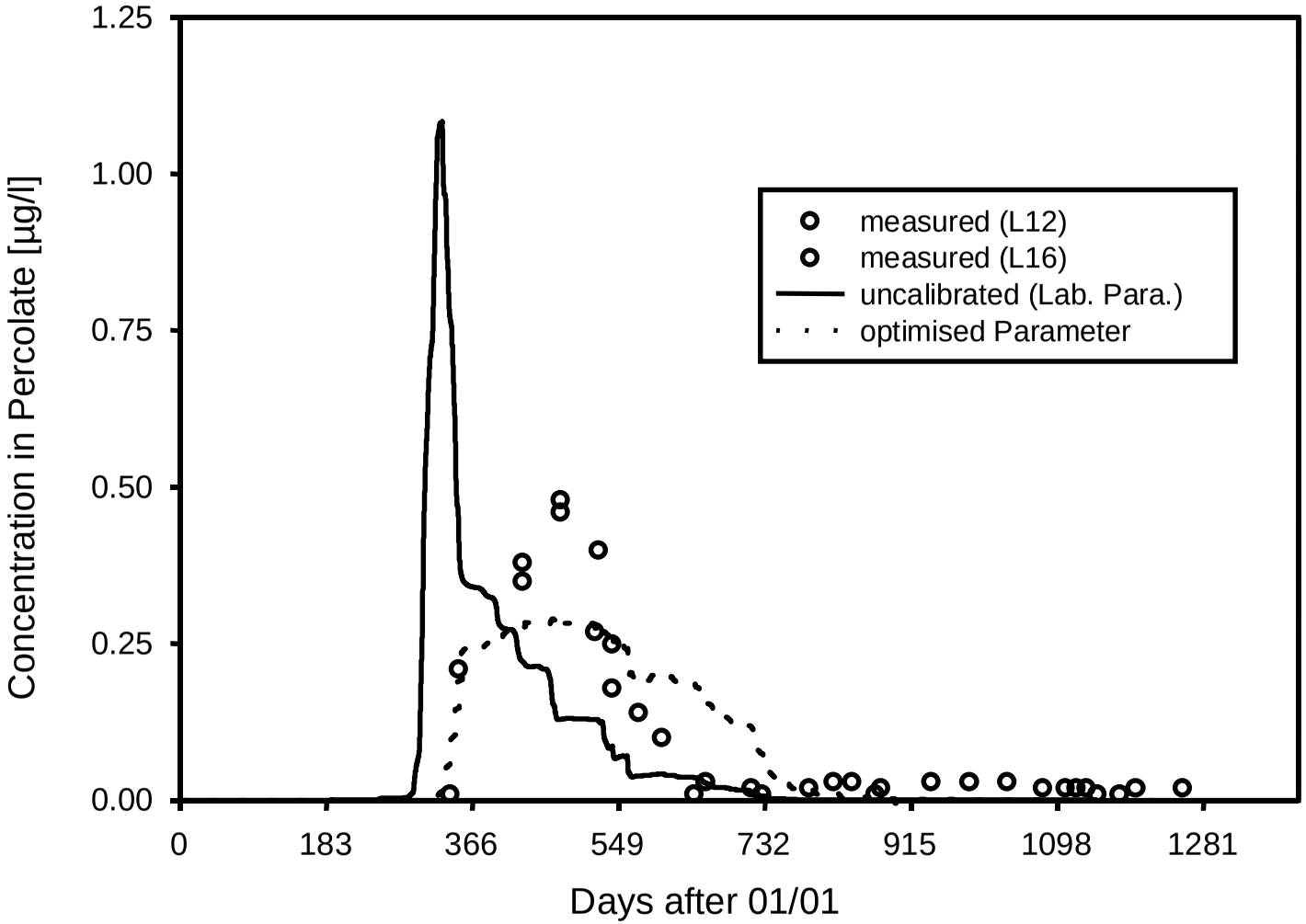
Measured and Simulated Residues of XXX in a field study using the initial and the optimised half life and the models PESTRAS and MACRO



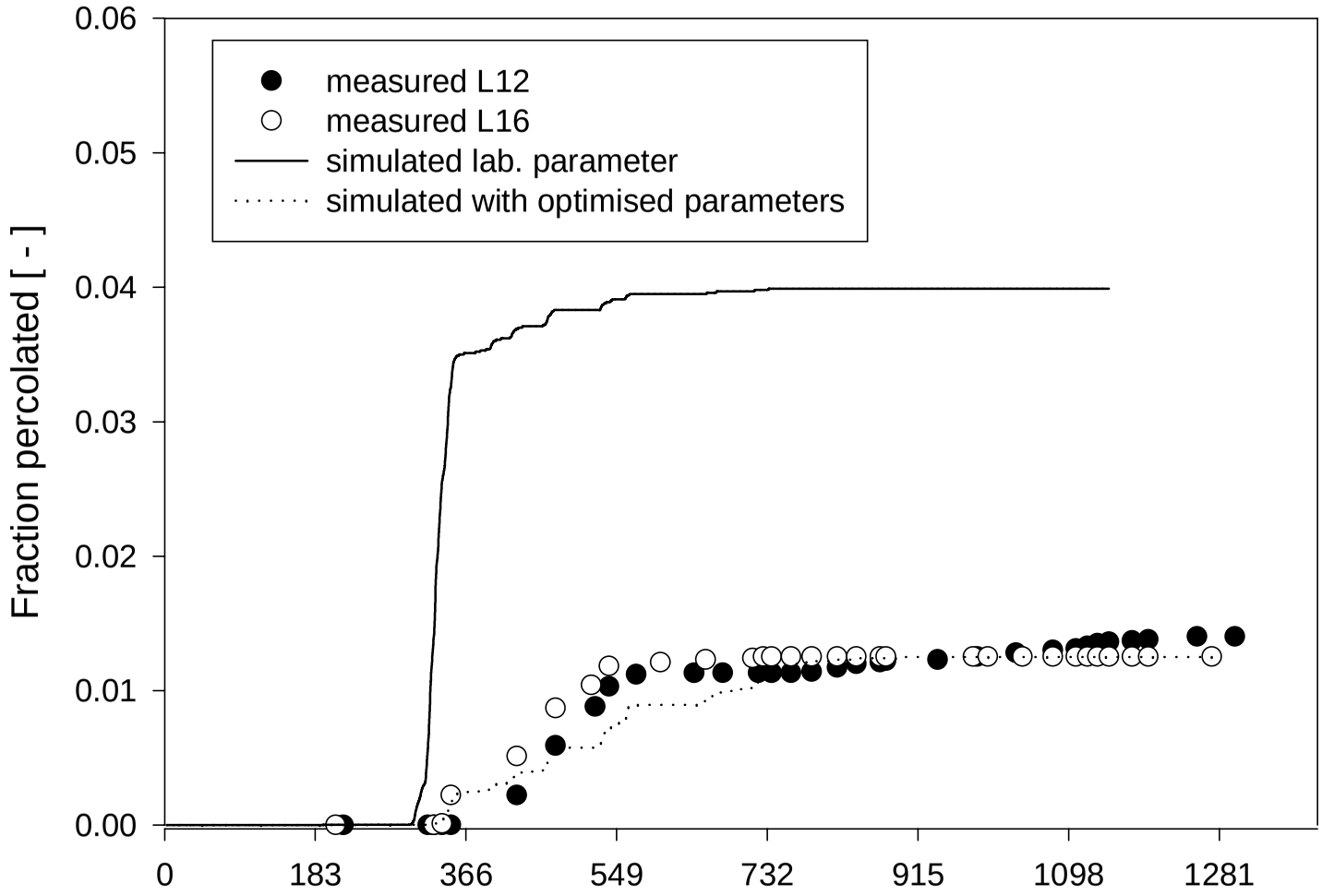
Comparison of Reference Half Lives of X determined from Laboratory Incubation Studies and Estimated with Inverse Modelling



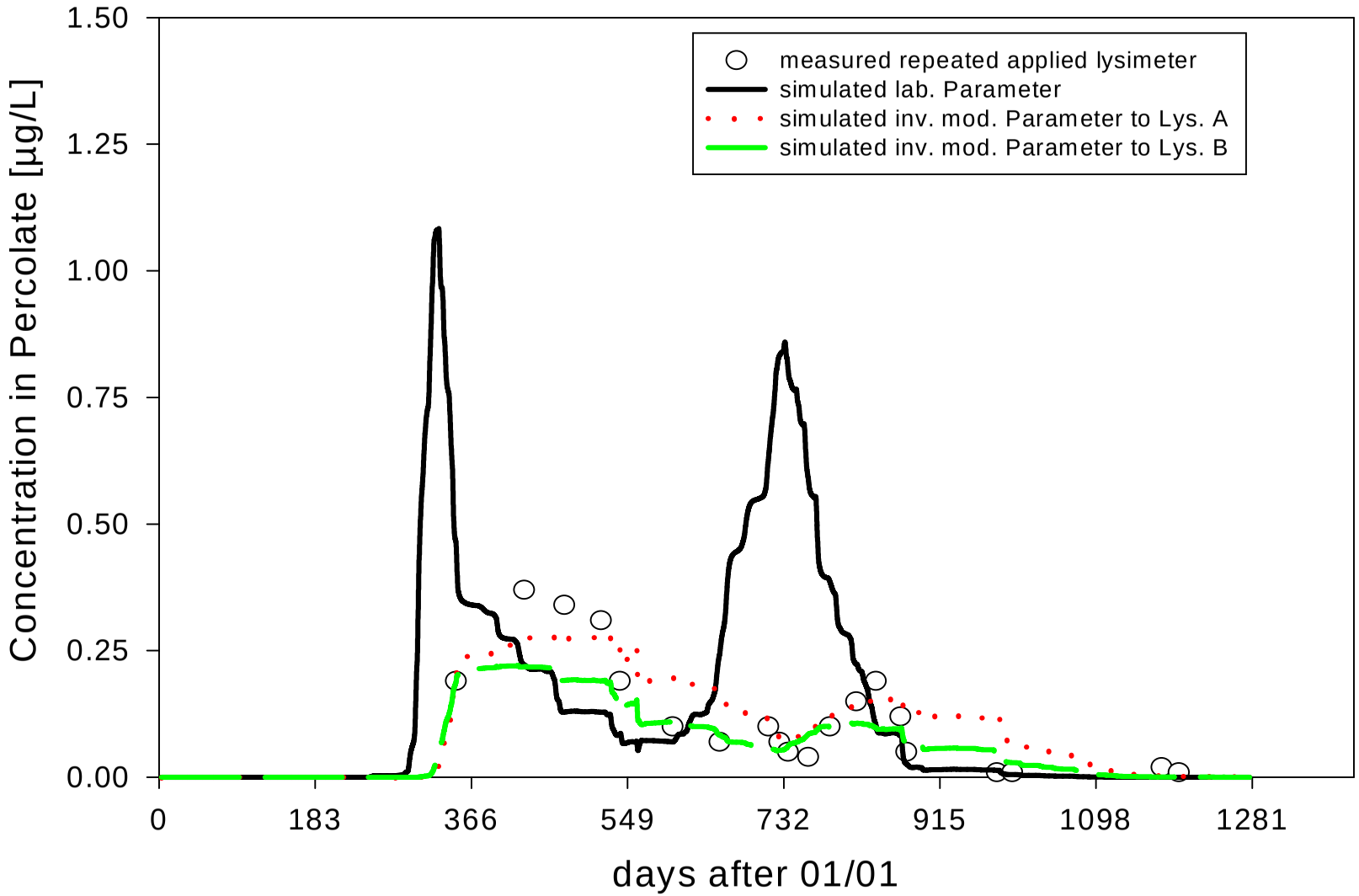
Optimisation Step (concentrations single applied lysimeter)



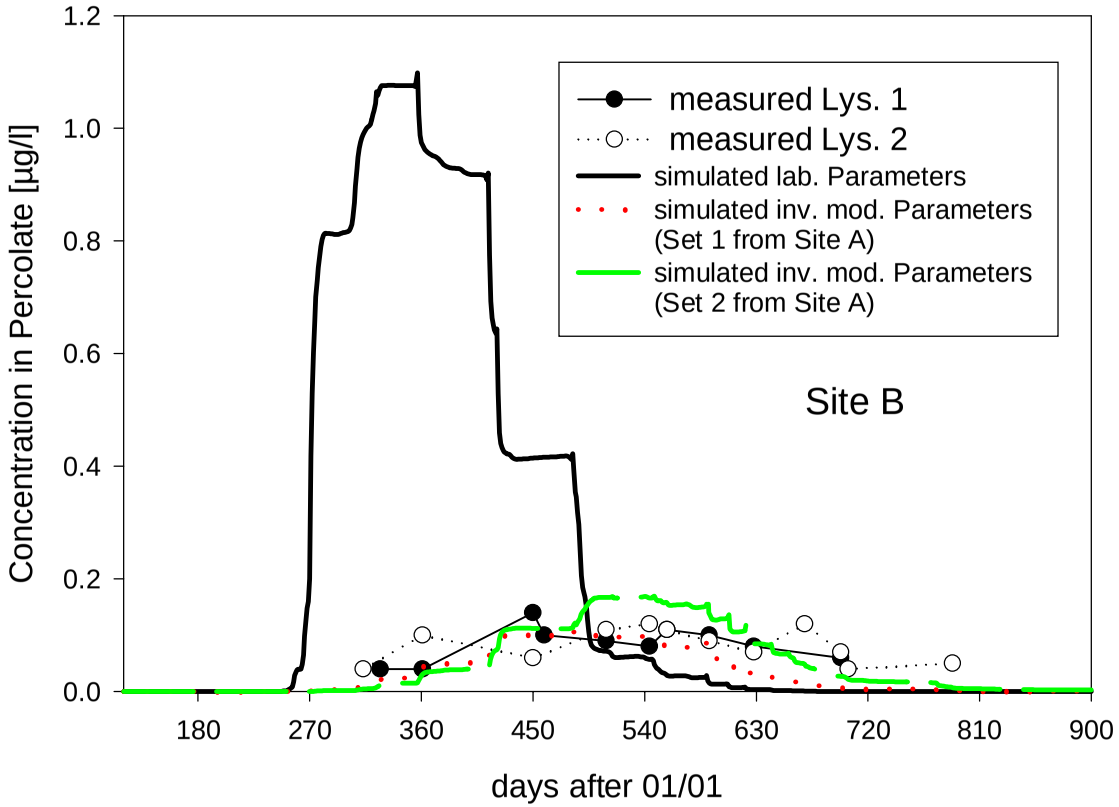
Optimisation Step (fraction percolated)



Validation Step (‚independent' repeated applied lysimeter)



Example for a validation/extrapolation step of inverse modelled parameters



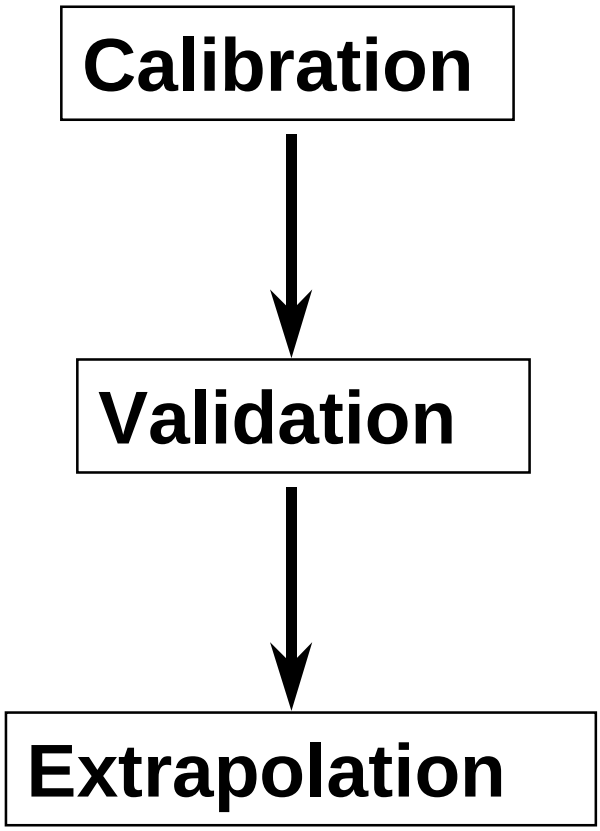
Standardisation:
Proposal for the Standardisation Step

Replace:

Standardized Result of Field-/Lysimeter Study:

$$S_{F/L} = M_{F/L} / C_{F/L} * C_{SS}$$

Include:



Resume:
What should be considered for Inverse Modelling

- **appropriate simulation model**
  (sophisticated water/solute transport routines; ETP with Penman or Makkink;
  Temp./Moist. Reduction Factors for degradation; Freundlich sorption)

- **data set of good quality**
  (from the most realistic system and scale of interest; e.g. field lysimeter;
  BTC with enough data points; residue profiles)

- **appropriate opimisation shell**

- **suitable stepwise approach**
  -> 1. Calibration
  2. Validation (on independent data set)
  3. Extrapolation

- **‚experienced' model user**