

Estimation of Key E-fate Parameters

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

Principles of Inverse Modeling

Calibration

- lysimeter trials
- field trials

Validation

Extrapolation

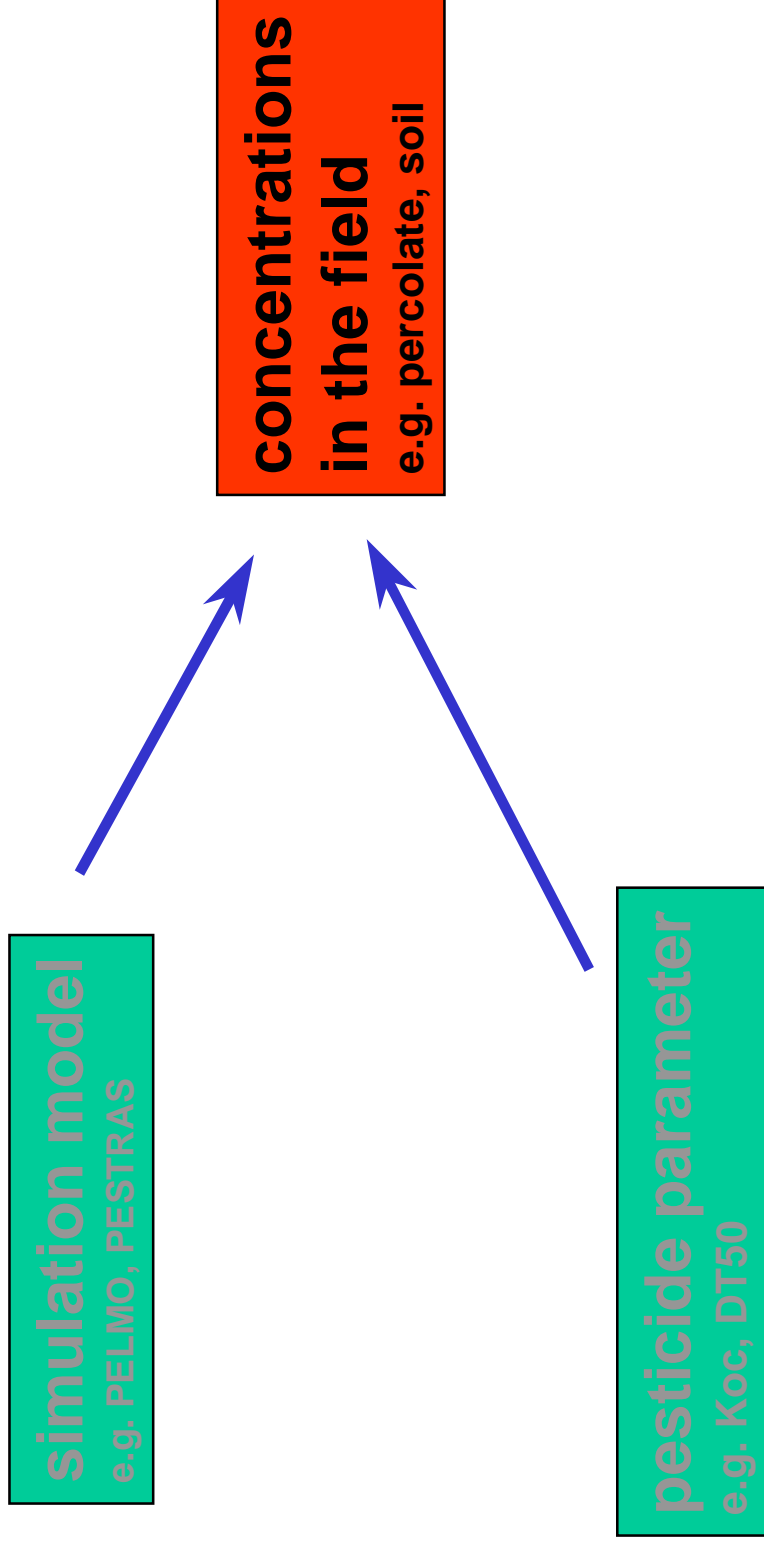
What is 'Inverse Modelling' ?

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.

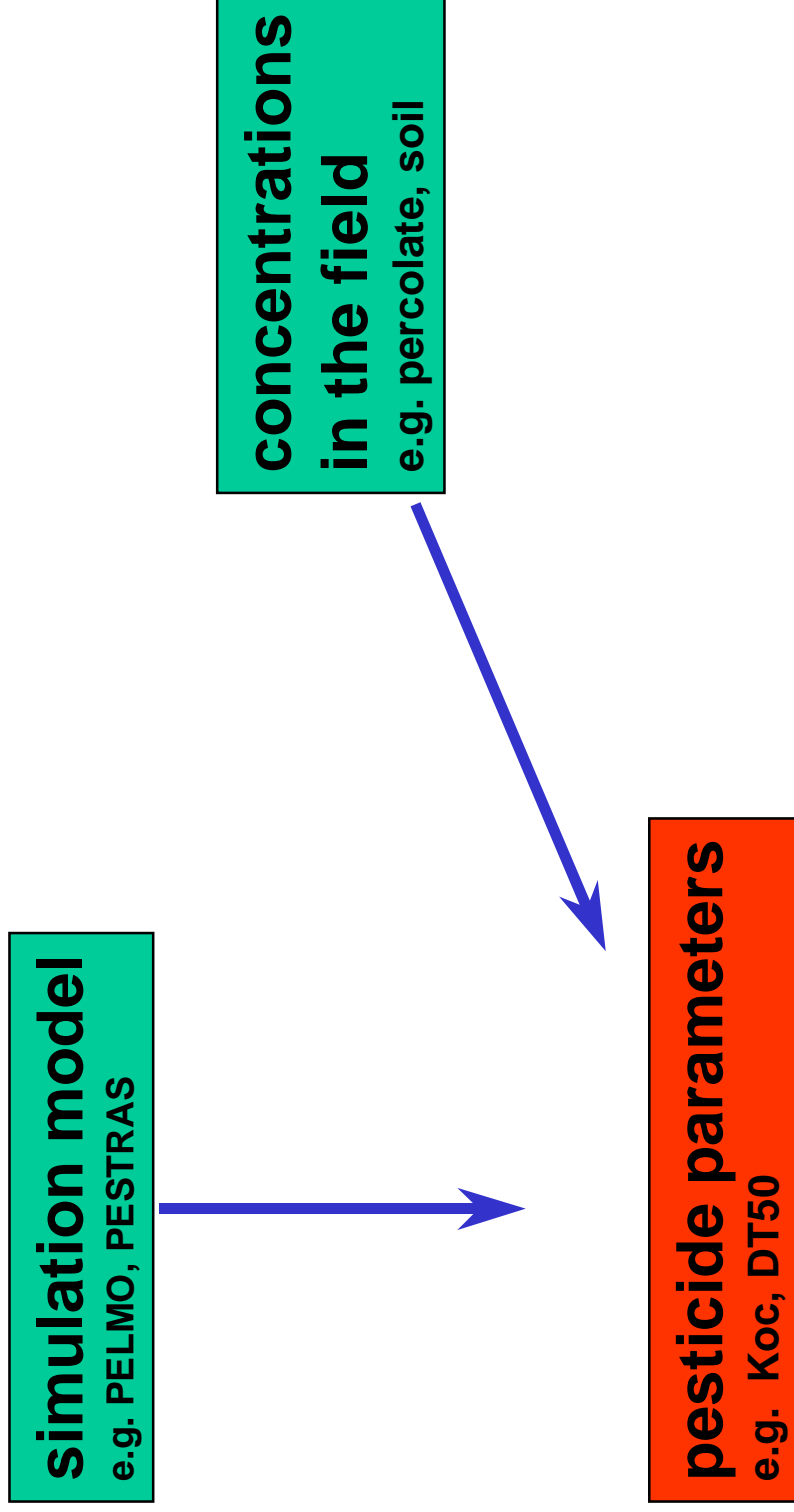
What is the difference between
'inverse' and 'usual' modelling?

1. 'Usual' Modelling:

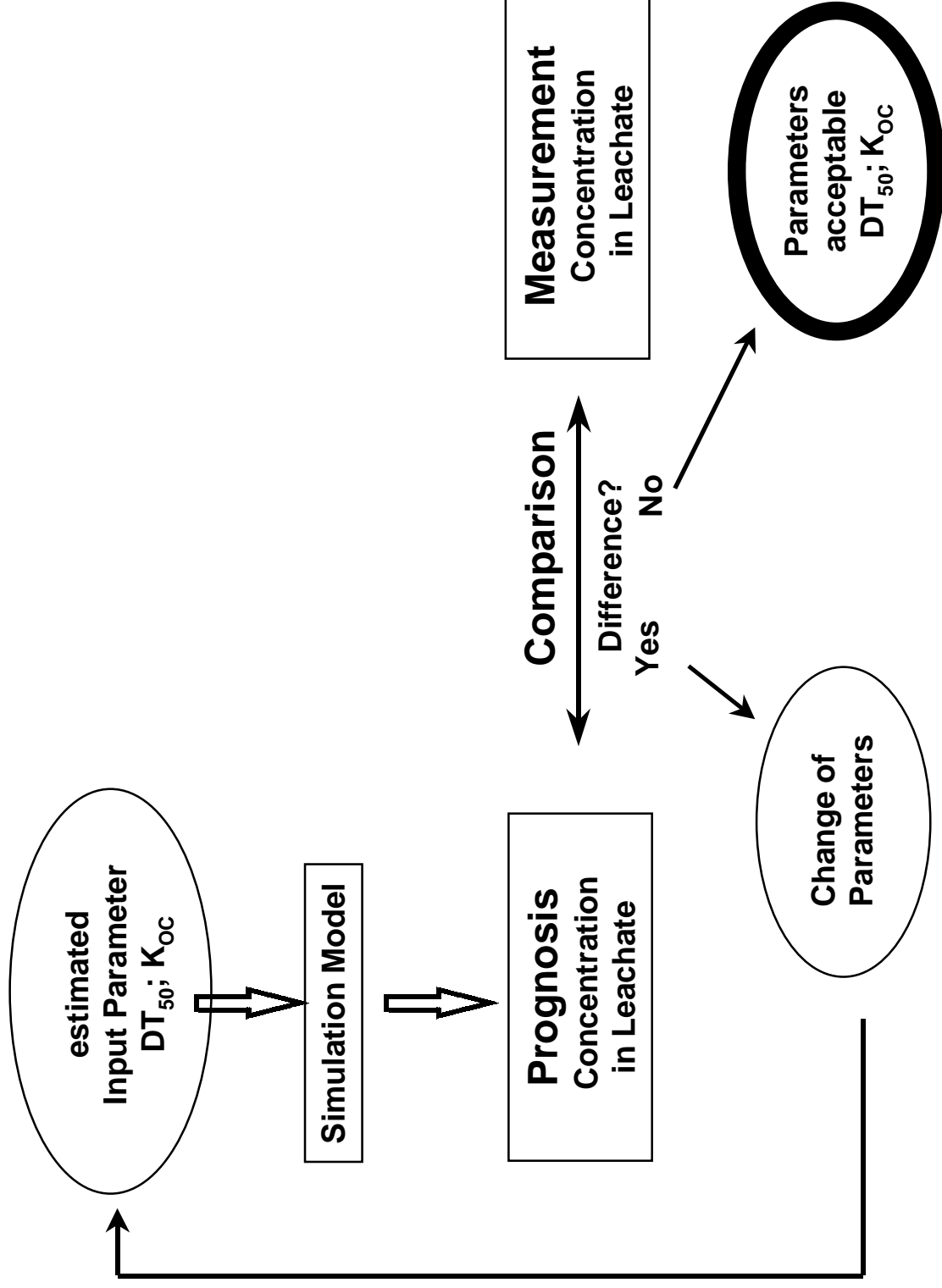


What is the difference between
'inverse' and 'usual' modelling?

-1. 'inverse' modelling:



The Principle of Inverse Modelling

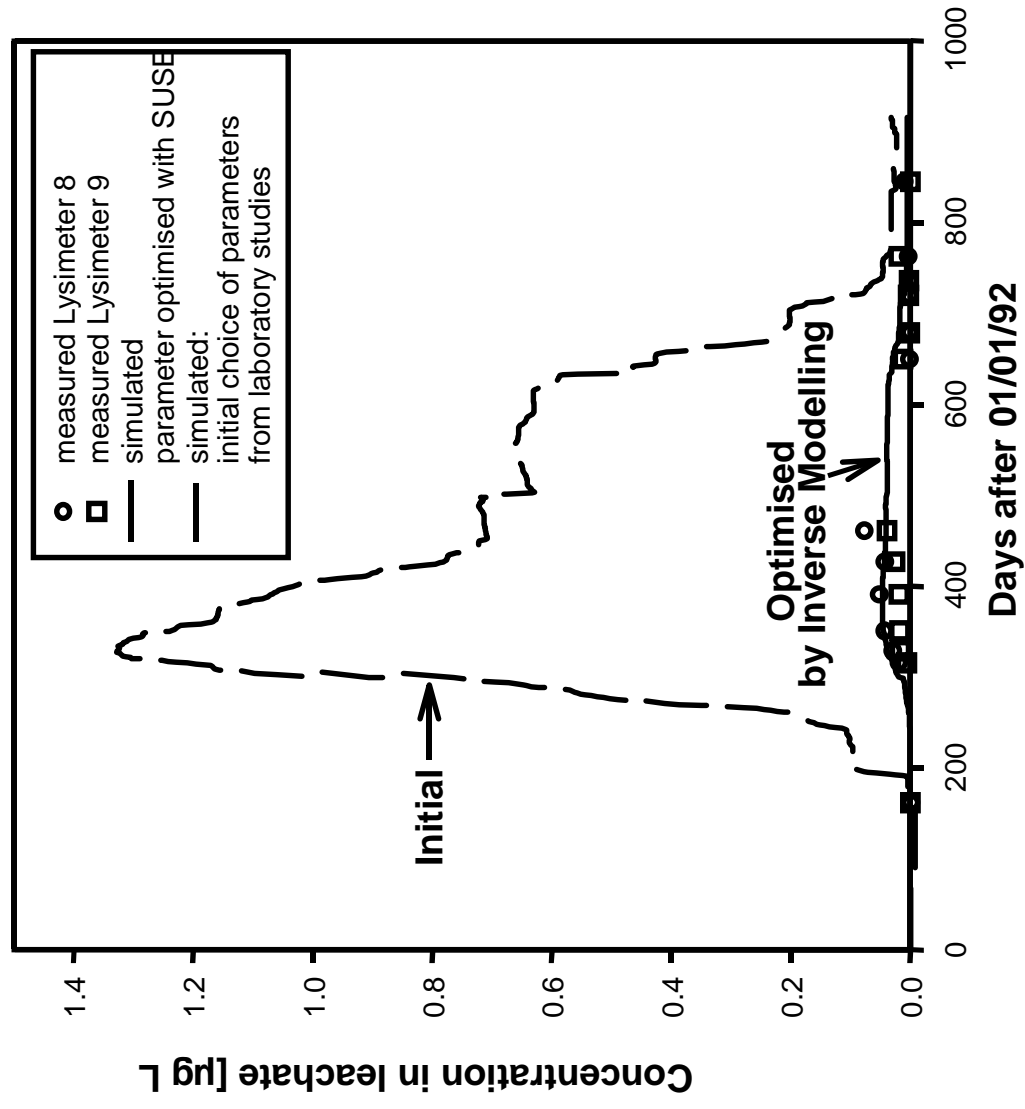


Estimation of Key E-fate Parameters
Sensitivity Analysis of Model Input Parameters

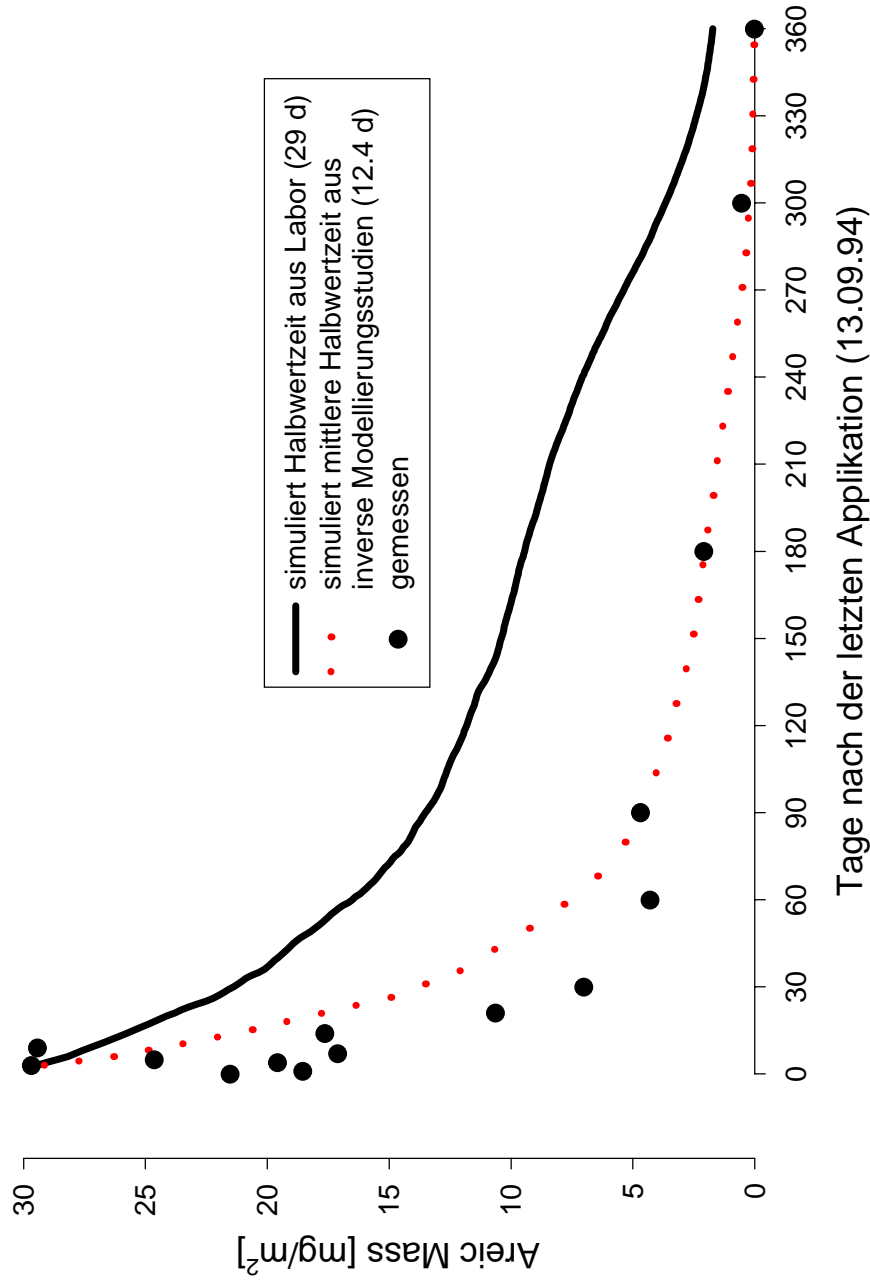
Parameter	Rank	# NRC
Freundlich Exponent	1	5 - 7
DT50	2	2 - 3
KOM	3	-1 - -3
TSCF	4	-2
Temp. factor	5	0 - -1
Moisture factor	6	0 - 0.5

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

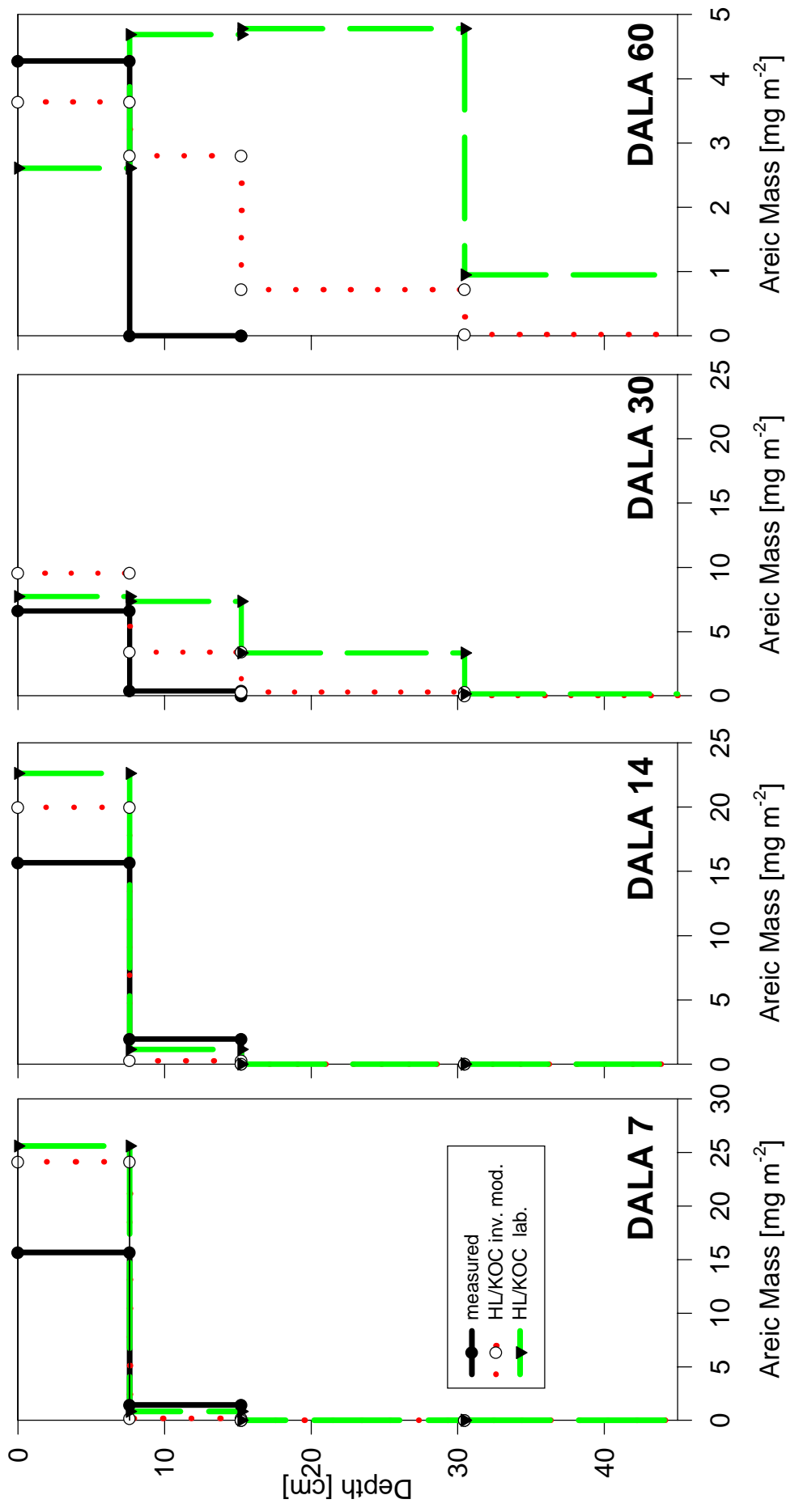
Inverse Modelling: Calibration Phase



Inverse Modelling: Validation Phase

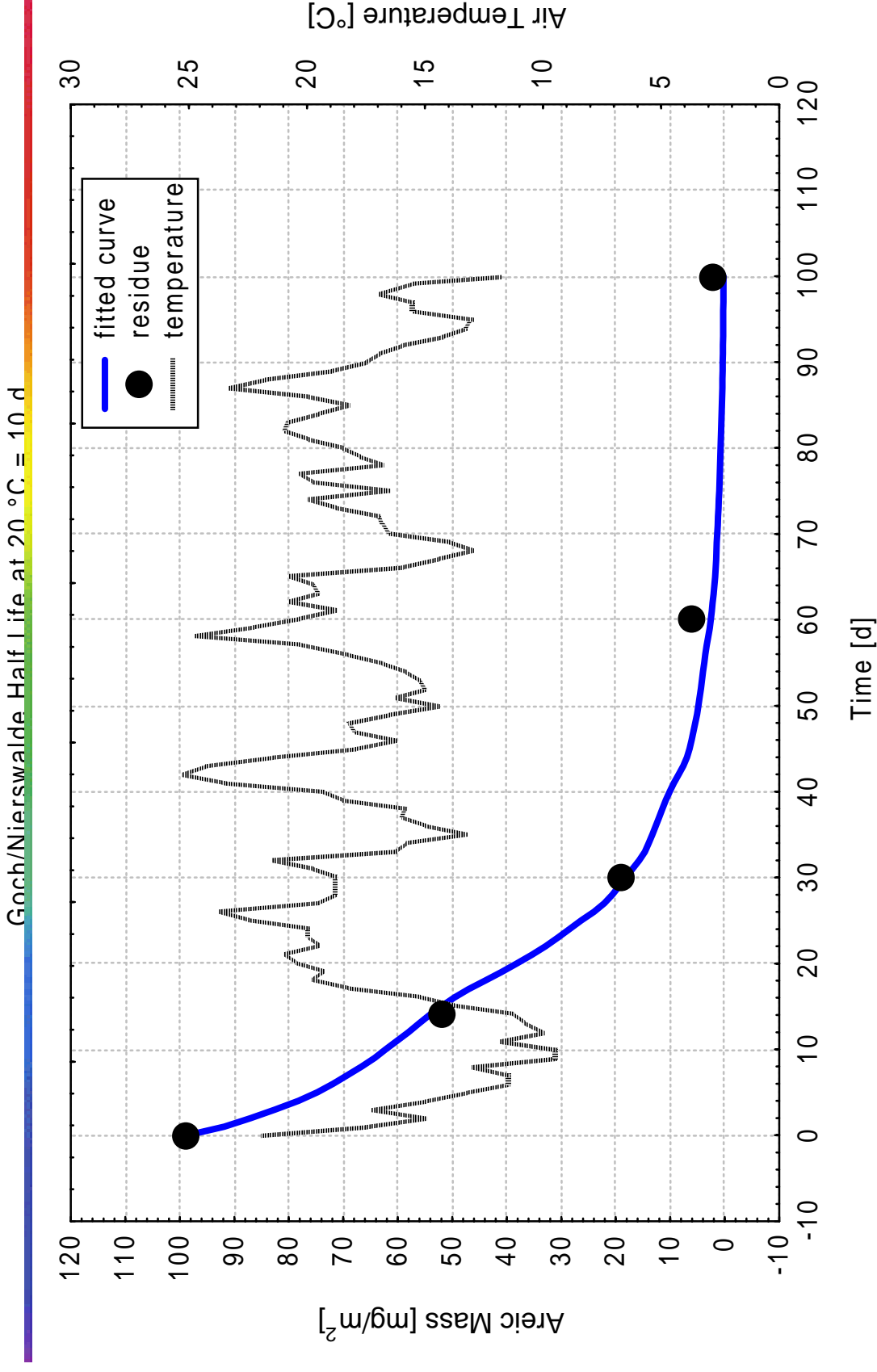


Validation Step of Inverse Modelled Parameters in an Independent Field Leaching Study



Estimation of Key E-fate Parameters

Inverse Modeling of Field DT50 at Reference Temperature



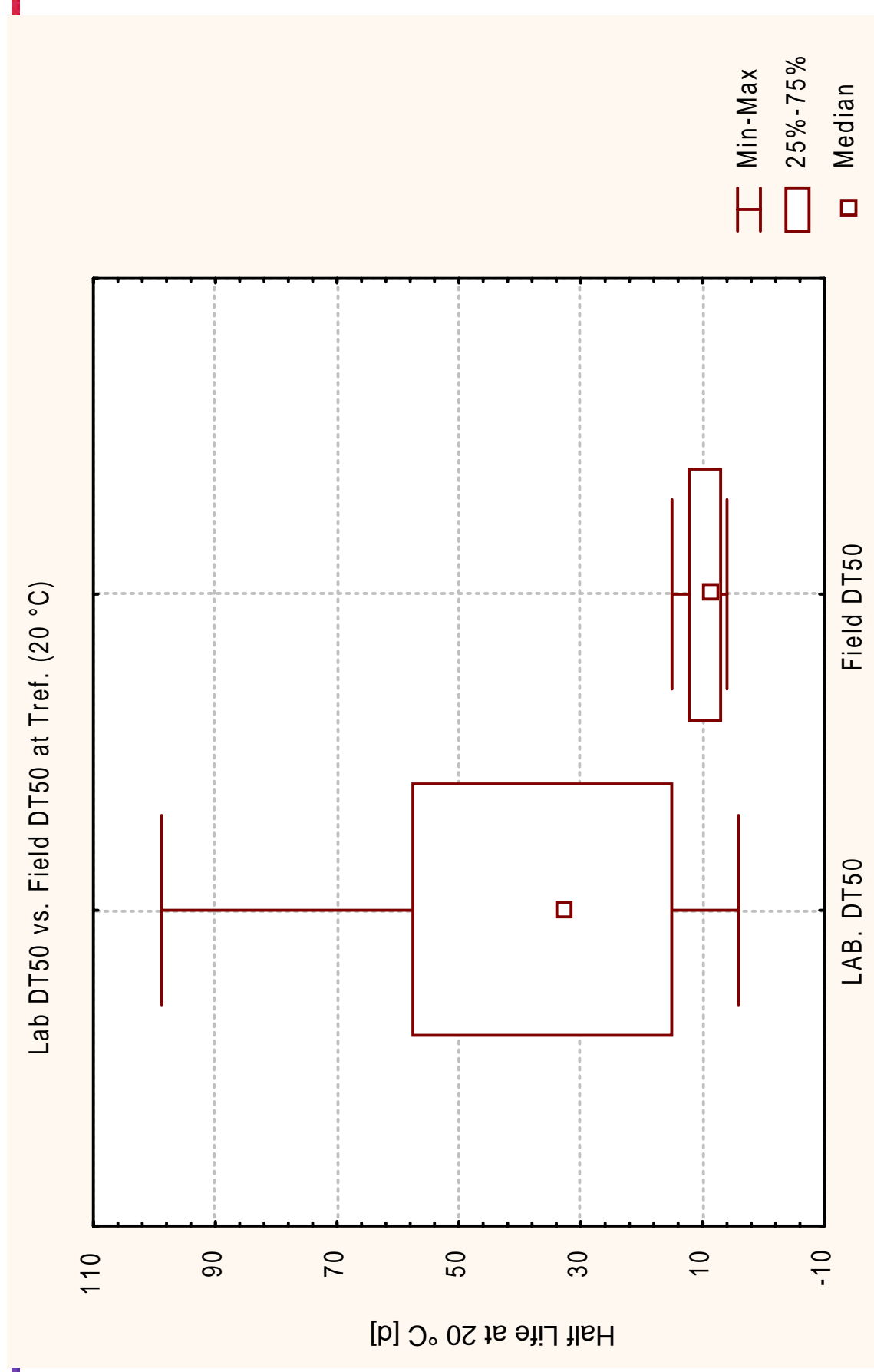
Estimation of Key E-fate Parameters

Standardisation of DT50field to Reference Temperature

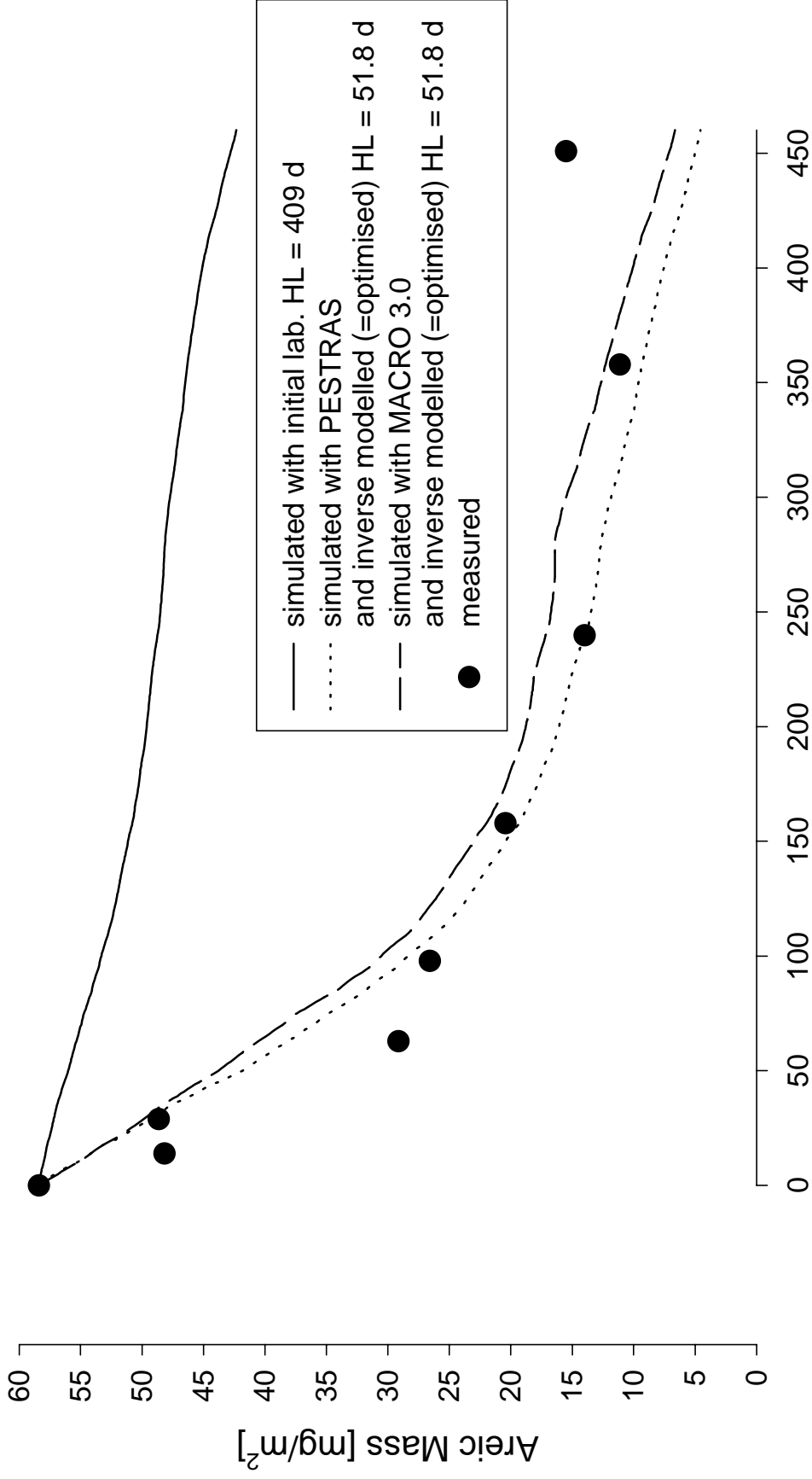
Site	average temperature [°C]	Half Life fitted 1 st order [d]	Half Life 20°C daily temperature correction [d]
Goch/Nierswalde	17.5	14	10
Havixbeck	15.6	13	7
Limburgerhof	19.0	9	8
Holzen	15.2	22	15
Stetten	17.1	17	12

Estimation of Key E-fate Parameters

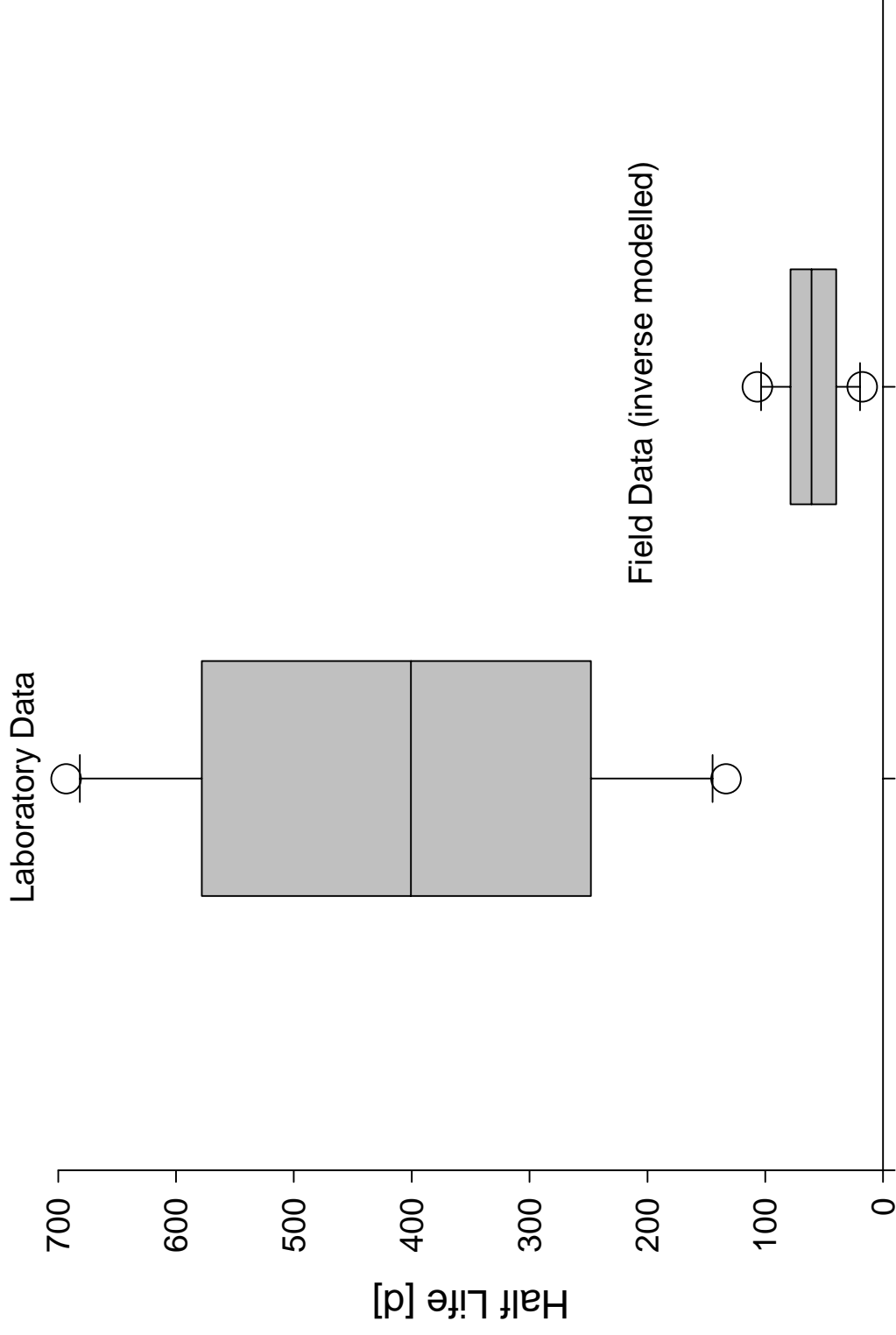
Lab. vs. Field DT50 at Reference Temperature



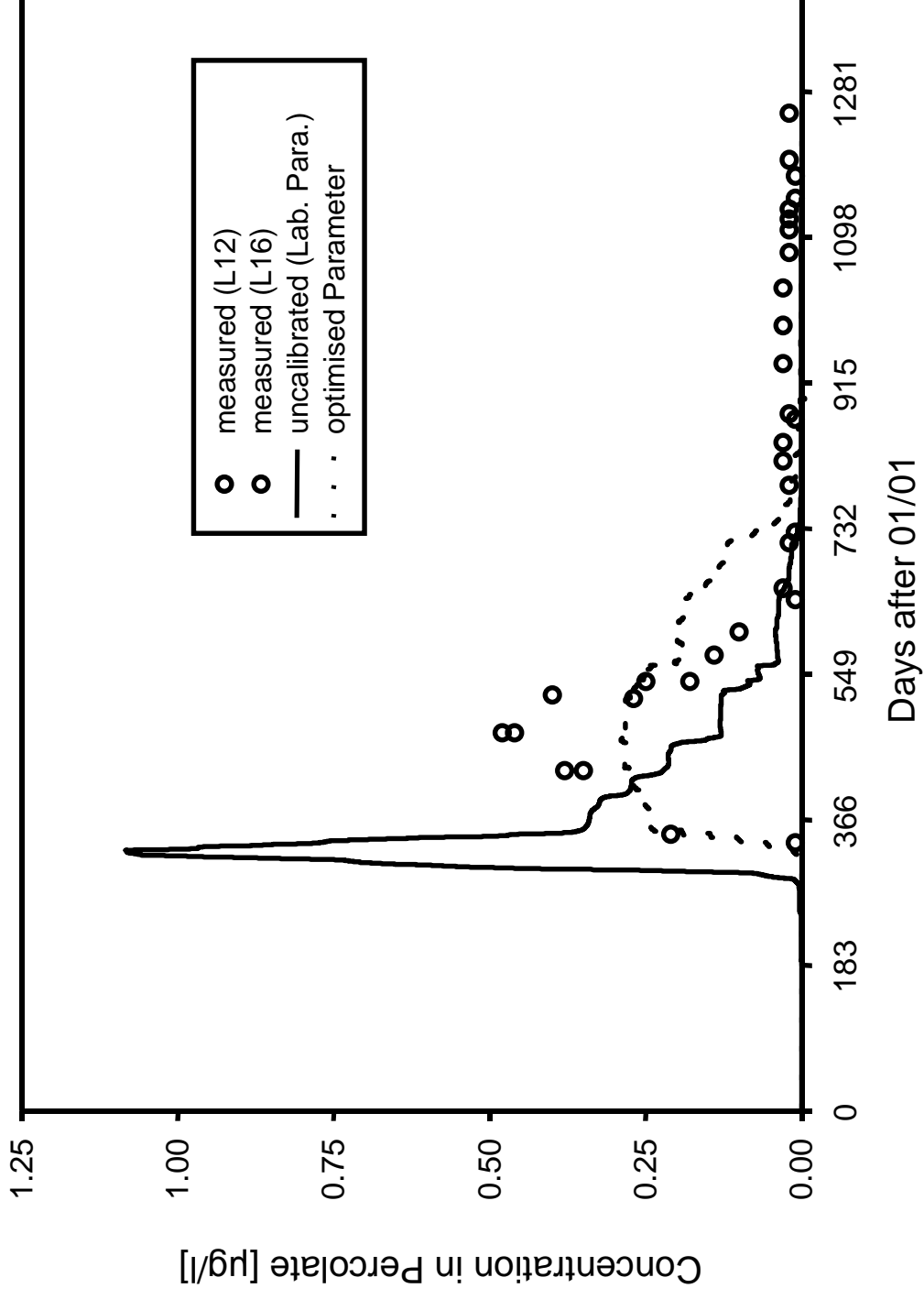
Measured and Simulated Residues of XXX in a field study using the initial and the optimised half life and the models PESTRAS and MACRO



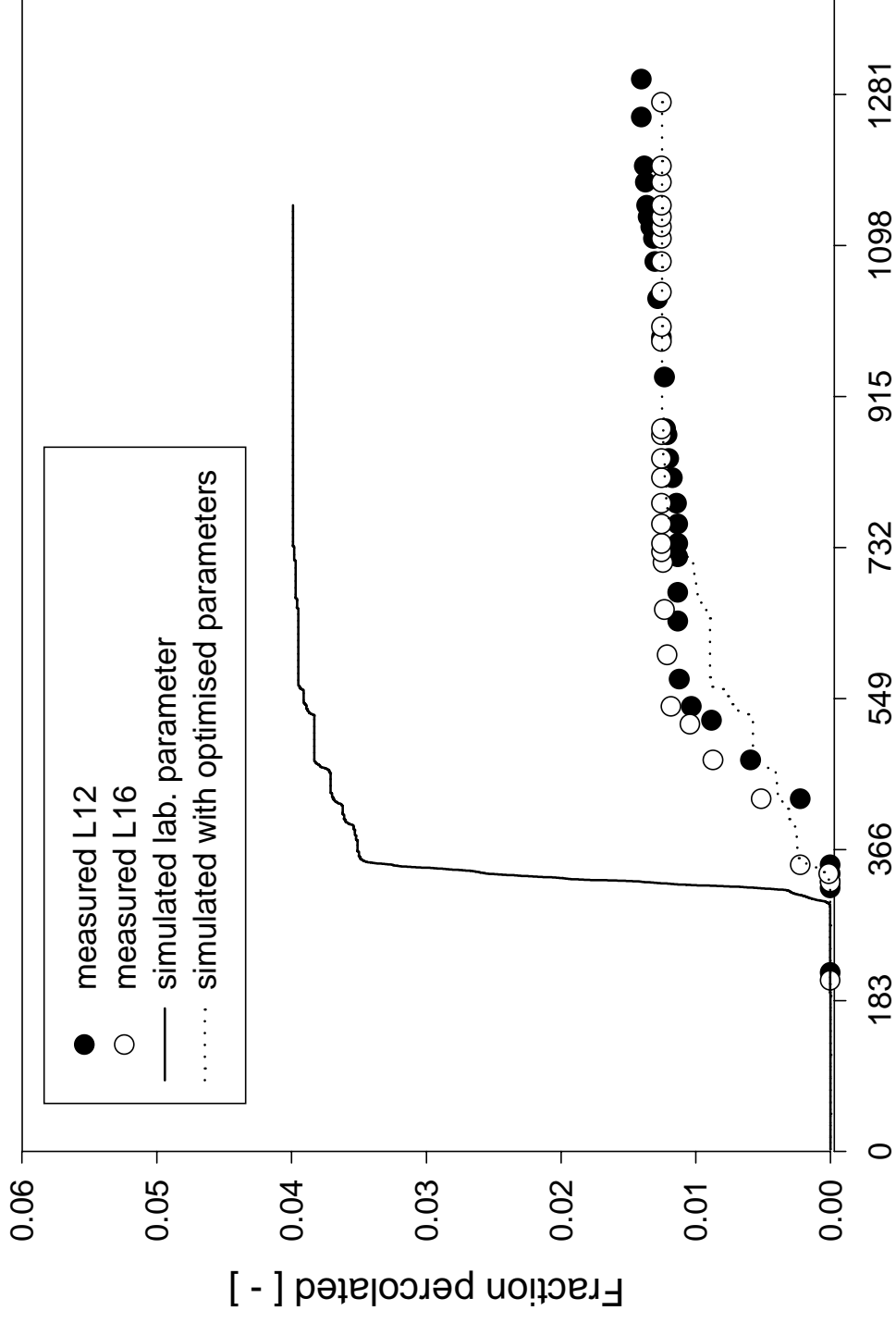
Comparison of Reference Half Lives of X determined from Laboratory Incubation Studies and Estimated with Inverse Modelling



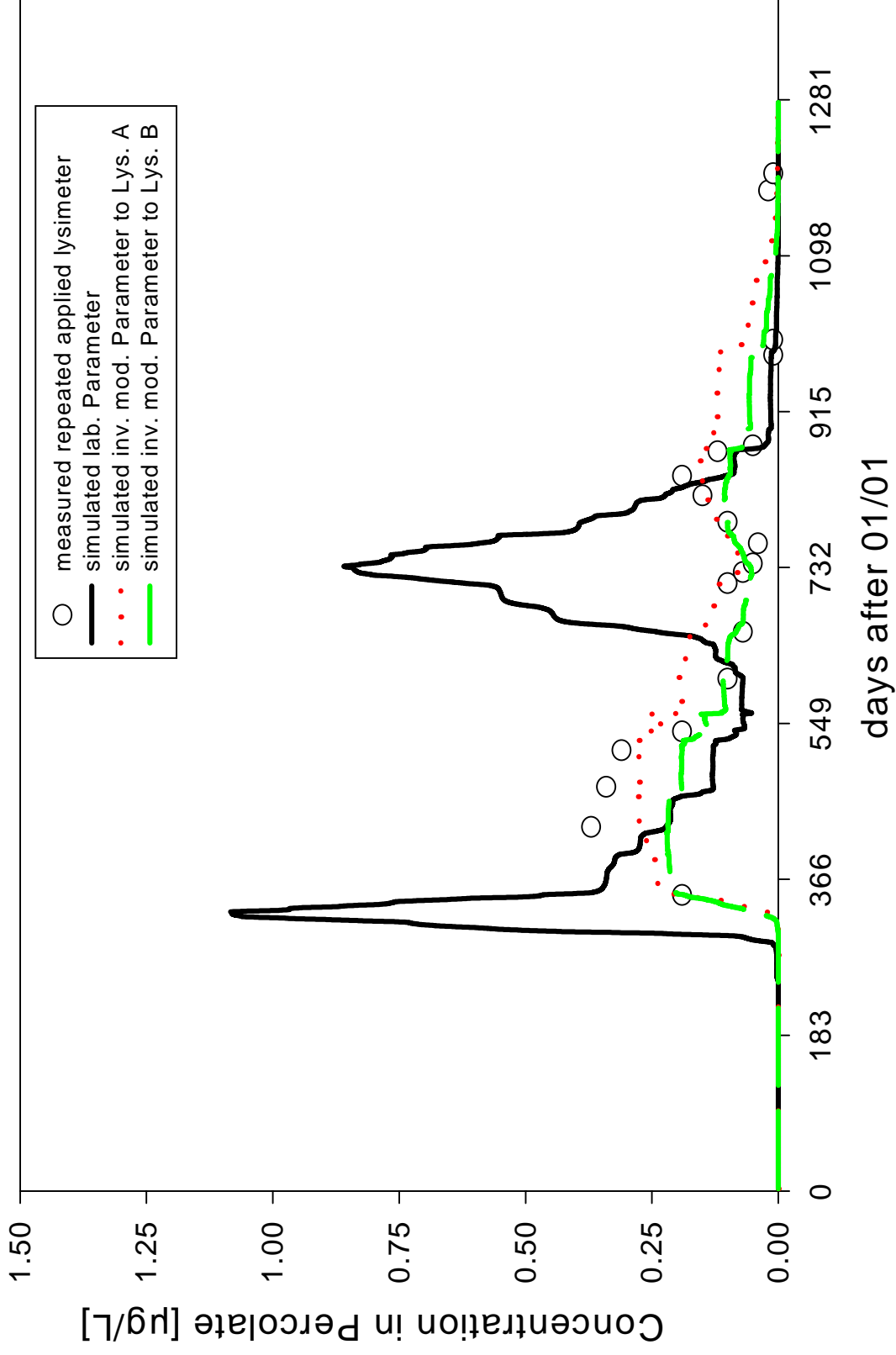
Optimisation Step (concentrations single applied lysimeter)



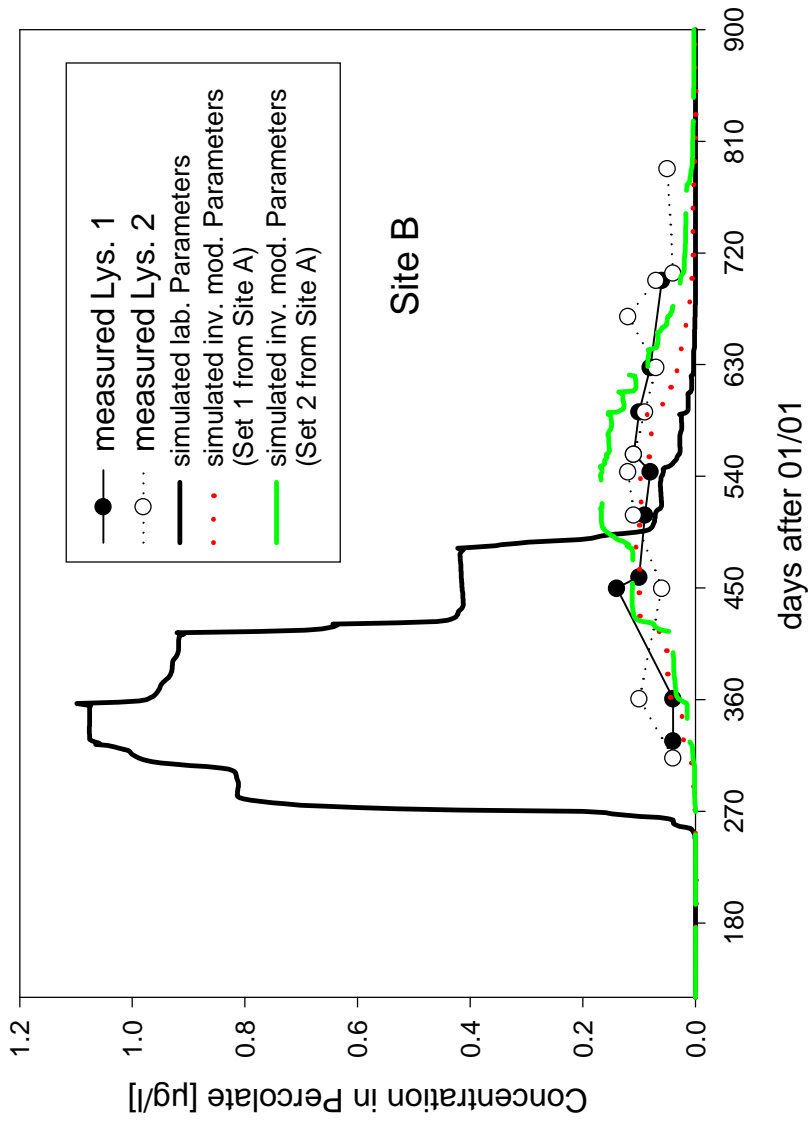
Optimisation Step (fraction percolated)



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:

Calibration



Validation



Extrapolation

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 optimisation shell**
- **suitable stepwise approach**
 - > 1. Calibration
 - 2. Validation (on independent data set)
 - 3. Extrapolation
- **,experienced' model user**