

Shell+Model Combinations for a data set

Bernhard Gottesbüren (BASF)

Use of different model + shell combinations for
Inverse Modelling with the same data set

Data set
PEST+PELMO
SUSE + PESTRAS
Results and Resume

Shell+Model Combinations for 1 data set

Description of the Data-set and shell+model

DATASET

- 4 lysimeters at site A (years 1-3)
- +
- 2 lysimeters at site B (years 4-5)

- same crop, same soil,
but
- different weather, different application rate

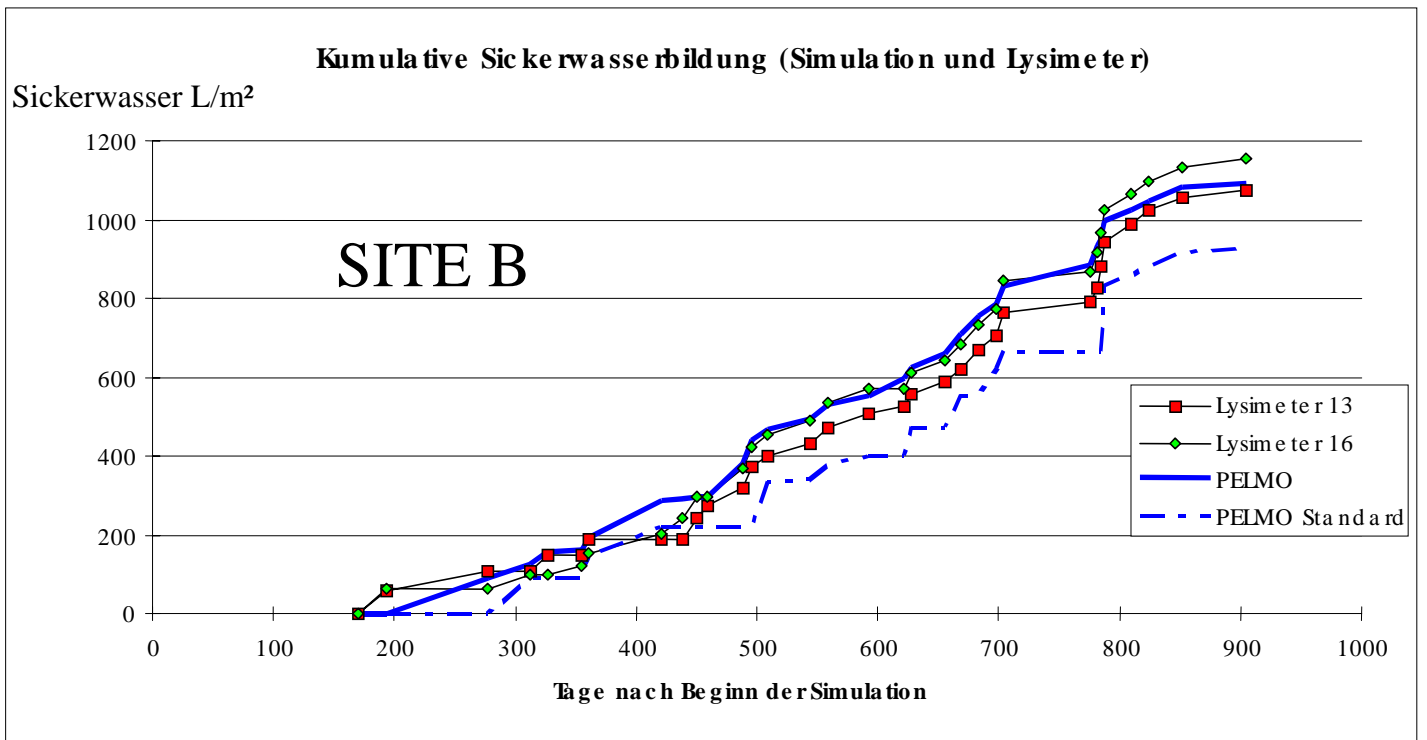
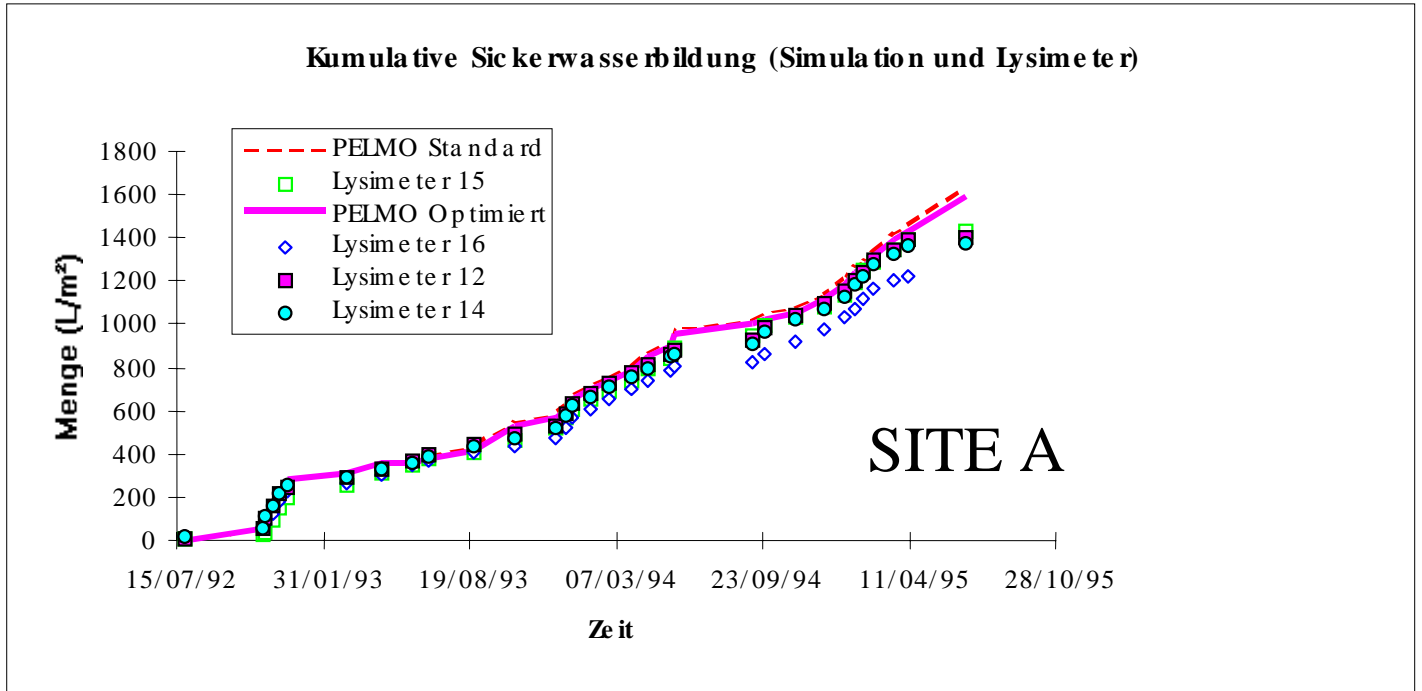
SHELL+MODEL COMBINATION

- PEST (Levenberg Marquardt) + PELMO 3.0

- SUSE (Simplex) + PESTRAS 3.1

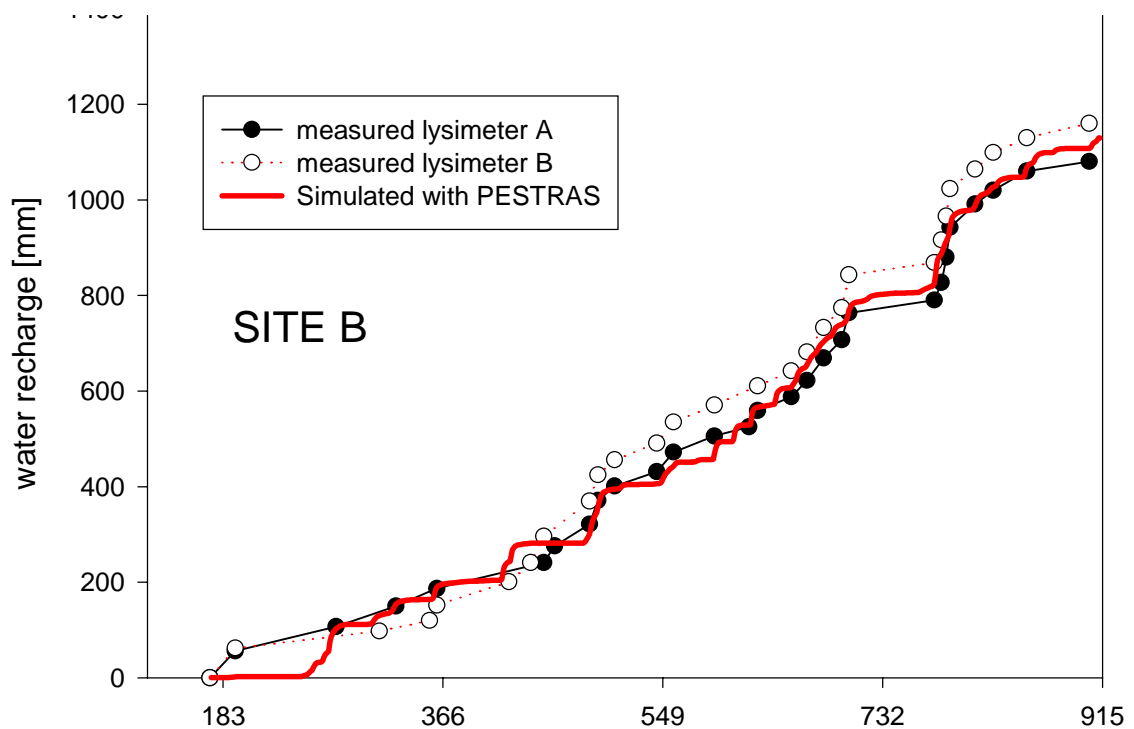
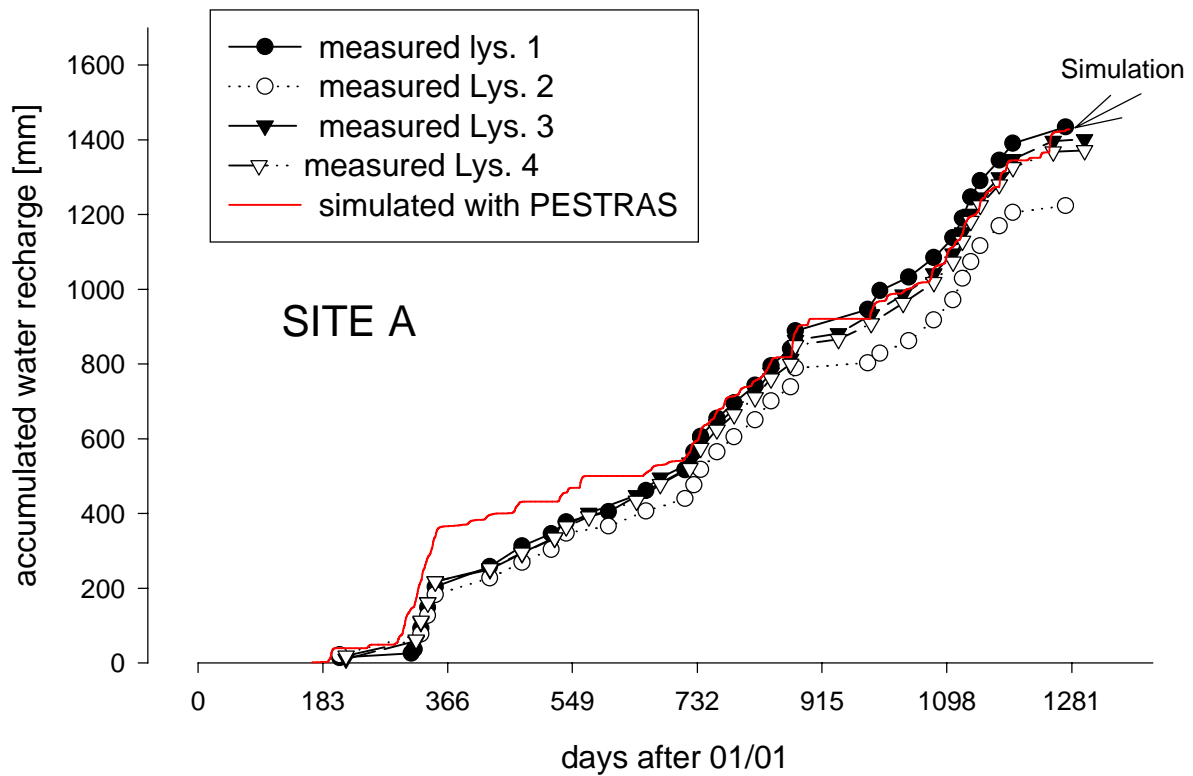
Shell+Model Combinations for 1 data set

Simulation of the water recharge with PELMO



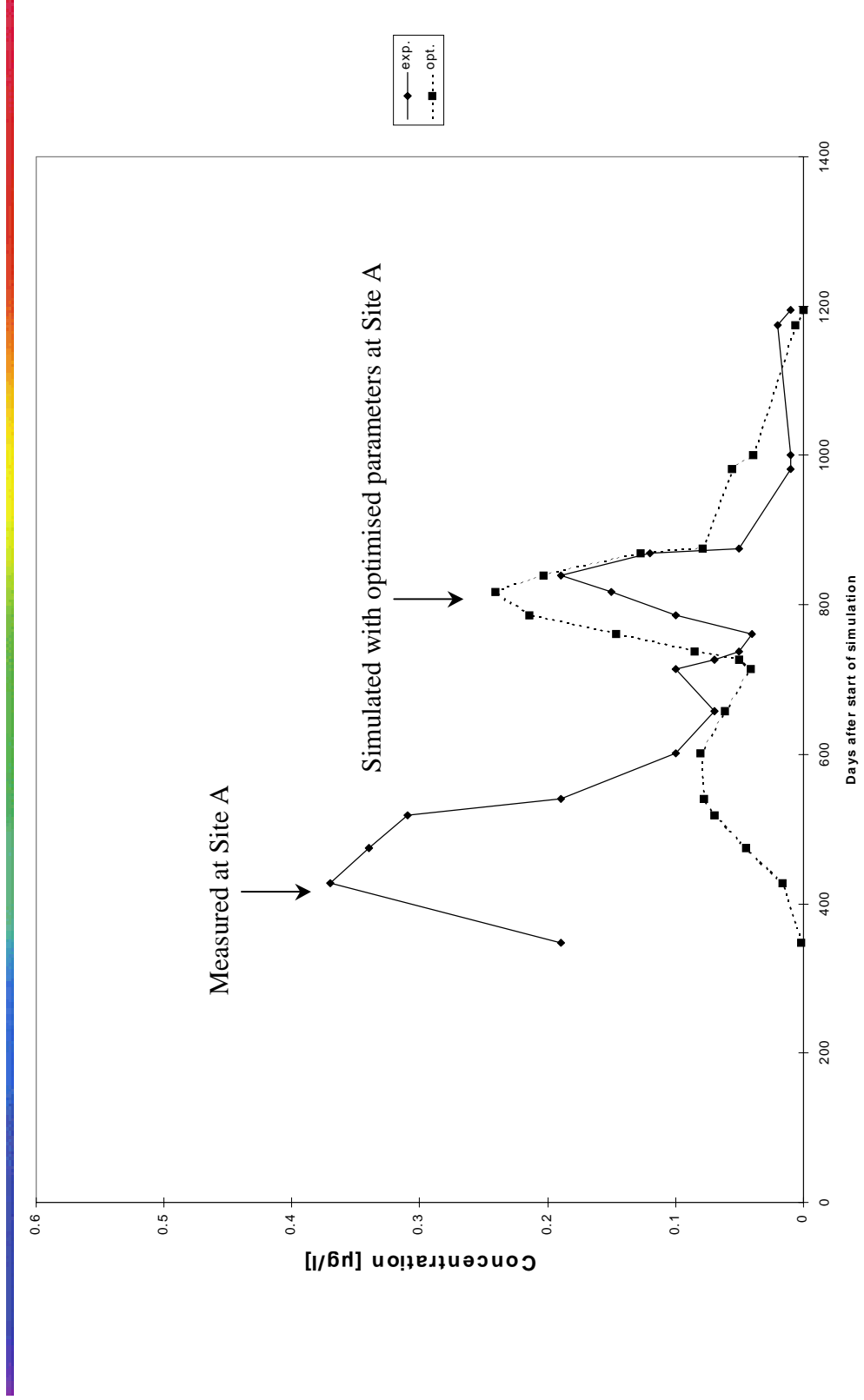
Shell+Model Combinations for 1 data set

Simulation of the water recharge with PESTRAS

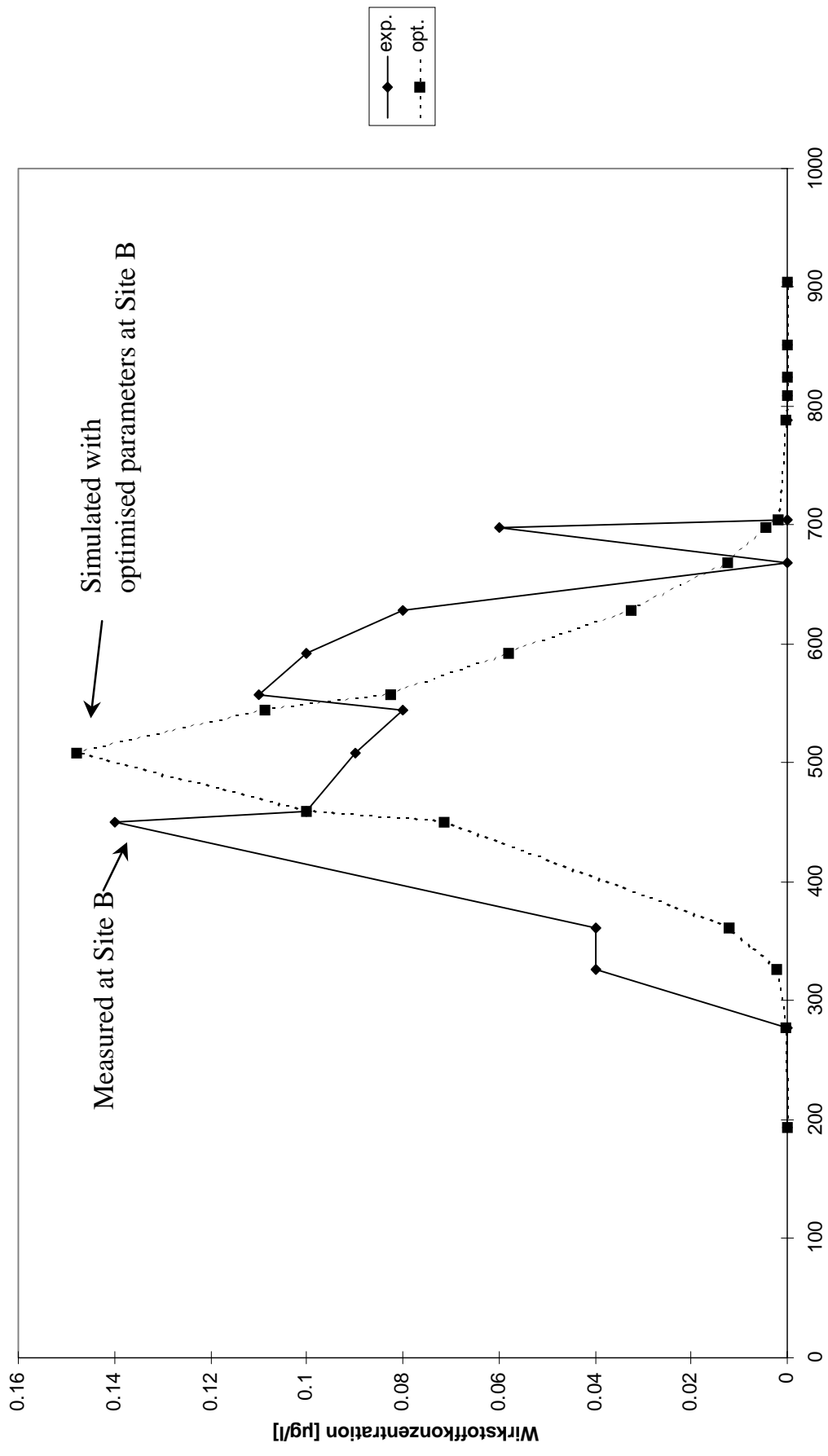


Shell+Model Combinations for 1 data set

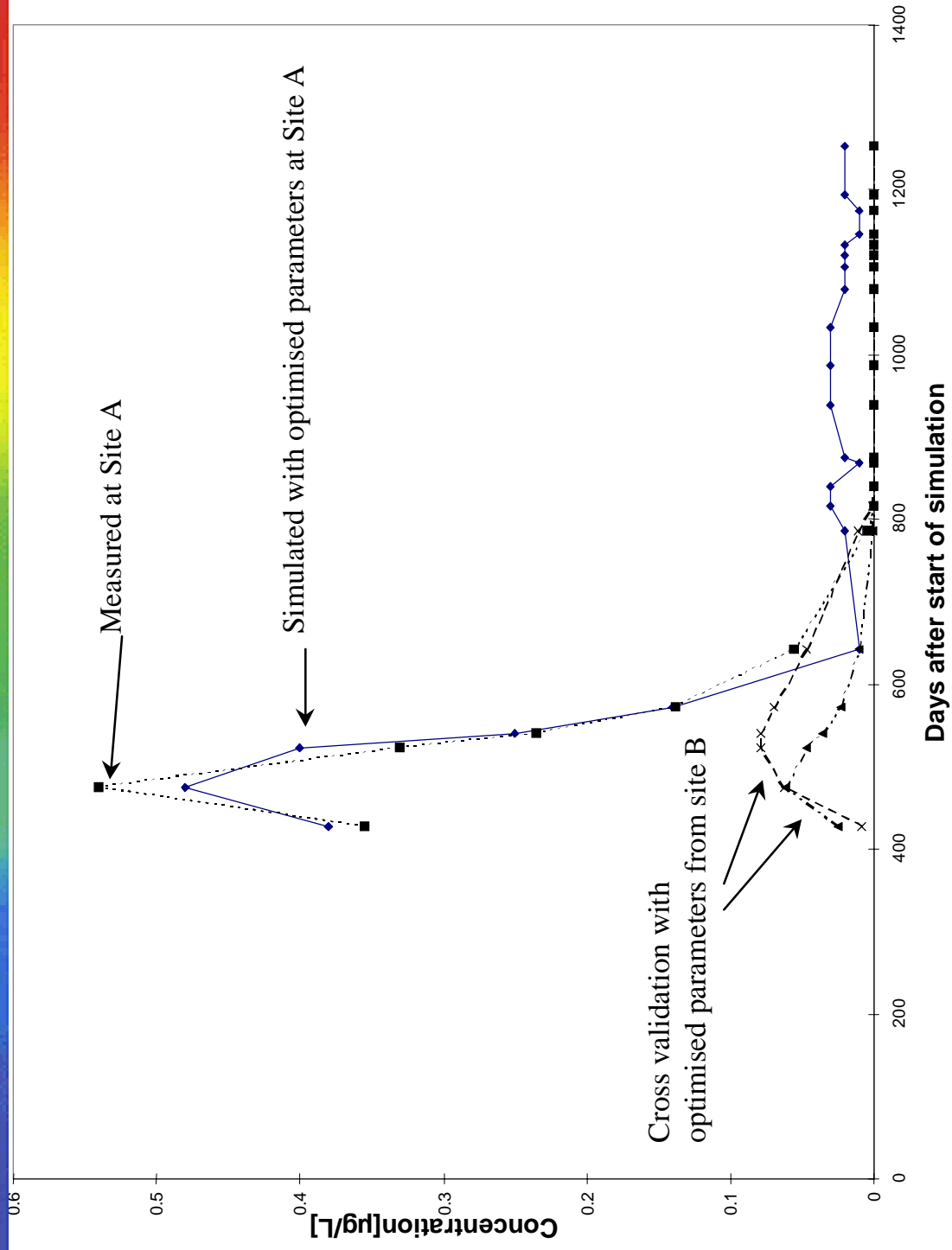
PEST + PELMO example 1



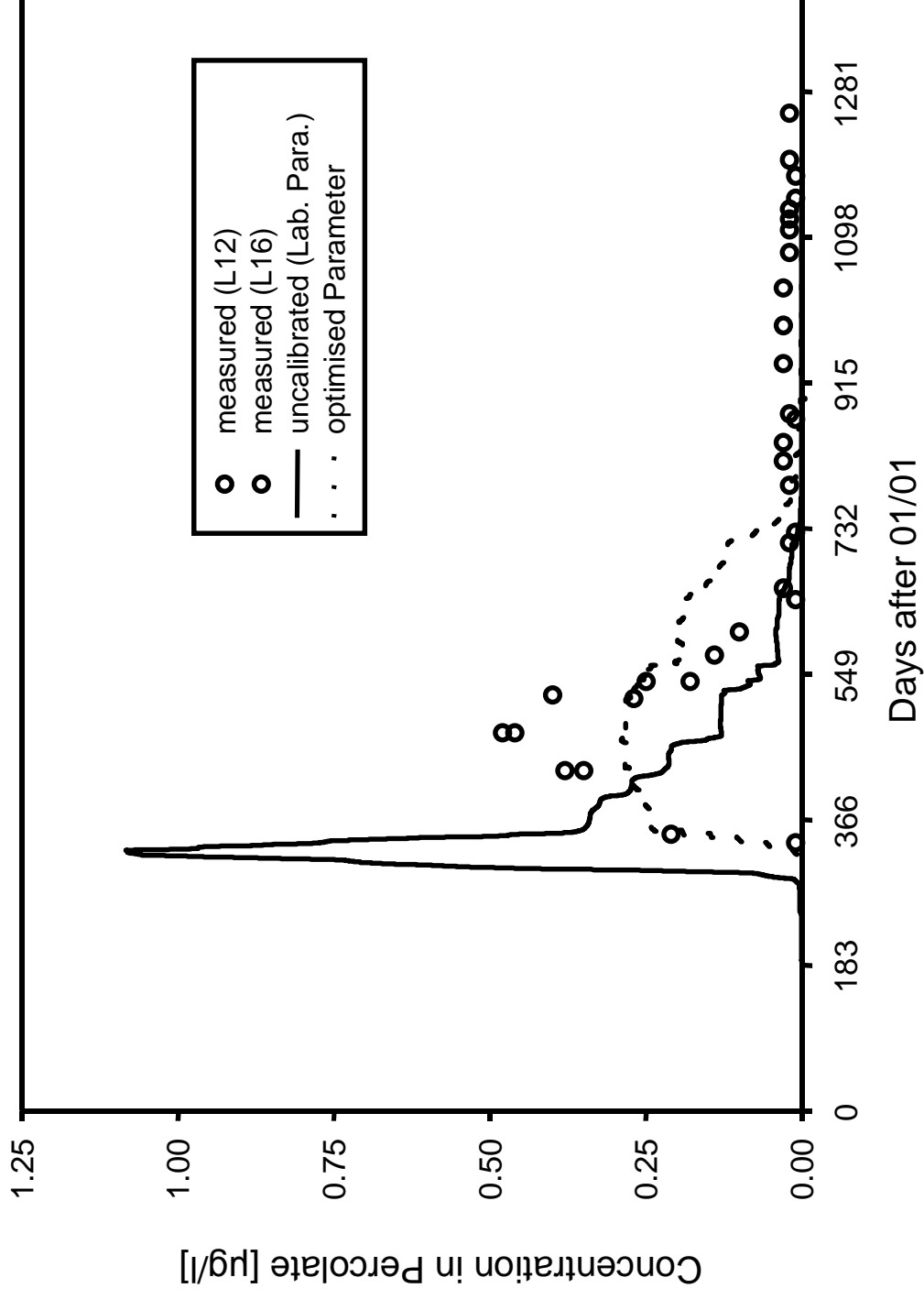
Shell+Model Combinations for 1 data set PEST + PELMO example 2



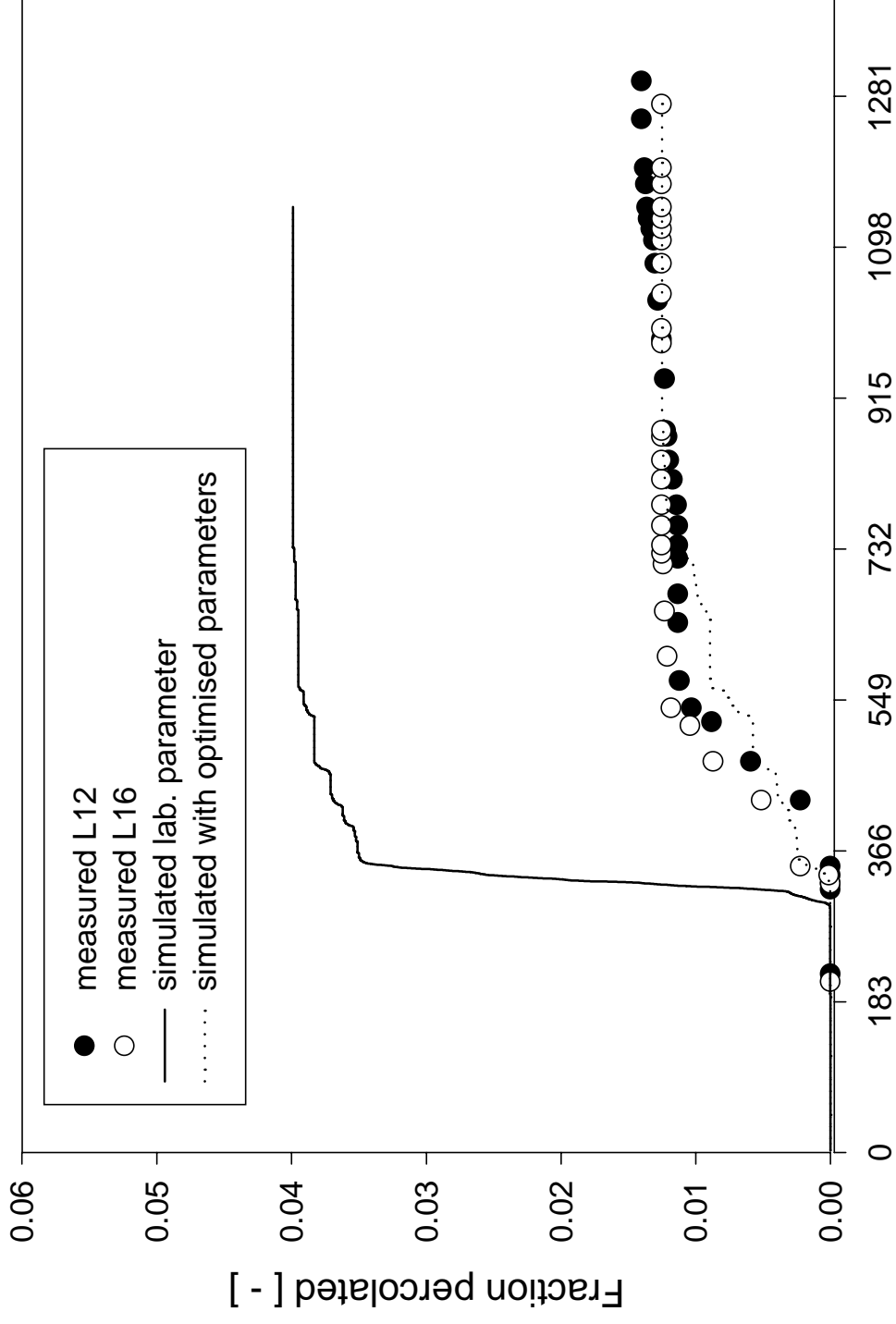
Shell+Model Combinations for 1 data set PEST + PELMO cross validation 2



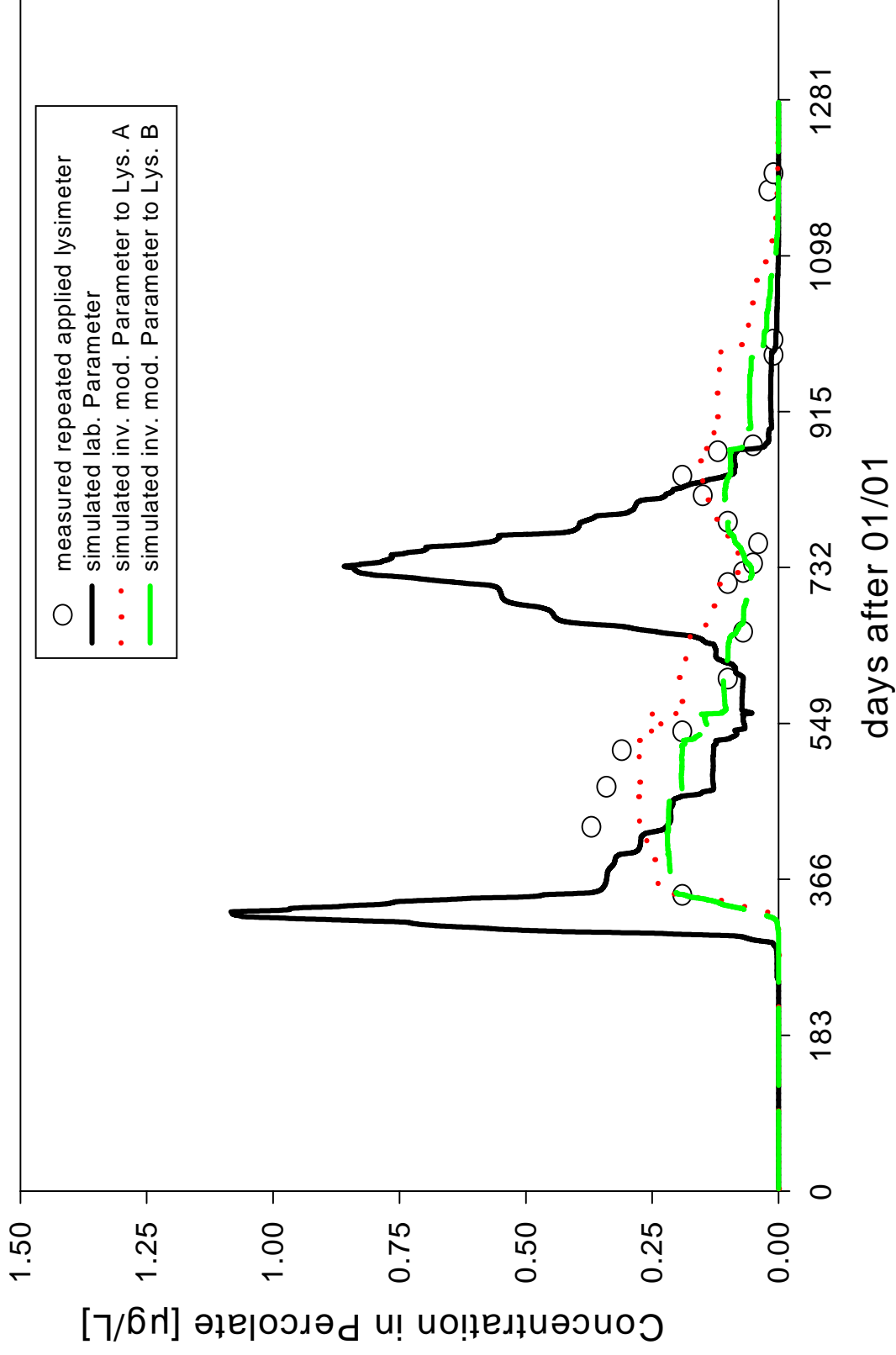
Optimisation Step (concentrations single applied lysimeter)



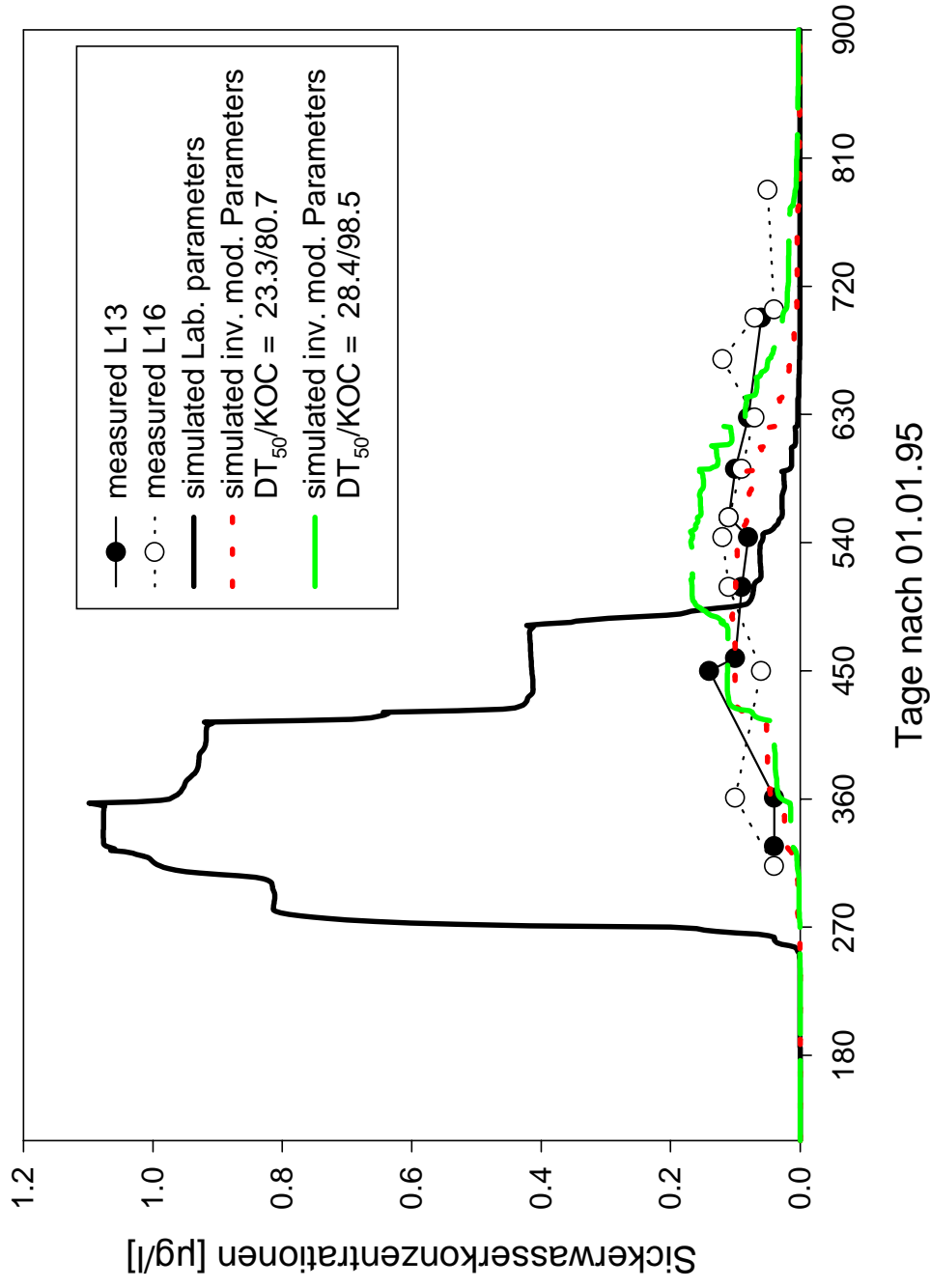
Optimisation Step (fraction percolated)



Validation Step (,independent' repeated applied lysimeter)




Example for a validation/extrapolation step of inverse modelled parameters



Shell+Model Combinations for 1 data set

PEST + PELMO vs. SUSE+PESTRAS optimised parameters



Parameter	DT50 [d]	K_{oc} [dm³/kg]
Laboratory Parameter	25	12
PESTRAS	23- 28	81-98
PELMO	17-28	11-22

Shell+Model Combinations for 1 data set

Resume simulations with PELMO

- At both experimental sites nearly identical KOC values but different DT50 were obtained
- Water recharge could be calibrated fairly well
- Optimised KOM-values were similar in all lysimeters but Optimised DT50-values were different
- In 50% of the studies the peak concentrations in the first recharge period could not be simulated correctly with PELMO
(although water percolation pattern seemed to be correct)
- Crossvalidation was only partially successful
- -> Problem to simulate exact breakthrough curves of reactive substances with capacity type of model
- > the required fine resolution of water transport on a daily basis can not be expected from a capacity model, (which on the other hand provides good prognoses of the long-term behaviour of pesticides)

Shell+Model Combinations for 1 data set

Resume simulations with PESTRAS

- Optimised DT50 are in the range of measured field DT50
- Optimised KOM are higher than measured K_{OM} Adsorption but equal to measured K_{OM} Desorption.
- The water recharge and the breakthrough of the compound could be simulated fairly well in all 6 lysimeter studies
- The laboratory parameter combinations were unsuitable
- The BTC of the compound in lysimeters at site B could be simulated very well with optimised parameters from site A