

Investigations on inverse modelling as a tool  
for estimating degradation and sorption  
parameters for pesticides

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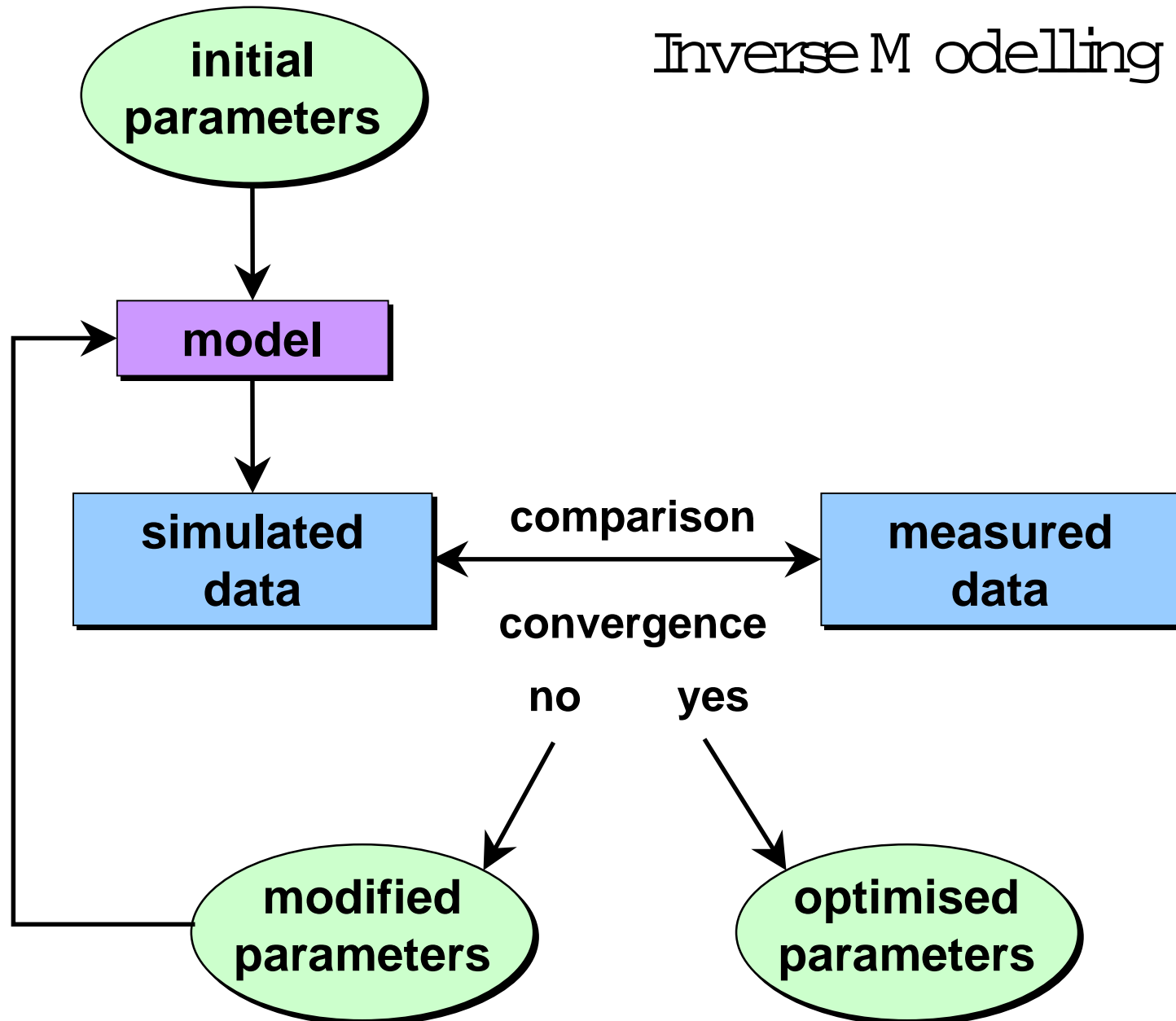
**Cranfield University**

**Silsoe, Bedford**

**UK**

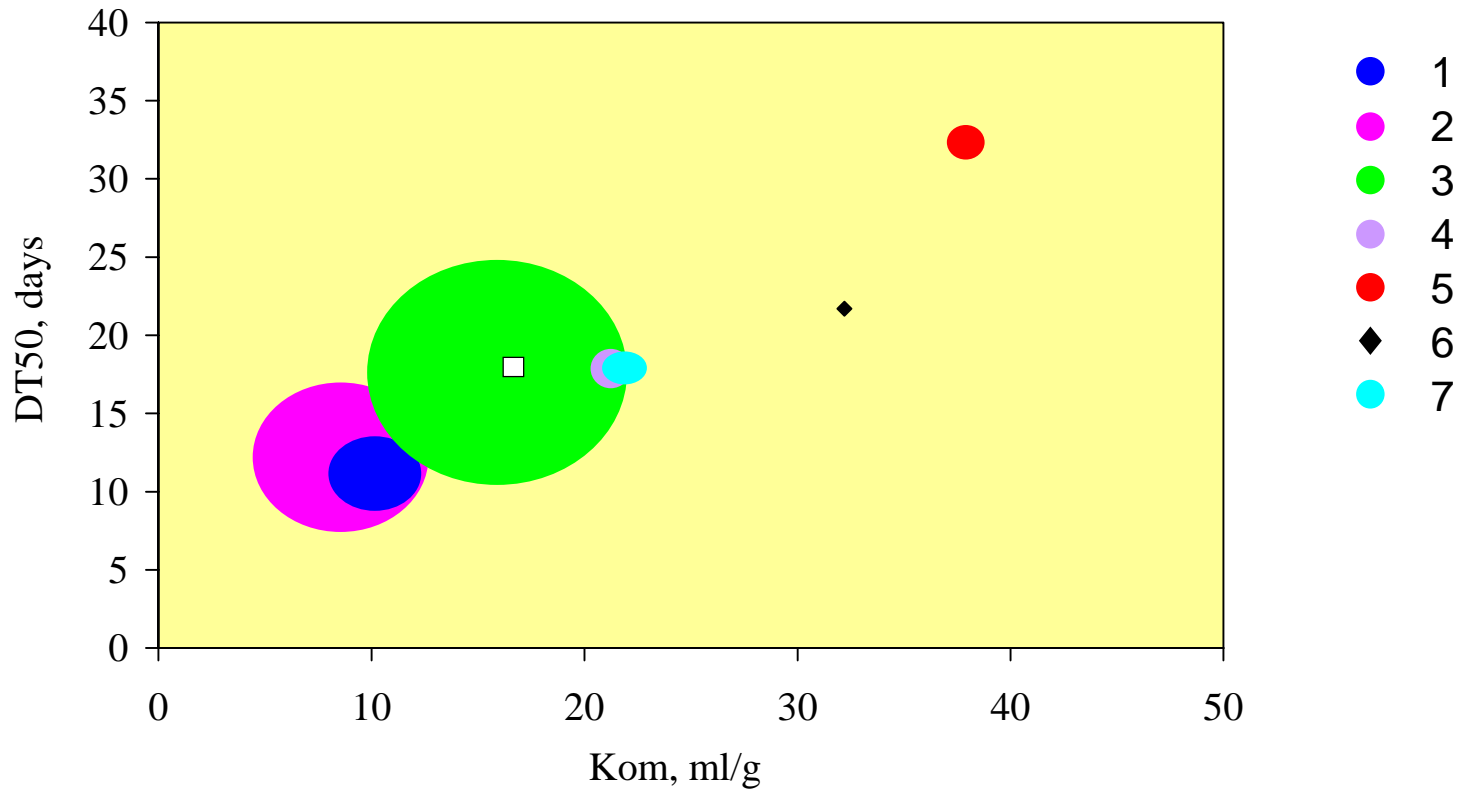


# Inverse Modelling

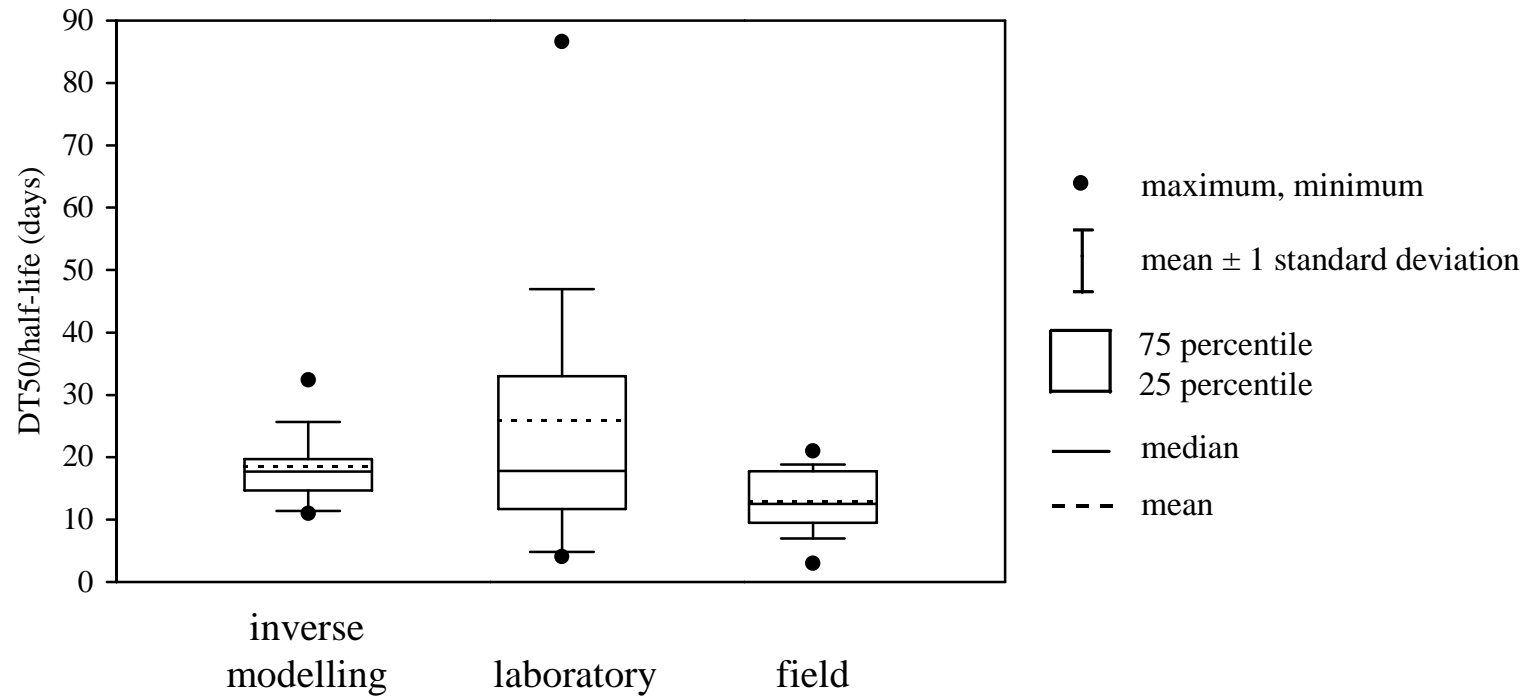


<b>Aim:</b>	<b>Estimation of DT50 and Kom values of a pesticide</b>
<b>Experimental data:</b>	<b>Leaching of the pesticide through seven undisturbed sandy loam soil lysimeters</b>
<b>Model:</b>	<b>PESTRAS 3.1.3</b>
<b>Starting values:</b>	<b>Median of 21 laboratory half-lives (17.8 days) Median of 11 experimental Kom values (16.4 ml g<sup>-1</sup>)</b>
<b>Inverse modelling package:</b>	<b>PEST, SUSE</b>

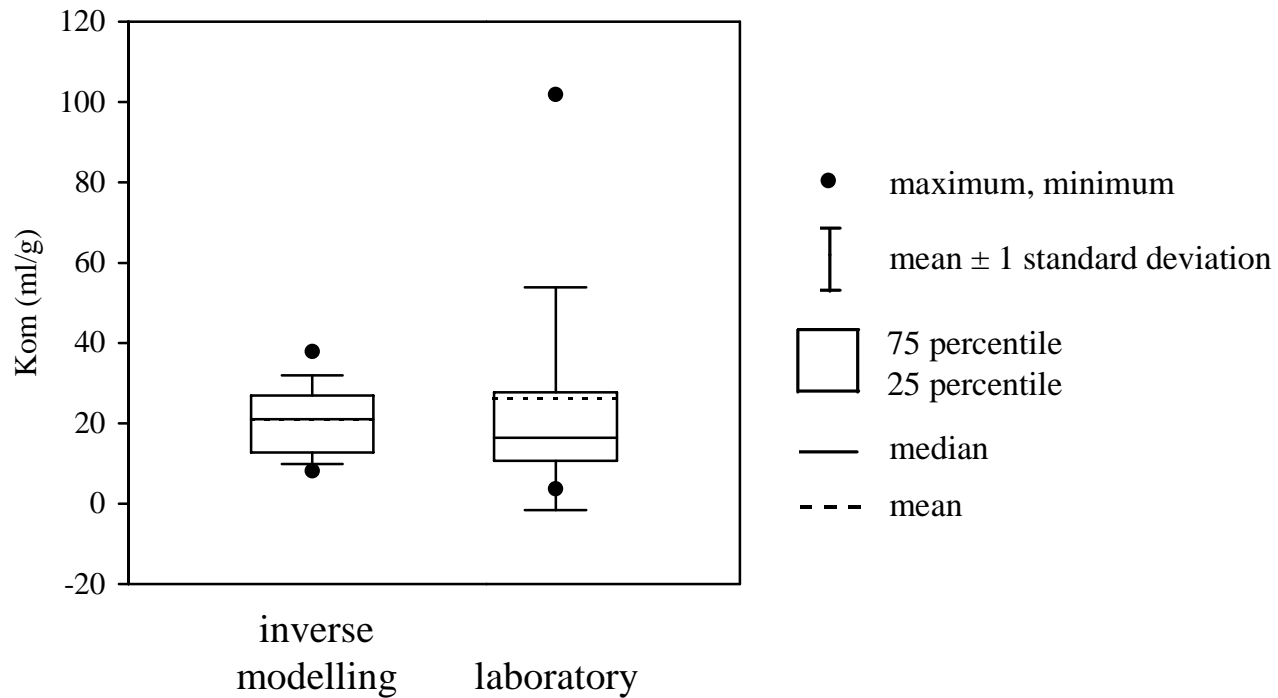
Combinations of  $K_{om}$  and DT50 values  
optimised by PEST  
(95% confidence intervals)



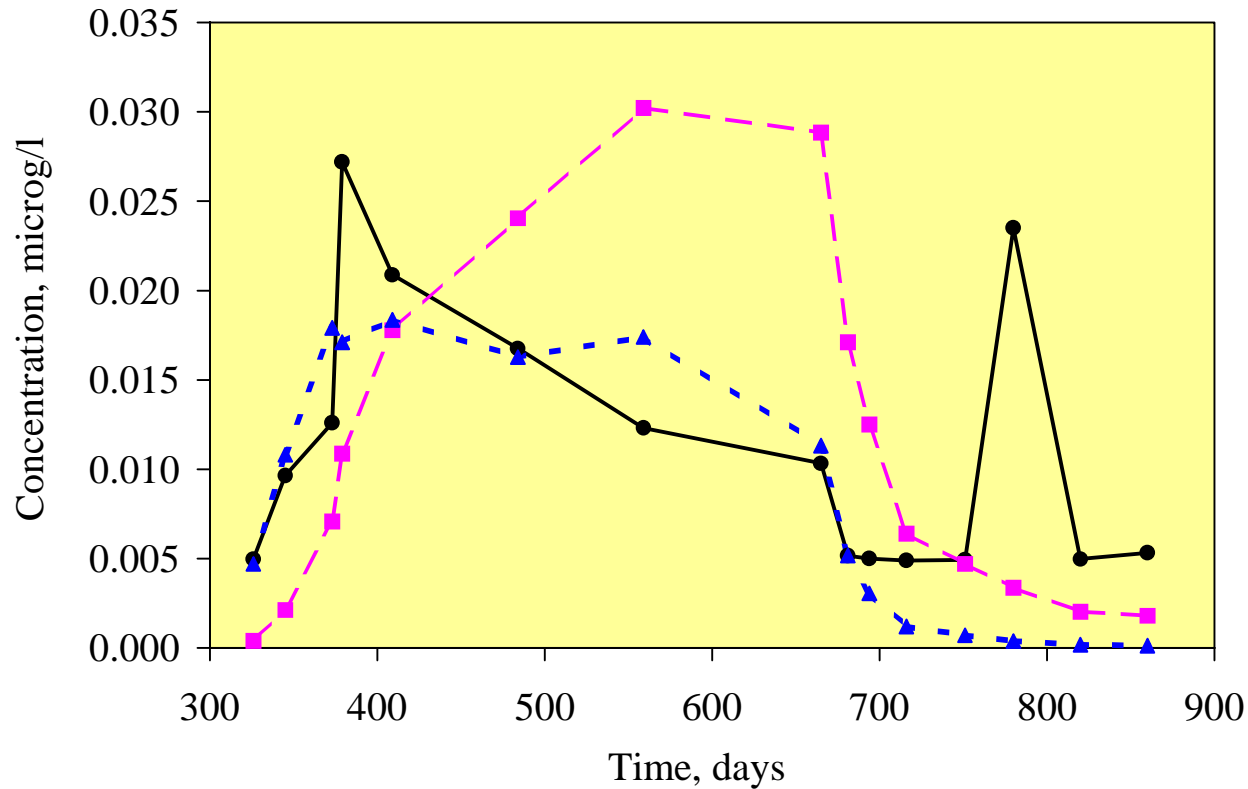
# Box & Whisker Plots of DT50 values



# Box & Whisker Plots of Kom values

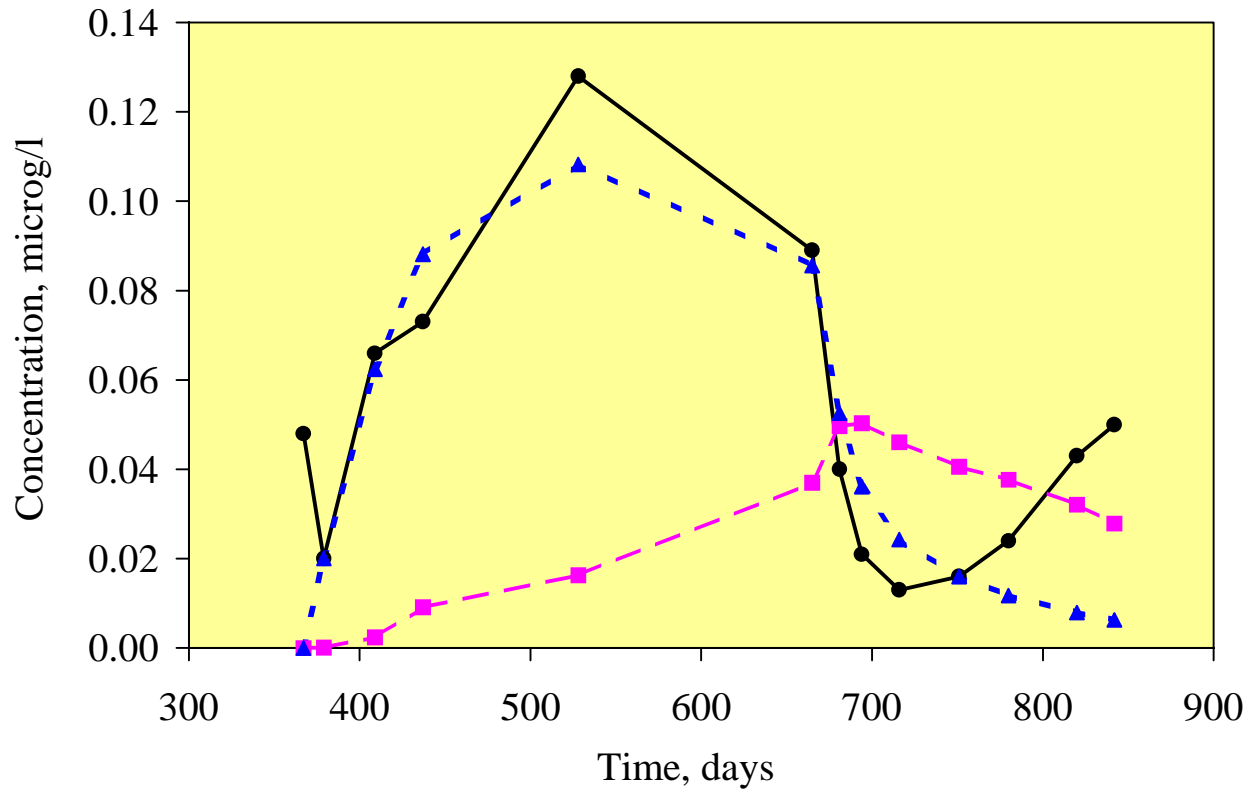


# Observed and simulated concentrations in leachate Lysimeter 1



—●— Observed values    -■- Initial Kom, DT50    -▲- Optimised Kom, DT50

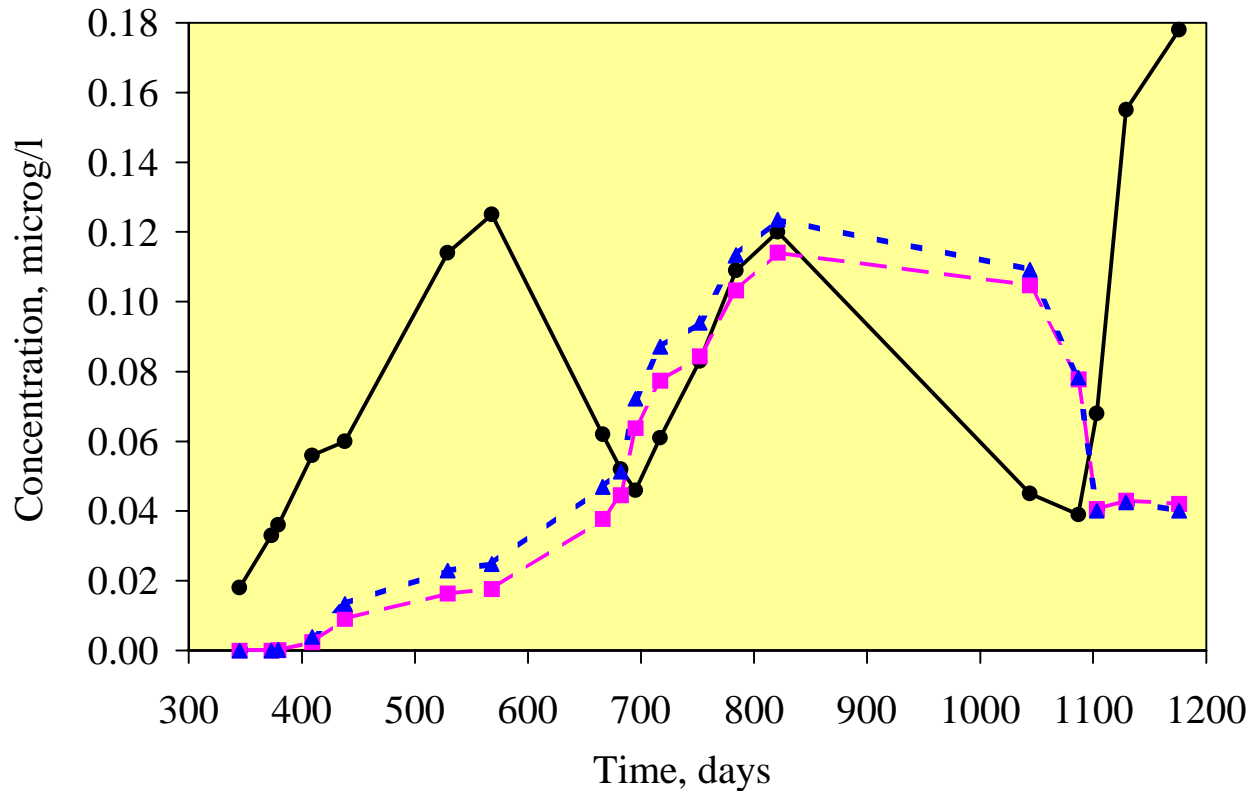
# Observed and simulated concentrations in leachate Lysimeter 2



—●— Observed values    -■- Initial Kom, DT50    -▲- Optimised Kom, DT50

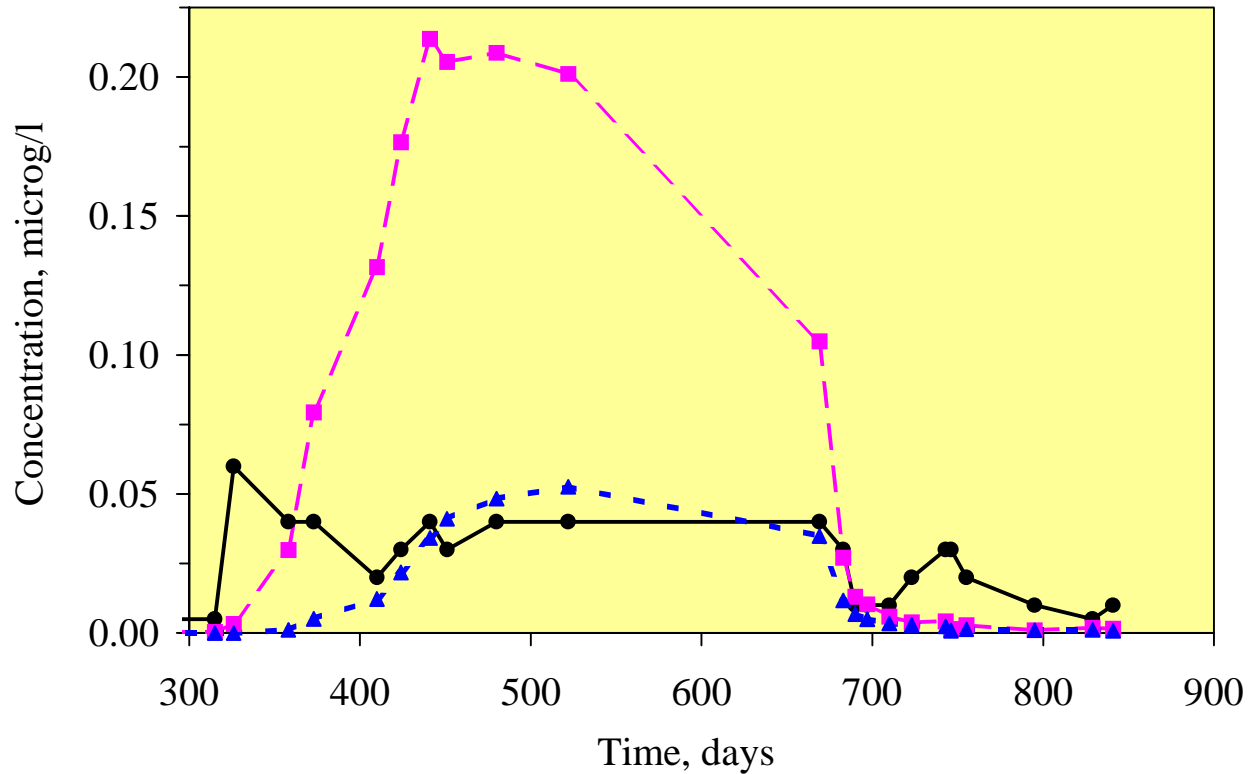


# Observed and simulated concentrations in leachate **Lysimeter 3**



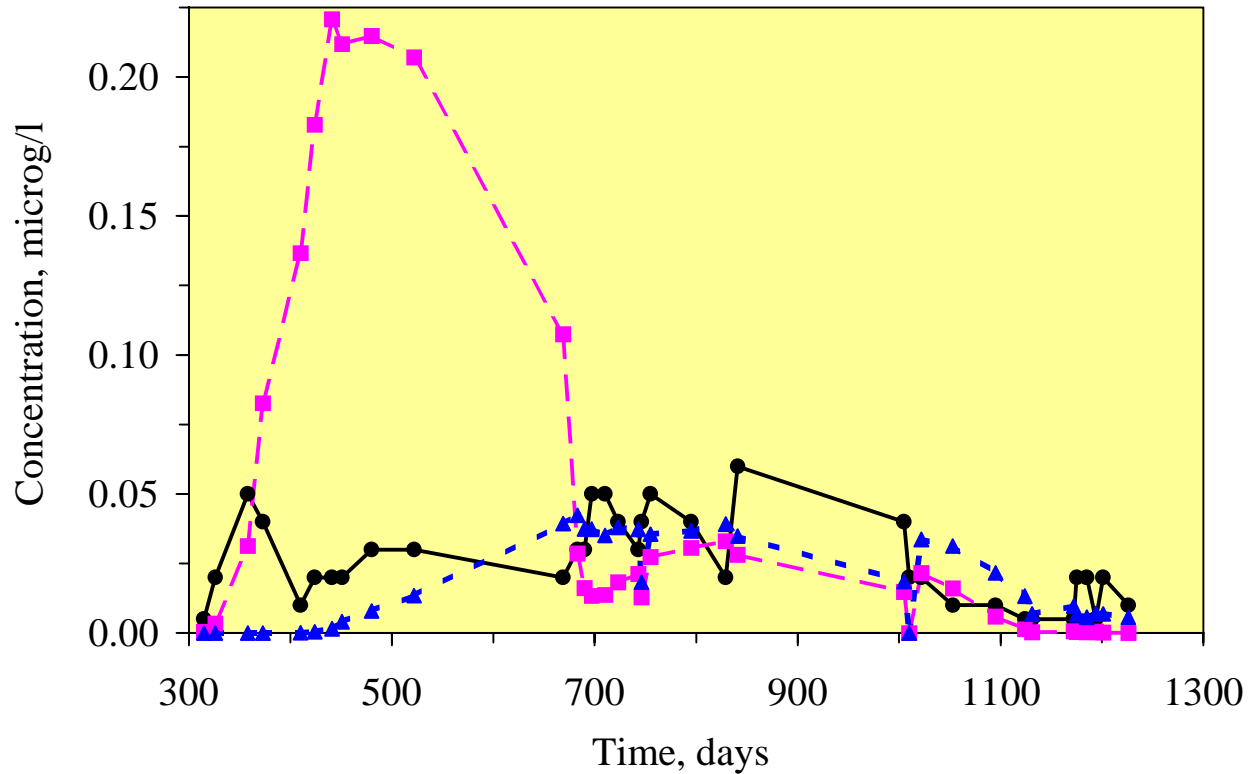
—●— Observed values    -■- Initial Kom, DT50    -▲- Optimised Kom, DT50

# Observed and simulated concentrations in leachate Lysimeter 4



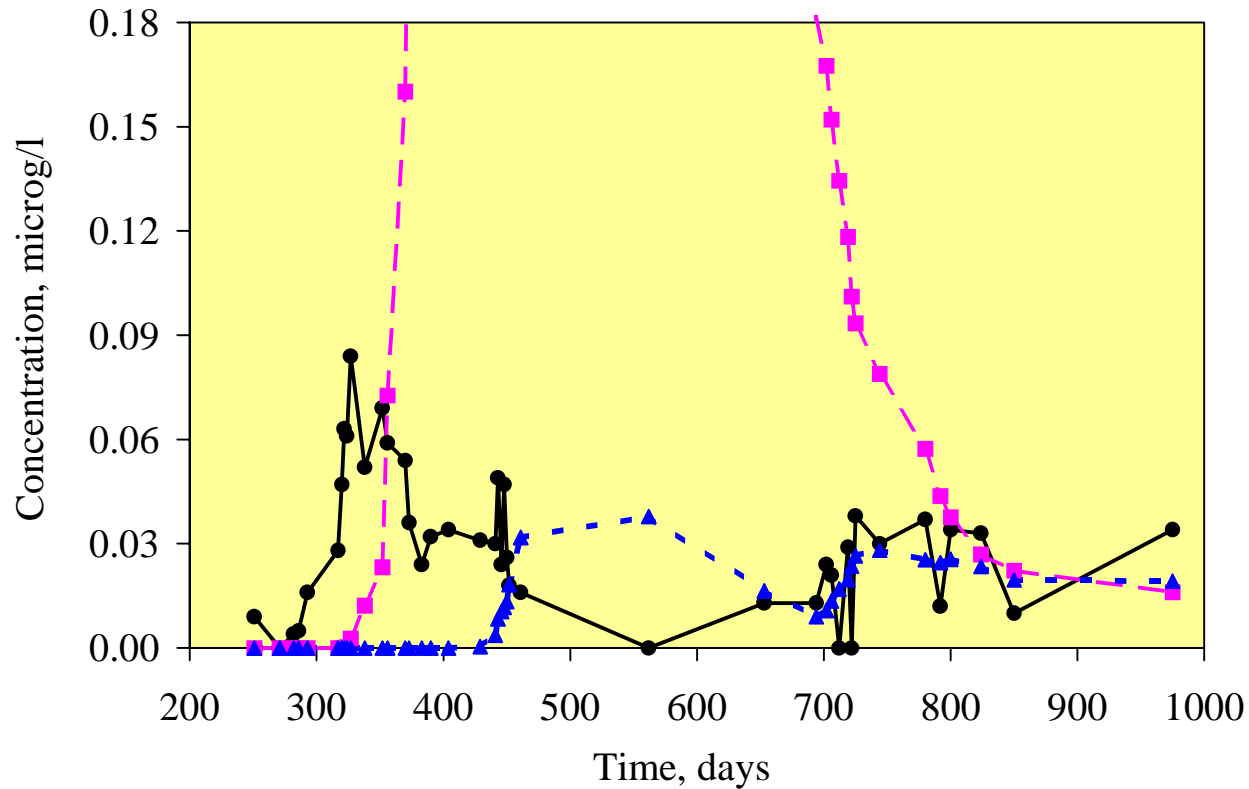
—●— Observed values    -■- Initial Kom, DT50    -▲- Optimised Kom, DT50

# Observed and simulated concentrations in leachate Lysimeter 5



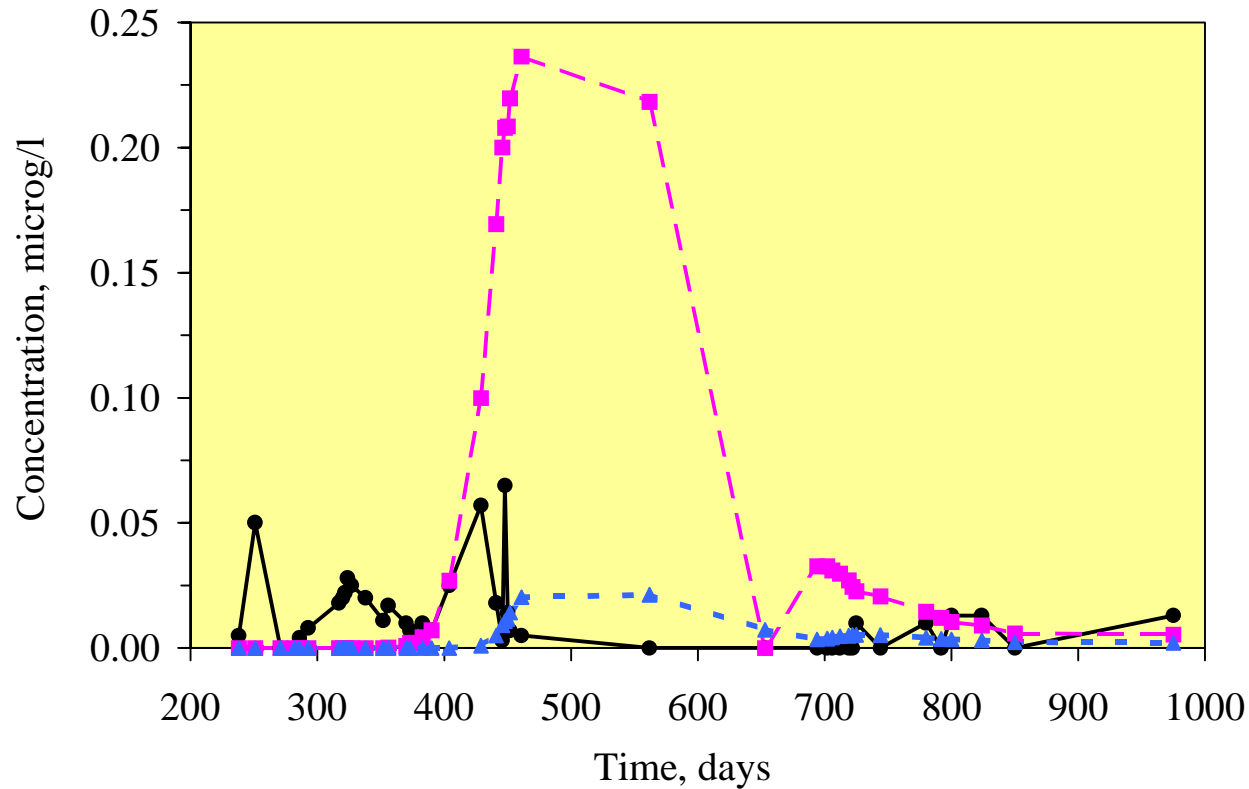
—●— Observed values    -■- Initial Kom, DT50    -▲- Optimised Kom, DT50

# Observed and simulated concentrations in leachate Lysimeter 6



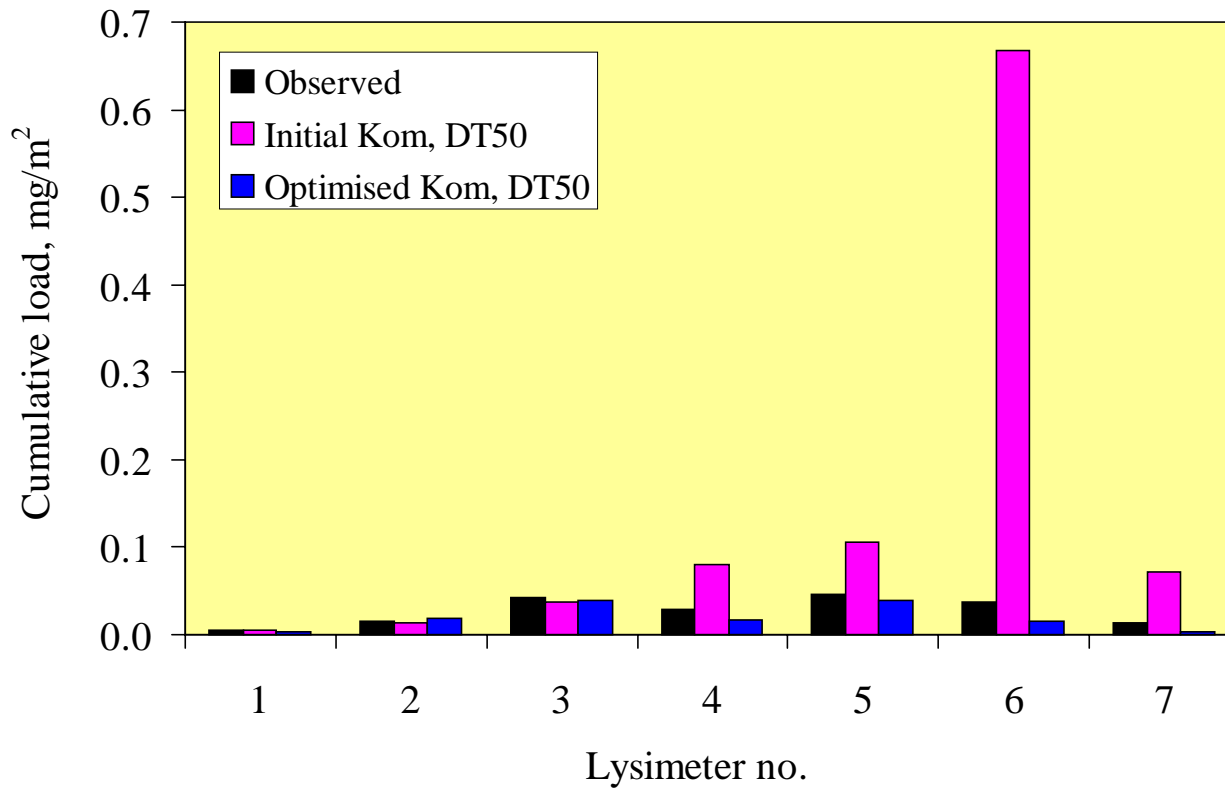
—●— Observed values    -■- Initial Kom, DT50    -▲- Optimised Kom, DT50

# Observed and simulated concentrations in leachate Lysimeter 7



—●— Observed values    —■— Initial Kom, DT50    -▲- Optimised Kom, DT50

# Cumulative loads



# Conclusions

- **PESTRAS failed to simulate pesticide leaching through the lysimeters on the basis of median laboratory  $K_{om}$  and DT50 values. Leaching was matched better for most lysimeters when individual  $K_{om}$  and DT50 values derived by inverse modelling were used.**
- **$K_{om}$  and DT50 values derived by inverse modelling were reasonable.**
- **The median of  $K_{om}$  and DT50 values derived by inverse modelling was not markedly different from that of experimental data, but the variability of inverse modelling results was smaller.**
- **Inverse modelling has the potential to provide pesticide sorption and degradation data relevant to the field situation.**