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

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Inverse Modelling

Initial parameters

Model

Simulated data

Comparison

Convergence

No

Yes

Modified parameters

Optimised parameters

Measured data
Aim: Estimation of DT50 and Kom values of a pesticide

Experimental data: Leaching of the pesticide through seven undisturbed sandy loam soil lysimeters

Model: PESTRAS 3.1.3

Starting values: Median of 21 laboratory half-lives (17.8 days)
Median of 11 experimental Kom values (16.4 ml g⁻¹)

Inverse modelling package: PEST, SUSE
Combinations of Kom and DT50 values optimised by PEST
(95% confidence intervals)
Box & Whisker Plots of DT50 values

- Maximum, minimum
- Mean ± 1 standard deviation
- 75 percentile
- 25 percentile
- Median
- Mean

Box plots for inverse modelling, laboratory, and field data.
Box & Whisker Plots of Kom values

- maximum, minimum
- mean ± 1 standard deviation
- 75 percentile
- 25 percentile
- median
- mean

Kom (ml/g)

inverse modelling laboratory
Observed and simulated concentrations in leachate

Lysimeter 1

<table>
<thead>
<tr>
<th>Time, days</th>
<th>Observed values</th>
<th>Optimised Kom, DT50</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.005</td>
<td>0.010</td>
</tr>
<tr>
<td>0.015</td>
<td>0.020</td>
<td>0.025</td>
</tr>
<tr>
<td>0.030</td>
<td>0.035</td>
<td>0.040</td>
</tr>
</tbody>
</table>
Observed and simulated concentrations in leachate

Lysimeter 2

- Observed values
- Initial Kom, DT50
- Optimised Kom, DT50
Observed and simulated concentrations in leachate

Lysimeter 3

![Graph showing concentration over time for observed and simulated values in Lysimeter 3.]
Observed and simulated concentrations in leachate

Lysimeter 4

![Graph showing observed and simulated concentrations in leachate for Lysimeter 4. The x-axis represents time in days, ranging from 300 to 900, and the y-axis represents concentration in microg/l, ranging from 0.00 to 0.20. The graph includes observed values, initial Kom, DT50, and optimised Kom, DT50.]
Observed and simulated concentrations in leachate

Lysimeter 5

![Graph showing observed and simulated concentrations](image)
Observed and simulated concentrations in leachate

Lysimeter 6

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- Observed values
- Initial Kom, DT50
- Optimised Kom, DT50
Observed and simulated concentrations in leachate

Lysimeter 7

![Graph showing observed and simulated concentrations over time.](image-url)
Cumulative loads

The diagram shows cumulative loads for different lysimeters. The y-axis represents the cumulative load in mg/m², ranging from 0 to 0.7. The x-axis indicates lysimeter numbers from 1 to 7. Three lines represent different conditions:

- Observed
- Initial Kom, DT50
- Optimised Kom, DT50

The observed load is the lowest, followed by initial Kom, DT50, and then optimised Kom, DT50. The load values are significantly higher for lysimeter 6.
Conclusions

- PESTRAS failed to simulate pesticide leaching through the lysimeters on the basis of median laboratory Kom and DT50 values. Leaching was matched better for most lysimeters when individual Kom and DT50 values derived by inverse modelling were used.

- Kom and DT50 values derived by inverse modelling were reasonable.

- The median of Kom 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.