Uncertainty Analysis of the GeoPEARL Pesticide Leaching Model

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The GeoPEARL model

- 1D-model describing the fate of pesticides in the soil-plant system
- Calculates drainage of pesticides into surface water and leaching to groundwater
- Applied at grid nodes to create spatial images
- Used to verify the Dutch Pesticide Authorisation procedure
GeoPEARL has many inputs, mainly soil, landuse, climate and hydrology.
Why uncertainty analysis of GeoPEARL?

- Authorities must know how accurate the results of the model are if these results are to be used in legislation and policy making
- Information about uncertainty can be used to take better decisions (i.e., risk analysis)
- It provides insight into how best to improve results or save costs without deteriorating the results
This study

- Considered only the propagation of uncertainty in soil and pesticide properties (for three characteristic pesticides, named A, B and D)
- Used a Monte Carlo simulation approach
- Also quantified the contribution of individual error sources to the output
- Model output is defined as the 90 percentile of the spatial distribution of the temporal median of the leaching concentration at 1m depth
Uncertain soil properties

For each horizon:

- Thickness – truncated normal, parameters derived from Soil Information System (SIS)
- Texture – triplet {clay-silt-sand}, truncated normal, parameters from SIS, cross-correlated
- Organic matter content – truncated lognormal, parameters from SIS
- Hydraulic conductivity – random sampling from Staring series per soil type
- Water retention characteristic – random sampling from Staring series per soil type
Uncertain pesticide properties

- Half-life of transformation in soil – lognormal, parameters from literature
- Coefficient of sorption on organic matter – lognormal, parameters from literature
Summary of Monte Carlo method

- Repeat many times (in our case 1000 times):
  - Simulate a possible reality from the probability distribution of the uncertain inputs
  - Run model with simulated input and store result
- Compute and report statistics of the stored results (e.g. mean, standard deviation, proportion that exceeds critical threshold)
Systematic spatial sample of 258 grid points

- Sampling error was considered negligible (but this was not checked!)
- At each point 1000 Monte Carlo runs of GeoPEARL
- Next 90 percentile (P90) of 258 GeoPEARL outputs computed for each of the 1000 runs
- Variability in the 1000 P90 values conveys uncertainty about true P90
Results: uncertainty in GeoPEARL output

- Large uncertainty in P90, particularly for substance A
- Box-plots all above regulatory limit of 0.1 $\mu$g·L$^{-1}$
- Reject all three pesticides with certainty
1000 Monte Carlo runs was sufficient.

\[
\text{var}(m_{P90}) = \frac{\sigma_{P90}^2}{N}
\]

\[
\text{var}(S_{P90}^2) = \frac{1}{N} \left( \frac{\tau_{P90}^4 - \sigma_{P90}^4 \cdot \frac{N - 3}{N - 1}}{N} \right)
\]

**Table 2**
Estimated mean and variance of P90 and associated sampling error standard deviations.

<table>
<thead>
<tr>
<th>Pesticide</th>
<th>Mean of P90 (µg/L) Mean</th>
<th>SD</th>
<th>Variance of P90 (µg/L)^2 Mean</th>
<th>SD</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>7.168</td>
<td>0.033</td>
<td>1.063</td>
<td>0.045</td>
</tr>
<tr>
<td>B</td>
<td>4.202</td>
<td>0.016</td>
<td>0.258</td>
<td>0.012</td>
</tr>
<tr>
<td>D</td>
<td>0.3922</td>
<td>0.0034</td>
<td>0.0119</td>
<td>0.0007</td>
</tr>
</tbody>
</table>
Including uncertainty causes a systematic shift in P90
What is the main source of error?

Percentage variance explained by uncertain inputs

<table>
<thead>
<tr>
<th>Substance</th>
<th>Organic matter</th>
<th>Other soil properties</th>
<th>Half-life</th>
<th>Sorption</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance D</td>
<td>0</td>
<td>0</td>
<td>60</td>
<td>20</td>
</tr>
<tr>
<td>Substance A</td>
<td>7</td>
<td>1</td>
<td>54</td>
<td>41</td>
</tr>
<tr>
<td>Substance B</td>
<td>7</td>
<td>0</td>
<td>87</td>
<td>10</td>
</tr>
</tbody>
</table>
Conclusions

- Uncertainty in 90 percentile of the spatial distribution of pesticide leaching concentration is very large.
- However, when the regulatory limit of 0.1 µg·L⁻¹ is used, then uncertainty does not impair decision-making.
- Pesticide properties (notable the half-life) are a much greater source of uncertainty than soil properties.
- Accuracy improvement of GeoPEARL output must be achieved by reducing the uncertainty about pesticide properties.
- Reducing uncertainty about pesticide properties is difficult because this requires extensive experiments and modelling of the interaction between soil and pesticides.
Thank you