From lower to higher tiers in the assessment of pesticide leaching to GW: a case study

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PLO548 project

- Aim: To assess the feasibility of using probabilistic approaches for assessing pesticide exposure within the context of pesticide registration

- Objectives of phase I:
  - To characterise uncertainty in pesticide fate modelling
  - To investigate the robustness of Monte Carlo approaches
  - To prepare case studies which demonstrate the use of probabilistic approaches
PLO548 outputs


Probabilistic approaches to pesticide fate modelling: a case study
Case study

- Aim: demonstrate the applicability of probabilistic approaches to a GW assessment
  - Atrazine (Syngenta kindly provided some of their data)
  - Increasing complexity, from FOCUS through Monte Carlo modelling to scenario-based modelling
  - PEARL and MACRO simulations
  - FOCUS: use of three combinations of Koc / DT50 + use of different application dates
  - MC: based on the worst-case FOCUS scenario
  - Scenario-based modelling: first step towards integrating the diversity of environmental conditions at the national level

FOCUS modelling

80th concentrations predicted by PEARL for the four scenarios relevant to UK conditions

<table>
<thead>
<tr>
<th>Scenario</th>
<th>80th percentile concentration (µg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Châteaudun</td>
<td>0.084</td>
</tr>
<tr>
<td>Hamburg</td>
<td>0.041</td>
</tr>
<tr>
<td>Kremsmünster</td>
<td>0.060</td>
</tr>
<tr>
<td>Okehampton</td>
<td>0.206</td>
</tr>
</tbody>
</table>
### Better case, worse case

<table>
<thead>
<tr>
<th></th>
<th>Koc</th>
<th>Field DT50</th>
</tr>
</thead>
<tbody>
<tr>
<td>Median case</td>
<td>50th percentile</td>
<td>91.5 ml/g</td>
</tr>
<tr>
<td></td>
<td>50th percentile</td>
<td>43 days</td>
</tr>
<tr>
<td>Better case</td>
<td>75th percentile</td>
<td>116 ml/g</td>
</tr>
<tr>
<td></td>
<td>25th percentile</td>
<td>29 days</td>
</tr>
<tr>
<td>Worse case</td>
<td>25th percentile</td>
<td>79 ml/g</td>
</tr>
<tr>
<td></td>
<td>75th percentile</td>
<td>60 days</td>
</tr>
</tbody>
</table>

### Refined FOCUS modelling

(multiple combinations of Koc and DT50)

80th concentrations predicted by PEARL for the four scenarios relevant to UK conditions for three combinations of Koc and DT50

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Better case</th>
<th>Median case</th>
<th>Worse case</th>
</tr>
</thead>
<tbody>
<tr>
<td>Châteaudun</td>
<td>&lt;0.001</td>
<td>0.084</td>
<td>1.307</td>
</tr>
<tr>
<td>Hamburg</td>
<td>&lt;0.001</td>
<td>0.041</td>
<td>0.597</td>
</tr>
<tr>
<td>Kremsmünster</td>
<td>&lt;0.001</td>
<td>0.060</td>
<td>0.815</td>
</tr>
<tr>
<td>Okehampton</td>
<td>0.001</td>
<td>0.206</td>
<td>1.903</td>
</tr>
</tbody>
</table>
Influence of the application date

- Aim: investigate the influence of the application date considered on FOCUS predictions
- Base case: application 7 days after emergence
- Application varied between emergence and emergence + 15 days (+ or – 7 days compared to base case)

Refined FOCUS modelling (variation of application date)
Monte Carlo modelling

- Based on the 20-year PEARL predictions for the Okehampton scenario (worst-case scenarios)
- Data for Koc and DT50 available (20 and 61 values, respectively)
- PDF fitting exercise. Triangular distributions used in the end
- MC analysis with 500 runs repeated 10 times with different seed numbers
Monte Carlo modelling

Monte Carlo modelling: pros and cons

- Monte Carlo modelling
  - Is widely used in other fields of science
  - Helpful for considering the uncertainty in modelling predictions resulting from that in pesticide properties

- Not informative about the relevance of the scenario used
- Numerous subjective choices involved
- Repeatability issues
- Does not move the regulatory process significantly forward
Scenario-based modelling

- The aim is to provide a relatively simple framework which reflects the diversity in soils and climate at the national scale
- 4 soil and 4 climate scenarios
- 30-year simulations with MACRO
- Results for individual scenarios are weighted according to the abundance of the scenario across England & Wales
- Three combinations of Koc and DT50 used (first-step towards accounting for the variability in Koc and DT50)

Climatic scenarios

- Average annual rainfall
- Wheat growing area
Definition of representative soil series

Rep. Soil 1 7%
Rep. Soil 2 16%
Rep. Soil 3 15%
Rep. Soil 4 9%
Rep. Soil 5 4%
Rep. Soil 6 3%
Not relevant 46%
Scenario-based modelling

Example of intermediate results

Simulations for the Ludford representative soil series

Scenario-based modelling

Weighting of results

- Extracting of 30-year average concentrations of atrazine in leaching for each of the 48 scenarios simulated
- Weighting according to the abundance of the scenario in the E&W landscape

<table>
<thead>
<tr>
<th>Soil type</th>
<th>Extent of soil within each climatic scenario (%)</th>
<th>Total extent (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>&lt;625 mm AAR</td>
<td>625-750 mm AAR</td>
</tr>
<tr>
<td>Not overlying aquifers</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Not vulnerable a</td>
<td>0.7</td>
<td>2.9</td>
</tr>
<tr>
<td>Enborne</td>
<td>0.7</td>
<td>1.3</td>
</tr>
<tr>
<td>Hall</td>
<td>0.2</td>
<td>0.8</td>
</tr>
<tr>
<td>Cudmorey</td>
<td>0.2</td>
<td>1.3</td>
</tr>
<tr>
<td>Ludford</td>
<td>0.8</td>
<td>4.1</td>
</tr>
<tr>
<td>Total</td>
<td>2.6</td>
<td>10.3</td>
</tr>
</tbody>
</table>

Impermeable or peaty soils

- Derivation of cumulative distribution charts
Scenario-based modelling

Final results

- Better case
- Median case
- Worse case

Scenario-based modelling: pros and cons

- Covers the full range of vulnerability at a large scale
- Computational effort compatible with the use of MACRO
- Provides useful additional information
- Does not account for the variability in pesticide properties (although a simple approach to do this was demonstrated)
- Subjectivity in the selection of the scenarios
### Where to from there? (1/3)
#### Higher tier & uncertainty

- Spatially distributed modelling on a “pixel base”
  - GeoPEARL, GeoPELMO-type work
  - Higher tier or first tier? Still is an assessment of chromatographic leaching to groundwater on the basis of concentrations in soil
- Uncertainty: uncertainty in pesticide properties could be accounted for routinely
- Are we ready to face the consequences? (e.g. red spots and their consequences on land value)
- Towards more relevance of environmental fate predictions in the overall risk assessment (GW and SW)

### Where to from there? (2/3)
#### Higher tier

- Possible refinement: be more realistic & move beyond the one-metre depth
  - Use of models which can simulate the fate of pesticides from the soil surface to and in the groundwater (in the root zone - unsaturated zone - saturated zone continuum)
  - MARTHE refined as part of the PEGASE project
  - Very similar to any root zone model for the soil part
  - Blind modelling (dilution or attenuation in the unsaturated and saturated zones), site-specific modelling (explain detections/concentrations in the GW or in springs), GW vulnerability mapping, scenario-based modelling
Where to from there? (3/3)

Uncertainty

- We need to:
  - account for the uncertainties we can reasonably easily account for (e.g. pesticide properties)
  - Know about the more subtle uncertainties that are always ignored in our modelling (modeller subjectivity, model selection, model parameterisation, etc.)
    - Research perspective
    - Decision-making perspective
- Uncertainty and variabilities can have a major influence on risk assessment results: let's deal with them!