European Scenarios for Exposure of Soil Organisms to Plant Protection Products

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Work done by the Working group
Persistence in Soil/fate

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Background

• Generally excepted European scenarios for exposure of soil organisms not available

• There is a need for such scenarios: ongoing discussion in PRAPer on PEC_{soil}

• Development of tiered exposure assessment approaches for soil organisms in which scenarios play an important role
End points for the assessment: which ERC?

• First step in exposure assessment: identify which type of concentration gives best correlation to effect.

• This is the Ecotoxicologically Relevant Concentration (ERC)

• Ecotox workgroup delivered two types of ERCs:
  – Concentration in total soil (mg kg\(^{-1}\))
  – Concentration in the liquid phase (mg l\(^{-1}\))
  – Averages over soil layers of different depths
End points for the assessment: which percentile?

• Target defined by risk managers: 90\textsuperscript{th} percentile concentration in a number of climatic zones

• Practical considerations: The overall 90\textsuperscript{th} percentile concentration within the three regulatory zones proposed in the new Regulation concerning the placing of PPPs on the market
The regulatory zones

- Good general correspondence with climatic zones
- Only anomaly: Denmark, which has a Central European climate
What is the 90th spatial percentile?
Scenarios for annual crops and conventional tillage

• Largest surface area and most PPP applications, so good starting point

• Ploughing depth: 20 cm

• EFSA ecotox workgroup defined following types of ERC:
  – concentration in total soil (CT) and in pore water (CL)
  – averages over layers 0-1, 0-2.5, 0-5 and 0-20 cm
Tiered assessment scheme for annual crops and conventional tillage

Core of presentation (development of Tier-4 scenarios approximately the same)

1. Conservative scenarios for analytical model (arable land and all substances)
2. Realistic worst-case scenarios for numerical models (arable land and all substances)
3. Crop- and/or substance specific scenarios for analytical model
4. Crop- and/or substance specific scenarios for numerical models

Two parallel schemes: One for each ERC
Procedure for deriving Tier-2 scenarios: a systematic approach

1. Data compilation
2. Selection of model for vulnerability mapping
3. Derivation of the target spatial percentile with consideration of uncertainty about pesticide properties and soil properties
4. Selection of scenarios that meet the target spatial percentile for multiple pesticides
5. Scenario parameterization
6. Simulation with the comprehensive fate models (e.g. PEARL and PELMO)

End-points:
Overall 90th percentile of the concentration in total soil and the concentration in the liquid phase
Data compiled by JRC at a resolution of 1x1 km²:

- EU-Soil map
- Topsoil organic matter
- Climatic data from WorldClim (temperature and precipitation)
- Corine land use data
Selection of model for vulnerability mapping

Development

- Data compilation
- Selection of model for vulnerability mapping
- Derivation of the target spatial percentile with consideration of uncertainty about pesticide properties and soil properties
- Selection of scenarios that meet the target spatial percentile for multiple pesticides
- Scenario parameterization
- Simulation with the comprehensive fate models (e.g. PEARL and PELMO)
- End-points: Overall 90th percentile of the concentration in total soil and the concentration in the liquid phase
What is vulnerability mapping?

- Vulnerability maps can be used to find locations where the concentration is equal to a certain spatial percentile.

Absolute concentration versus vulnerability score (zone South)

<table>
<thead>
<tr>
<th>Concentration in total soil (mg/kg)</th>
<th>Vulnerability score (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non arable</td>
<td>Non arable</td>
</tr>
<tr>
<td>&lt; 2.5</td>
<td>0 - 20</td>
</tr>
<tr>
<td>2.5 - 3.5</td>
<td>20 - 40</td>
</tr>
<tr>
<td>3.5 - 4.5</td>
<td>40 - 60</td>
</tr>
<tr>
<td>4.5 - 5.5</td>
<td>60 - 80</td>
</tr>
<tr>
<td>&gt; 5.5</td>
<td>80 - 100</td>
</tr>
</tbody>
</table>

- Grid cell with the highest concentrations score 100% and the grid cell with the lowest concentrations scores 0%.
Model requirements

• The model used for scenario selection must:
  – Use data that are available for the entire EU-27
  – Give the same vulnerability score as the Tier-2 model

• We selected an analytical model that simulates degradation and tillage of PPPs in a single soil compartment
PERsistence in Soil Analytical Model (PERSAM)

Four spatial parameters:
- Organic matter
- Bulk density
- Mean temperature
- Mean water content

\[ C_{T,ini} = \frac{DOSE}{\rho z_{rel}} \]

\[ C_{T,peak} = C_{T,ini} + C_{T,plateau} \]

\[ C_{L} = \frac{C_{T}}{\theta / \rho + f_{om} f_{om,K} K_{om,ref}} \]

Example for a tillage depth of 20 cm
Temperature Arrhenius weighted

In this way a better estimation of the total degradation is given
Derivation of target spatial percentile

Development

- Data compilation
- Selection of model for vulnerability mapping
- Derivation of the target spatial percentile with consideration of uncertainty about pesticide properties and soil properties
- Selection of scenarios that meet the target spatial percentile for multiple pesticides
- Scenario parameterization
- Simulation with the comprehensive fate models (e.g. PEARL and PELMO)

End-points:
Overall 90th percentile of the concentration in total soil and the concentration in the liquid phase
The "true" 90th percentile shifts towards higher values if uncertainty in PPP properties and soil properties is considered.
The 95\textsuperscript{th} spatial percentile is used in the remainder of this exercise.

- 90\textsuperscript{th} overall percentile corresponds to the 95\textsuperscript{th} percentile of the cumulative probability density function resulting from \textit{median} pesticide properties and \textit{median} soil properties \textit{if a CV of 25\% is assumed}.

- \textit{See further Vanderborght et al., Pest. Manag. Sci., in press.}
Other choices could have been made – see presentation of Jos

percentiles of $DegT50$

worst of four

median

EXAMPLE

Contour plot of percentiles for concentration in total soil

median $DegT50$ → 95$^{th}$ spatial percentile
worst of four $DegT50$ → 73$^{rd}$ spatial percentile
Scenario selection

- Data compilation
- Selection of model for vulnerability mapping
- Derivation of the target spatial percentile with consideration of uncertainty about pesticide properties and soil properties
- Selection of scenarios that meet the target spatial percentile for multiple pesticides
- Scenario parameterization
- Simulation with the comprehensive fate models (e.g. PEARL and PELMO)

End-points:
Overall 90th percentile of the concentration in total soil and the concentration in the liquid phase
Select all grid cells with the target vulnerability score

• Target vulnerability = 95 ± 1%
Scenarios must apply to all PPP-depth combinations

- Different PPPs and evaluation depths may give different rankings and therefore different target scenarios

- But the scenarios must apply to all relevant PPPs and evaluation depths

- To deal with this problem, vulnerability maps are created for 38 PPP-depth combinations and these maps are overlain
Overlay procedure

38 vulnerability maps

Result is a map where all PPP-depth combinations are within the target vulnerability range
Scenarios closest to the scenario with median properties of all candidates
### Properties of CT scenarios

<table>
<thead>
<tr>
<th></th>
<th>$f_{om}$ (%)</th>
<th>$T_{mean}$ (°C)</th>
<th>Texture</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>11.8</td>
<td>4.7</td>
<td>Coarse</td>
</tr>
<tr>
<td>Central</td>
<td>8.6</td>
<td>8.0</td>
<td>Coarse</td>
</tr>
<tr>
<td>South</td>
<td>4.8</td>
<td>11.0</td>
<td>Medium fine</td>
</tr>
</tbody>
</table>

### Properties of CL scenarios

<table>
<thead>
<tr>
<th></th>
<th>$f_{om}$ (%)</th>
<th>$T_{mean}$ (°C)</th>
<th>Texture</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>2.3</td>
<td>8.2</td>
<td>Medium</td>
</tr>
<tr>
<td>Central</td>
<td>1.8</td>
<td>9.1</td>
<td>Medium</td>
</tr>
<tr>
<td>South</td>
<td>1.1</td>
<td>12.8</td>
<td>Medium</td>
</tr>
</tbody>
</table>
Scenario parameterisation

Development

- Data compilation
- Selection of model for vulnerability mapping
- Derivation of the target spatial percentile with consideration of uncertainty about pesticide properties and soil properties
- Selection of scenarios that meet the target spatial percentile for multiple pesticides
- Scenario parameterization
- Simulation with the comprehensive fate models (e.g. PEARL and PELMO)
- **End-points:** Overall 90th percentile of the concentration in total soil and the concentration in the liquid phase
PEARL and PELMO parameters

• Soil profiles and soil parameters: derived by pedotransfer functions

• Dispersion length 2.5 cm

• Crop data from FOCUS

• Daily weather data from MARS and scaled to WorldClim
Simulation with PEARL and PELMO

**Development**

1. Data compilation
2. Selection of model for vulnerability mapping
3. Derivation of the target spatial percentile with consideration of uncertainty about pesticide properties and soil properties
4. Selection of scenarios that meet the target spatial percentile for multiple pesticides
5. Scenario parameterization
6. Simulation with the comprehensive fate models (e.g. PEARL and PELMO)

**End-points:**
- Overall 90th percentile of the concentration in total soil and the concentration in the liquid phase
Normal FOCUS procedure: 20 years simulations

Concentration in total soil (mg/kg)

26 annual applications

Example: simulation with EFSA_PEARL

The peak
Results – the maximum concentration

- Differences between zones small:
  - P90 of CT: factor of 2 – 5
  - P90 of CL: factor of 1 – 1.5

- Small differences due to opposite trend of organic matter and temperature in the EU
  - North: Organic matter high; temperature low
  - South: Organic matter low, temperature high
Tier-2 must apply to all crops

- Scenario selection done for total surface area of annual crops

- End-point is the 90th percentile of the exposure concentration within the intended area of use of a PPP

- Safety factors needed to ensure that Tier 2 is sufficiently conservative
Development of safety factors

- Simulations done for 18 crops or groups of crops as available in the CAPRI crop database provided by JRC

- For each crop $P_{95\text{crop}}/P_{95\text{annual}}$ is calculated

- The safety factor is the maximum of all these ratios
CAPRI: an extremely valuable resource
Results: P95 for all crops

- Sun flowers
- Texture crops
- Common wheat
- Sugar beets
- Rye
- Root crops
- Rapes
- Pulses
- Vegetables
- Industrial crops
- Other fodder
- Other cereals
- Oats
- Maize
- Flowers
- Barley
- All annual
### Safety factors

#### Safety factor for CT scenario

<table>
<thead>
<tr>
<th>Region</th>
<th>Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>1.74</td>
</tr>
<tr>
<td>Central</td>
<td>1.16</td>
</tr>
<tr>
<td>South</td>
<td>1.07</td>
</tr>
</tbody>
</table>

#### Safety factor for CL scenario

<table>
<thead>
<tr>
<th>Region</th>
<th>Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>North</td>
<td>1.02</td>
</tr>
<tr>
<td>Central</td>
<td>1.15</td>
</tr>
<tr>
<td>South</td>
<td>1.13</td>
</tr>
</tbody>
</table>
Conclusions/relevance for authorisation

• A systematic approach has been developed for the selection of tier 2 and higher tier scenarios. A validation study by an independent contractor showed that the procedure is reproducible.

• This procedure explicitly considers the uncertainty of PPP-properties and soil properties by using a higher spatial percentile.

• The procedure is generic and can also be applied to e.g. leaching scenarios and the national scale.
Final remark

• The full dataset will be made available by JRC, so that notifiers can also do Tier 3 and Tier 4 studies

• This will also make tier 2C of the new FOCUS GW report operational

Calculations: MetaPEARL
Thanks !
How do PERSAM results compare to (Geo)PEARL results?

- Some differences in liquid phase concentration because of non-linear sorption in PEARL
- But correlation is good
- So PERSAM is defensible for scenario selection
<table>
<thead>
<tr>
<th>Kom</th>
<th>10</th>
<th>31</th>
<th>100</th>
<th>316</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td></td>
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<td></td>
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<td></td>
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<td>1000</td>
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</tbody>
</table>

Not relevant, because these PPPs exceed 0.1 μg/l in groundwater.
Example: properties of selected scenarios in zone ‘North’

Median temperature and organic matter