Effective approaches for Assessing the Predicted Environmental Concentrations of Pesticides

A project supporting the harmonised registration of pesticides in Europe


EU-FP5- Quality of Life programme
Who?

- Université catholique de Louvain (M. Vanclooster et al.)
- Alterra (J. Boesten et al.)
- Swedish university of agricultural sciences (N. Jarvis et al.)
- Forschungszentrum Jülich GmbH (P. Burauel et al.)
- Instituto de Recurso Naturales y Agrobiologica de Sevilla (E. Fernandez et al.)
- Universita Cattolica de Sacro Cuore (M. Trevisan et al.)
- Fraunhofer Institut für Umweltchemie und Okotoxikologie (M. Klein et al.)
- Rijksinstituut voor volksgezondheid en milieu (A. Tiktak et al.)
- Joint Research Centre (G. Bidoglio et al.)
Research context

Directive 91/414/EU: ‘Uniform principles’ for registration of crop protection products
   “...Use validated simulation models for PEC to groundwater, surface water and air…”

EU/DG-SANCO: FOCUS (Forum for the co-ordination of the pesticide fate models and their use) working groups
   • Develop guidelines on the selection and use of pesticide emission models
   • Define scenarios for the use of pesticide emission models in the process of registration
Objectives

To evaluate the validation status of PEC groundwater models

To evaluate the validation status of PEC groundwater scenarios (i.e. FOCUS scenario’s)

To propose new effective approaches considering
  • preferential flow
  • volatilization
Pan-European agri-environmental data
i.e. FOCUS Groundwater Scenario

Fate and transport model for the soil crop continuum
- PEARL
- MACRO
- PELMO

Pan-European PEC

Valid?
Validating local scale PEC groundwater models
Research method

1. Input Data
2. Model
3. Model Output
4. Model OK?
   - No: Improvement of model concepts
   - Yes: Accept

Field Data
Local PEC model

Local scale agro-environmental data

Fate and transport model for the soil-crop continuum
  • PEARL
  • MACRO
  • PELMO

Local PEC
Local PEC model test sites
## Local PEC model test sites

<table>
<thead>
<tr>
<th>Location</th>
<th>Country</th>
<th>Climate</th>
<th>Soil Type</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lanna</td>
<td>Sweden</td>
<td>Cold humid</td>
<td>Silty clay over clay</td>
<td>Larsson and Jarvis, 1999</td>
</tr>
<tr>
<td>Brimstone</td>
<td>United Kingdom</td>
<td>Moderate sea climate</td>
<td>Cracking heavy clay</td>
<td>Bromilow et al., 1998; Harris and Catt, 1999; Armstrong et al., 2000.</td>
</tr>
<tr>
<td>Andelst</td>
<td>the Netherlands</td>
<td>Moderate sea climate</td>
<td>Medium clay</td>
<td>In press.</td>
</tr>
<tr>
<td>Vredepeel</td>
<td>the Netherlands</td>
<td>Moderate sea climate</td>
<td>Sand</td>
<td>Boesten and van der Pas, 1999, 2000</td>
</tr>
<tr>
<td>Lebrija</td>
<td>Spain</td>
<td>Mediterranean</td>
<td>Silty (drained marshland)</td>
<td>Andreu et al., 1996, Rieu et al, 1998;</td>
</tr>
<tr>
<td>Coria</td>
<td>Spain</td>
<td>Mediterranean</td>
<td>Silty clay loam</td>
<td>In press.</td>
</tr>
<tr>
<td>Bologna</td>
<td>Italy</td>
<td>Mediterranean</td>
<td>Loam</td>
<td>Araldi, 1997, Scarabello, 1999</td>
</tr>
</tbody>
</table>
Evaluation protocol for the local scale PEC model

- Blind validation (neither laboratory or field data)
  - Evaluate generic parameter identification procedures (pedo-transfer functions, environmental fate data base, …)
- Calibration using laboratory data
  - Evaluate local scale parameter identification approach
- Calibration using field data
  - Evaluate inverse modelling approach
- Blind prediction
Evaluation protocol for the local scale PEC model

• Phased approach
  – Water, solute, heat and pesticide fate evaluated separately

• Use of standardised evaluation criteria
  – Graphical and numerical criteria
Target objective

- Soil moisture in the profile
- Soil temperature
- Soil water drainage
- Groundwater position
- Bromide in profile, drainage water and groundwater
- Active substance in profile, drainage water and groundwater
- Products: bentazone, ethoprophos, imidacloprid, aclonifen, isporoturon, chloridazon
Exemple
measured and predicted drainage

[Graph showing measured and predicted drainage with time periods from 09-94 to 01-96 on the x-axis and drainage in mm/day on the y-axis.]
Bromure content (g/m³)

Depth (cm)

0 5 10 15 20 25 30

0 20 40 60 80 100

measured

predicted

Bromure content (g/m³)

Depth (cm)
bromide concentration in drainage

predicted
measured
Bentazone content (mg/m$^3$) vs. Depth (cm)

- Measured values
- Predicted values

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Bentazone content (mg/m$^3$) vs. Depth (cm)

- **Measured**
- **Predicted**

Depth (cm)

- 0
- 20
- 40
- 60
- 80
- 100

Content (mg/m$^3$)

- 0
- 20
- 40
- 60
- 80
- 100
- 120

Herbicide concentration in drainage water

- **Bentazone concentration in drainage water**

  - Concentration (µg/l)
  - Measured
  - Simulated

  - Dates: 09-94 to 01-96

  - Units: µg/l
Some remarks: weak points on the procedure

- No benchmarking on analytical solutions
- No stochastic validation approach (No ‘statistical’ validation test is done since uncertainty propagation is not considered explicitly in the validation approach)
New modelling approaches for preferential flow and volatilization
Local scale PEC model improvement

Preferential flow
Exemple
Concentration in drainflow (ng dm\(^{-3}\))

- Drain set 1
- Drain set 2
- Simulated
Volatilization
Validating groundwater scenarios
Why scenario validation?

- The selection/definition of the “scenario”, which is a data model, is equally important than the selection/definition of the “leaching model”
- Bias in expert judgement cannot be excluded
- Prepare authorization procedures after 2012
- Prepare harmonized European higher tier assessment
Pan-European scale PEC model

Pan-European agri-environmental data
i.e. FOCUS Groundwater Scenario

Fate and transport model for the soil crop continuum
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Pan-European PEC
Definition of FOCUS groundwater scenario

"A representative combination of crop, soil, climate and agronomic parameters to be used in modeling; representative means in this context that the selected scenarios should represent physical sites known to exist, i.e. the combination of crop, soil, climate and agronomic conditions should be realistic" (FOCUS, 1995).

A combination of parameter values selected in such a way that the leaching calculated with pesticide leaching models using these parameter values equals the 90th percentile of leaching inside the corresponding FOCUS area.
Evaluation/validation of a groundwater scenario?

**Validation level 1**: Are FOCUS scenarios combinations of parameter values selected in such a way that when used in pesticide PEC modeling the calculated leaching equals the 90th percentile of leaching inside the corresponding FOCUS area, as obtained from measurements?

**Validation level 2**: Are FOCUS scenarios combinations of parameter values selected in such a way that when used in pesticide PEC modelling the calculated leaching equals the 90th percentile of leaching inside the corresponding FOCUS area, as obtained from detailed and spatially distributed modeling results?
Validation level 1

Not possible for the time being since pan European data on pesticide concentration in groundwater are not available.
Validation level 2: Summary of the protocol

• Step 1: Identify the FOCUS area

• Step 2: Calculate probability of PEC groundwater with FOCUS scenario ➔ (PEC_FOCUS)

• Step 3: Calculate probability of PEC groundwater with detailed and spatially distributed pan European assessment model ➔ (PEC_PE)

• Step 4: Test: 90\textsuperscript{-th} perc. (PEC_PE) <> 90\textsuperscript{-th} perc. (PEC_FOCUS) ➔ Reject/accept
Spatially distributed approach  

Actual FOCUS approach

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Step 1: Definition of the FOCUS area’s
Definition of the FOCUS groundwater areas

<table>
<thead>
<tr>
<th>FOCUS AREA</th>
<th>mean annual rainfall</th>
<th>mean annual temperature</th>
<th>Corresponding scenario</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>&lt;600</td>
<td>&lt;5</td>
<td>Jokionen</td>
</tr>
<tr>
<td>2</td>
<td>&lt;600</td>
<td>[5-12.5]</td>
<td>Chateaudun</td>
</tr>
<tr>
<td>3</td>
<td>[600-800]</td>
<td>[5-12.5]</td>
<td>Hamburg/Chateaudun(Irr)</td>
</tr>
<tr>
<td>4</td>
<td>[800-1000]</td>
<td>[5-12.5]</td>
<td>Kremsmunster</td>
</tr>
<tr>
<td>5</td>
<td>[1000-1400]</td>
<td>[5-12.5]</td>
<td>Okehampton</td>
</tr>
<tr>
<td>6</td>
<td>&lt;600</td>
<td>&gt;12.5</td>
<td>Thiva/Sevilla</td>
</tr>
<tr>
<td>7</td>
<td>[600-800]</td>
<td>&gt;12.5</td>
<td>Thiva (Irr) /Sevilla (Irr)</td>
</tr>
<tr>
<td>8</td>
<td>[800-1000]</td>
<td>&gt;12.5</td>
<td>Piacenza</td>
</tr>
<tr>
<td>9</td>
<td>[1000-1400]</td>
<td>&gt;12.5</td>
<td>Porto</td>
</tr>
</tbody>
</table>

Define spatially
FOCUS area with arable land mask
The issue of grassland
Step 2: Definition of PEC_FOCUS: Trivial
Step 3: Definition of PEC_PE: Europearl
Approach in APECOP:

- **Step 1 (RIVM contribution: Tiktak and Denie):**
  Perform simulation with PEARL, using Pan European databases
  - PEARL is one of the FOCUS groundwater models;
  - Conceptual differences between FOCUS approach and regional scale model minimised;

- **Step 2 (UCL contribution: Pineros-Garcet and Van clooster):**
  Substitute the rest of the data with a statistical (meta)model approach:
  - Gives 100% coverage
  - We use an interpolation method, to make sure that the original data points are retained.
Parameterisation of EuroPEARL

• **Step 1:** Derivation of the unique combinations, based on climate and soil mapping units;

• **Step 2a:** Parameterisation of the soil profiles (linkage between soil map and Soil Profile Analytical Database of Europe, SPADE);

• **Step 2b:** Parameterisation of weather conditions for each individual plot;

• **Step 3:** Translation into model parameters, using pedotransfer functions etc.
Step 1: Derivation of Unique Combinations (UC)

Country
• Based on the SMU soil map

Soil Map (FAO)
• Created by JRC
• 1:1.000.000
• ‘STU’ info

FOCUS areas
• LU mask
• Precipitation and temperature maps
Step 1: Derivation of Unique Combinations (UC)

Unique combinations =>
- 1410 ‘calculation’ plots
- each UC contains:
  - SMU
  - Country
  - FA
Step 2a: Combine SPADE & SMU’s to PEARL profiles

Current status:

- SW and AUT not represented in SPADE
- 65% of the UC area parameterised
Future possibilities:

- Expansion to 75% possible
- Linking 2nd dominant STU to UC?
- Include more climatic parameters in construction UC's
- More detailed irrigation data
Step 2b: Combine daily weather & climate maps

9 time series (FOCUS)

9 Climate zones (10 x 10 km²)

Precipitation & temperature pattern 10 x 10 km²

Precipitation & temperature pattern for each UC

Scaling

Daily weather data for each UC

- Temperature
- Precipitation
- Potential evapotranspiration
Step 3: specific model parameters

- **Substance**
  - Substance properties, such as the half-live and the partitioning coefficient

- **Run**
  - Substance ID
  - Plot ID
  - Management ID
  - Start date
  - End date

- **Management**
  - Application date
  - Application type
  - Application dosage

- **Plot**
  - Plot ID
  - FOCUS Area ID
  - Land-use type ID
  - Soil profile ID
  - Groundwater depth group ID
  - Seepage flux and amplitude
  - Drainage characteristics

- **Soil profile**
  - Soil layer ID

- **Soil layer**
  - Soil physical unit ID
  - Layer thickness
  - Texture
  - Organic matter
  - pH

- **Soil physics**
  - Parameters of the Mualem-van Genuchten functions
  - Dispersion length

- **FOCUS Area**
  - Emergence date
  - Harvest date
  - Development stage ID
  - Critical pressure heads for drought stress and irrigation

- **Development stage**
  - LAI
  - Crop factor
  - Rooting depth

- **Spatially distributed variables**
Some preliminary results of EURO-PEARL
Fill out missing gaps: the EURO-PEARL meta-model?

- statistical model
- similar to kriging,
- useful and efficient in multidimensional parameter spaces.
What are the inputs and outputs of the metamodel?

Sand
Silt
Clay
OM
pH
AveWat
Bulk density
Temp_yr
Prec_yr
Eva_yr
Temp_spring
Prec_spring
Eva_spring
Temp_spring
Prec_spring
Eva_spring
GWLevel

mean year leaching concentration (atrazine)
What do we use for calibration?

- 656 combinations of the input parameters

\[ X_c = \begin{pmatrix} P1 & P2 & P3 \\ xc_{1,1} & xc_{1,2} & xc_{1,3} \\ xc_{2,1} & xc_{2,2} & xc_{2,3} \\ \vdots \\ xc_{116,1} & xc_{116,2} & xc_{116,3} \end{pmatrix} \]

\[ Y_c = \begin{pmatrix} yc_1 \\ yc_2 \\ \vdots \\ yc_{116} \end{pmatrix} \]
What do we use for validation?

- 72 combinations of the input parameters
- 72 Pearl outputs
How the calibration data where obtained?

- From +/-5400 unique combinations of soil and climate in the Netherlands, RIVM did Pearl simulations.

- From those simulations, 728 unique combinations were selected, having the following characteristics:
  - not irrigated
  - atrazine
  - non drained
  - maize

72 pts (10%, random) for validation  656 : calibration
Calibration results

Not surprising: it is calibrated to go through all calibrations points

predictions: \( \ln (\text{leaching (ug/l)} + 1) \)
Validation scatterplot

predictions: \( \ln (\text{leaching (ug/l)} + 1) \)
When and where will results be available

- Project deliverables available by march 2003

- Project results will be presented at the XII Pesticide chemistry symposium, Piacenza, Italy, May 2003

- Information

www.agro.ucl.ac.be/geru/recherche/projets/apecop-pub