Cranfield UNIVERSITY Silsoe

DEFRA PL0548

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

Igor Dubus, BRGM, France

i.dubus@brgm.fr

CRANFIELD CENTRE FOR ECOCHEMISTRY

Cranfield UNIVERSITY Silsoe

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

CRANFIELD CENTRE FOR ECOCHEMISTRY

Cranfield UNIVERSITY Silsoe

PLO548 outputs

- Dubus I.G., Brown C.D. & Beulke S. (2003). Sources of uncertainty in pesticide fate modelling. The Science of the Total Environment, 317:53-72.
- Dubus I.G. & Janssen P.H.M. (2003). Issues of replicability in pesticide fate modelling: a case study with a pesticide leaching model. Environmental Toxicology & Chemistry, 22:3081-3087.
- Dubus I.G., Brown C.D. & Beulke S. (2003). How much confidence should we assign to results of Monte Carlo modelling? Proceedings of the Piacenza conference.

CRANFIELD CENTRE FOR ECOCHEMISTRY

Cranfield UNIVERSITY Silsoe

PL0548

Probabilistic approaches to pesticide fate modelling: a case study

CRANFIELD CENTRE FOR ECOCHEMISTRY

Cranfield UNIVERSITY Silsoe

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

CRANFIELD CENTRE FOR ECOCHEMISTRY

Cranfield UNIVERSITY Silsoe

FOCUS modelling

80th concentrations predicted by PEARL

for the four scenarios relevant to UK conditions

Scenario	80th percentile concentration (µg/l)
Châteaudun	0.084
Hamburg	0.041
Kremsmünster	0.060
Okehampton	0.206

CRANFIELD CENTRE FOR ECOCHEMISTRY

Better case, worse case

	Koc	Field DT50
Median case	50th percentile 91.5 ml/g	50th percentile 43 days
Better case	75th percentile 116 ml/g	25th percentile 29 days
Worse case	25th percentile 79 ml/g	75th percentile 60 days

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

	80th-percentile concentration (μg/l)		
Scenario	Better case	Median case	Worse case
Châteaudun	<0.001	0.084	1.307
Hamburg	<0.001	0.041	0.597
Kremsmünster	<0.001	0.060	0.815
Okehampton	0.001	0.206	1.903

Cranfield UNIVERSITY Silsoe

CRANFIELD CENTRE FOR ECOCHEMISTRY

Influence of the application date

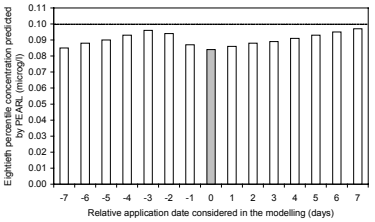
- Aim: investigate the influence of the application date considered on FOCUS predictions
  - Base case: application 7 days after emergence
  - Application varied between emergence and emergence + 15 days (+ or – 7 days compared to base case)

Cranfield UNIVERSITY Silsoe

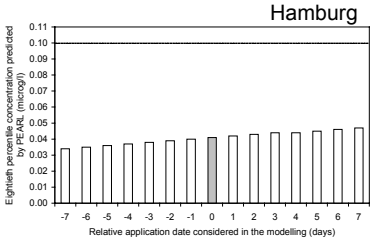
CRANFIELD CENTRE FOR ECOCHEMISTRY

Refined FOCUS modelling (variation of application date)

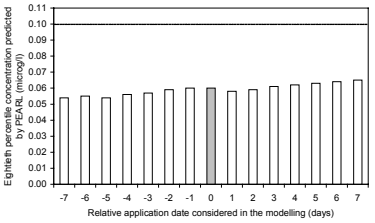
Châteaudun



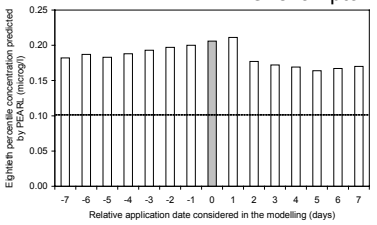
Hamburg



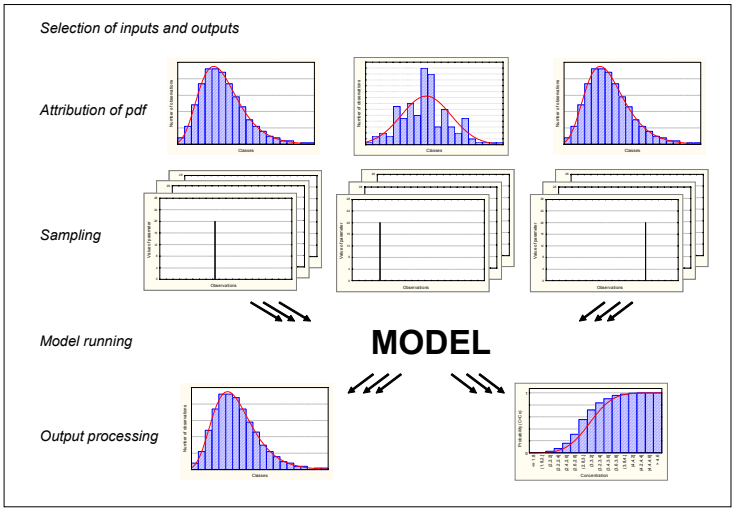
Kremsmünster



Okehampton



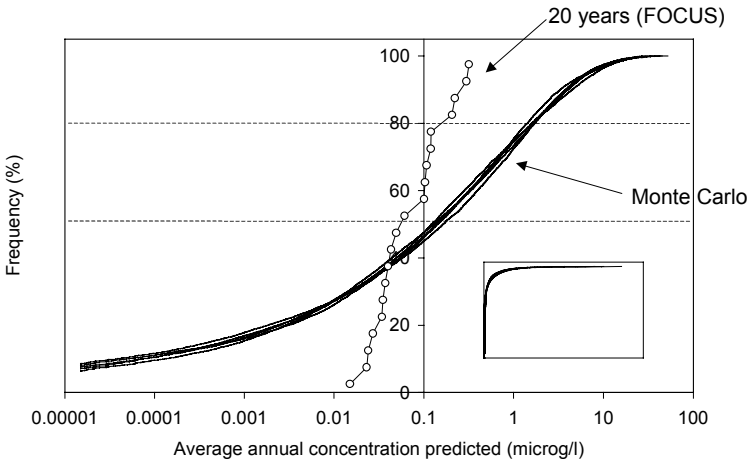
Monte Carlo modelling



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



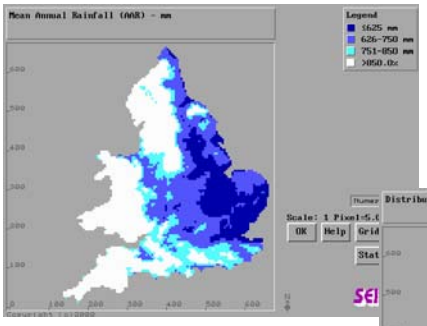
Monte Carlo modelling: pros and cons

- 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

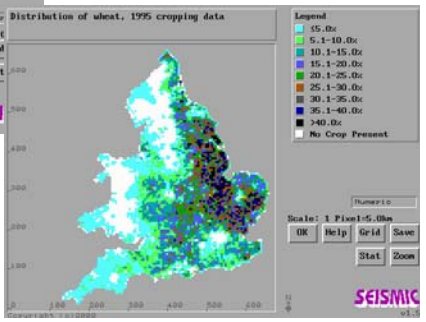
Scenario-based modelling

- 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

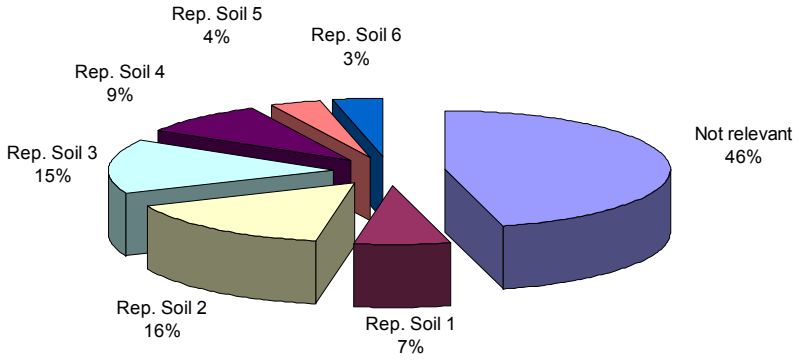


Average annual rainfall

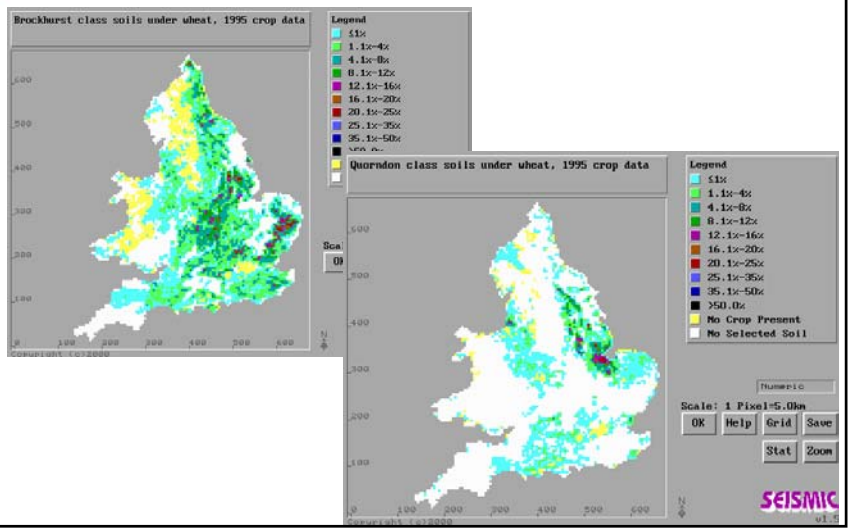


Wheat growing area

Definition of representative soil series



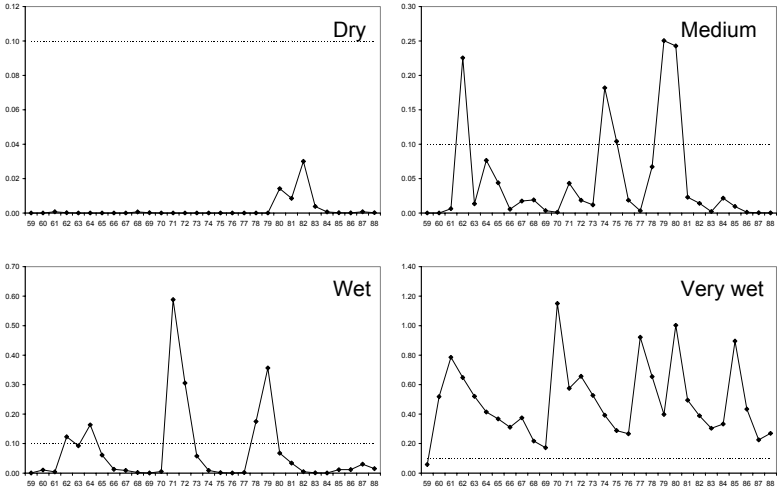
Definition of representative soil series



Cranfield UNIVERSITY Silsoe

CRANFIELD CENTRE FOR ECOCHEMISTRY

Scenario-based modelling
Example of intermediate results



Simulations for the Ludford representative soil series

Cranfield UNIVERSITY Silsoe

CRANFIELD CENTRE FOR ECOCHEMISTRY

Scenario-based modelling
Weighting of results

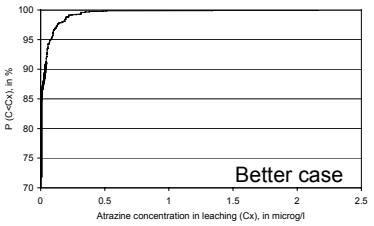
- Extracting of 30-year average concentrations of atrazine in leaching for each of the 48 scenarios simulated
- Weighting according to the abundance of the scenario in the E&W landscape

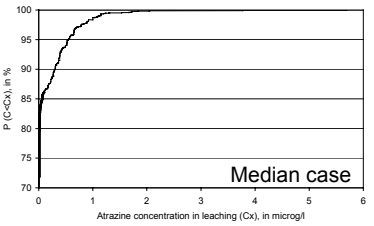
Soil type	Extent of soil within each climatic scenario (%)				Total extent (%)
	<625 mm AAR	625-750 mm AAR	751-850 mm AAR	>850 mm AAR	
Not overlaying aquifers	-	-	-	-	65.2
Not vulnerable [a]	0.7	2.9	3.4	0.8	7.8
Enborne	0.7	1.3	2.0	0.0	4.0
Hall	0.2	0.8	1.0	0.9	2.9
Cuckney	0.2	1.3	1.2	0.6	3.3
Ludford	0.8	4.1	4.1	7.8	16.8
Total	2.6	10.3	11.7	10.2	100.0

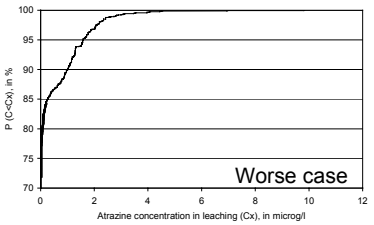
[a] Impermeable or peaty soils

- Derivation of cumulative distribution charts

Scenario-based modelling
Final results







	Probability of exceeding 0.1 µg/l (%)	95th percentile concentration (µg/l)
Better case (75th percentile Koc, 25th percentile DT50)	3.7	0.08
Median case (50th percentile Koc, 50th percentile DT50)	13.8	0.55
Worse case (25th percentile Koc, 75th percentile DT50)	17.7	1.58

Scenario-based modelling: pros and cons

- Scenario-based modelling
  - 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

Cranfield UNIVERSITY Silsoe

CRANFIELD CENTRE FOR ECOCHEMISTRY

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)

Cranfield UNIVERSITY Silsoe

CRANFIELD CENTRE FOR ECOCHEMISTRY

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

Cranfield UNIVERSITY
Silsoe

CRANFIELD CENTRE FOR ECOCHEMISTRY

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!