THE USE OF FOCUS PEARL IN AN AUTOMATED SPATIAL EXPOSURE MODELLING ASSESSMENT FOR THE PREDICTION OF ISOPROTURON CONCENTRATIONS IN GROUNDWATER

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Pesticide fate models currently employed in regulatory risk assessments are used to assess the likely movement of pesticides to surface waters and groundwater. These models depend critically on the degradation rate (DT_{50}) and sorption values (K_d, K_{OC}, K_{OM}) of a pesticide; therefore it is important to select these appropriately. Current regulatory modelling uses single endpoint values for degradation and sorption to describe a pesticide's availability in the soil environment. However, there is increasing data to suggest that pesticide degradation and sorption vary greatly across relatively short distances. The implications for exposure modelling of variable degradation rates and sorption values in soil on exposure modelling are examined below.

1. The Site and Sampling

• The site used was Deep Slade field (9 ha) at Horticulture Research International, Wellesbourne. The soil is a deep permeable coarse sandy loam of the Wick series that covers ca. 220,000 ha in England and Wales. The site was cropped with cereals in 2000.

• 108 soil samples were collected from Deep Slade field in 2000 and analysed in the laboratory

• Soil organic matter (SOM) and particle size distribution was determined for each soil sample

• Adsorption and DT_{50} values for isoproturon (IPU) for all 108 soil samples were determined and the distributions are given in Figure 1

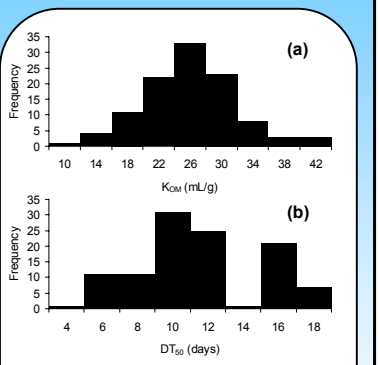

Figure 1 – Distribution of a) K_{OM} values and b) DT_{50} values for IPU in Deep Slade field

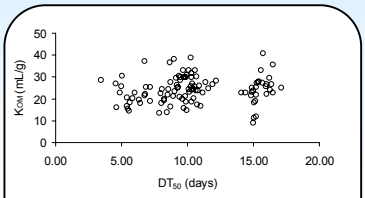

Figure 2 – Relationship between K_{OM} and DT_{50} values

• No correlation between K_{OM} and DT_{50} was observed (Figure 2)

2. Site-Specific Groundwater Simulations

Annual average concentrations of IPU in leachate at 1-m depth after 7 successive applications were simulated with PEARL v2.2.2

• A site-specific scenario was generated using :
  • A single soil profile obtained from the SEISMIC database
  • Pedotransfer functions
  • Weather data for 2000 for Wellesbourne
  • Crop parameters from the FOCUS groundwater scenario Okehampton

• The site-specific scenario for Deep Slade field was run using the experimental data above and the physico-chemical data obtained from the Pesticide Manual (2000)

• Median DT_{50} (10.49 days) and K_{OM} (24.19 mL/g) values for IPU (from the 108 soil samples) were used (with 1/n = 0.9)

• The annual average Predicted Environmental Concentration (PEC) in groundwater (GW) at 1 m depth in the 7th year was 0.012 µg/L (following a 6 year warm up period)

3. Spatial Modelling for Exposure in Groundwater

• The SENSAN software was interfaced with the pesticide leaching model PEARL v2.2.2

• The Freundlich exponent (1/n) was not calculated. Therefore, to examine the effect of the 1/n value on the calculated annual average PEC_{GW} values the model was run using three different 1/n values and the coupled measurements of DT_{50} and K_{OM}

• In addition, model runs were performed either using a median DT_{50} value with 108 site-specific measurements of K_{OM} or using a median K_{OM} value with site-specific DT_{50} values (with 1/n = 0.9 in both cases)

• The cumulative frequencies for the calculated annual average PEC_{GW} values at 1 m depth are given in Figure 3

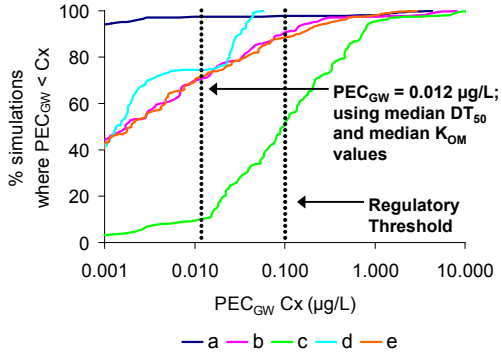

Figure 3 – Calculated PEC_{GW} values for 108 soil samples using coupled measurements of DT_{50} and K_{OM} and 1/n values of (a) 0.8, (b) 0.9 and (c) 1.0; (d) median K_{OM} and varying DT_{50} with a 1/n value of 0.9; (e) median DT_{50} and varying K_{OM} with a 1/n value of 0.9

• Varying the K_{OM} and using a median DT_{50} value had a greater effect on the annual average PEC_{GW} than *vice versa*

• The most significant effect on the calculated annual average PEC_{GW} value was observed by changing the Freundlich exponent (1/n value) from 0.8 to 1.0

• 98, 91 and 51% of the calculated annual average PEC_{GW} values are below the regulatory value of 0.1 µg/L for the simulations carried out using coupled measurements of DT_{50} and K_{OM} and 1/n values of 0.8, 0.9 and 1.0, respectively

• 100 and 88% of the calculated annual average PEC_{GW} values are below the regulatory value of 0.1 µg/L for the simulations carried out using either a median K_{OM} value and site-specific DT_{50} values or using a median DT_{50} value and site-specific K_{OM} values, respectively

4. Conclusions

• Predicted concentrations of IPU in leachate at 1 m depth ranged from 0.000 to 11.979 µg/L as derived from measured K_{OM} and DT_{50} values from samples collected from a single field, whereas the value based on median K_{OM} and DT_{50} values for all samples was 0.012 µg/L

• Correct parameterisation of the Freundlich exponent within PEARL v2.2.2 is critical in the estimation of accurate PEC_{GW}

• Using median DT_{50} and K_{OM} values in exposure modelling could result in risk assessments that under or over predict exposure to groundwater. Better characterisation of the variability in input parameters could result in more realistic risk assessments