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p-EMA (I): simulating the environmental fate of pesticides for a farm-level risk assessment system

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Abstract – A computer-based decision support tool (p-EMA) has been developed to support UK Government policy of optimising agricultural pesticide use. The system estimates risks to a wide range of taxonomic groups and environmental compartments using methods consistent with current regulatory assessments, but also allows adjustments to reflect formulation, the local conditions and the environmental costs and benefits of varying management practices. Simple models of the dispersion pathways of the pesticide in the local environment are used to estimate predicted environmental concentrations in the field and margin soil, surface water and groundwater. Exposure estimates are then combined with the toxicological properties of the pesticide in the form of toxicity:exposure ratios. Concentrations in groundwater are calculated on the basis of a meta-version of the MACRO model linked to environmental and pesticide databases. Surface water concentrations are taken as the maximum of those arising from inputs via spray drift and drainflow.

exposure / software / model / pesticide / ecological risk assessment

Résumé – p-EMA : Simulation de l'évolution des pesticides dans l'environnement pour un système d'évaluation du risque au niveau de l'exploitation. Un système expert d'aide à la décision (p-EMA) a été développé afin d'assister la démarche britannique d'optimisation de l'utilisation agricole de pesticides. Le système estime le risque d'impact environnemental sur un grand nombre d'organismes sur la base des mêmes méthodes utilisées dans l'homologation des produits de protection des plantes. Le système tient compte du type de formulation utilisé, des conditions environnementales locales et applique une approche perte-bénéfice vis-à-vis de l'environnement dans l'application de différentes alternatives de gestion de traitement. Des modèles simples de transfert de pesticides dans l'environnement sont utilisés pour estimer les concentrations dans le sol et les eaux de surface et souterraines. Ces concentrations sont comparées aux données écotoxicologiques sur la base d'un quotient toxicité/exposition. Les concentrations dans les eaux souterraines sont estimées à l'aide d'un émulateur du modèle de transfert MACRO combiné à des bases de données contenant les caractéristiques de l'environnement et des produits. Les concentrations dans les eaux de surface sont prises comme les valeurs maximales provenant du drainage et de la dérive des pulvérisations.

exposition / logiciel / modèle / pesticide / estimation du risque

1. INTRODUCTION

The use of pesticides to control agricultural pests and diseases is central to intensive, arable agriculture. Whilst there are clear benefits in productivity from these methods, many governments are committed to a long-term reduction in the total use of pesticides. In tandem with use reduction, the identification and minimisation of risks is essential to optimise the risk-benefit analysis. The environment is one of the areas where pesticides are seen to present a risk and the move towards integrated pest management has the reduction of this

risk at its heart. A number of instruments are available to control environmental risk from pesticides including restriction of chemical use and the imposition of taxes. Such schemes suffer because they must simplify the variability in the natural environment and regulate on the basis of scenarios at greatest risk. An alternative approach is to develop tools to assess risk at the local scale and support farm-level decisions on pesticide selection. This has the advantage that it can encompass local conditions whether they increase or mitigate risk and empowers the end user (farmer or pesticide advisor) who must ultimately implement any risk minimisation policy.

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This and two associated papers [11, 18] describe the development of p-EMA, a risk assessment system to guide use optimisation at the farm level. The methodology has been incorporated within the Environmental Management for Agriculture software package [17] which has been designed for use by farmers and their advisors to encourage more sustainable practices. The three papers treat environmental fate, ecological risk assessment and farm-level case studies, respectively.

To date, systems to promote and support more environmentally benign use of pesticides have relied either on hazard ranking or on very simplified indicators of risk. Levitan et al. [15] provide a thorough review of early work and highlight three issues: (a) creating an integrated assessment (most were groundwater-human toxicity based); (b) integrating environmental and economic information; and (c) balancing ease of use and complexity of process. Hazard-based systems rank compounds solely on their potential to cause harm with no consideration of the intensity or probability of environmental exposure. This is the approach used to date within EMA [16]. Label precautions for pesticide products were used as indicators for toxicity towards humans, animals, birds, aquatic life and bees and a site-specific summing system pointed the user towards selection of more benign chemicals. Fate was only considered through simple rule-basing such as weighting factors which varied with the distance between sprayed area and surface water. Potential for groundwater contamination was again hazard-based comprising an algorithm linking strength of sorption to soil and rate of degradation in soil [9], but not considering rate of application, soil type, depth to groundwater, etc.

Wijnands [22] describes a whole farm system to support integrated pest management where environmental exposure to pesticides for air, soil and groundwater compartments is calculated as a function of the application rate of the chemical and its vapour pressure, degradation rate in soil and mobility (strength of sorption), respectively. Roussel et al. [21] have developed a system based on fuzzy logic for pesticide use in Brittany, France (IPEST-B). Simple decision rules are used to assign an environmental effect score (0 to 1) based on whether a number of input parameters are 'favourable' or 'unfavourable'. For example, risk of contamination of groundwater and potential for harm to the population requires input related to pesticide properties, type of application, soil/geological conditions and acceptable daily intake for human consumption. SyPEP [19] adopts an alternative approach where exposure is explicitly considered via the SEPTWA model to estimate pesticide emissions to surface and groundwater. However, a single scenario is adopted to represent Belgian conditions and the system reverts to a standardised ranking index for pesticides with no consideration of local conditions. The environmental yardstick assesses the impact from pesticide use in the Netherlands and has a range of uses from management tool for farmers and agricultural consultants to a policy evaluation tool [20]. The calculation methods are risk-based, so that groundwater concentrations are calculated using the PESTLA leaching model and risk to aquatic organisms combines losses to surface water via drift with acute toxicity data for the compound. At the farm scale, the system comprises a number

of look-up tables with farmer inputs restricted to choice of chemical, dose rate, soil organic matter content, time and method of application and distance from sprayed area to surface water.

The reasons to maintain a relatively simple assessment of risk to the environment include few data requirements, short calculation times and transparency to the end user. However, simplifications are likely to fall short when trying to accommodate the differences between sites. It is clearly important that any system is broadly in tune with regulatory risk assessments which establishes the ultimate criteria of environmental acceptability. Any move away from regulatory procedures risks not only producing anomalies (e.g. a high impact score for a compound which has recently passed through the regulatory process), but also alienating industry and regulatory communities who are key stakeholders in the drive to minimise risk. The approach described in this and the associated papers [11, 18] seeks to make a more robust assessment of the risk to the local environment from pesticide use. The system is designed to provide scores which reflect both exposure and toxicity in a way which is consistent with current regulatory procedures, but also allows adjustments to reflect the local conditions and the environmental costs and benefits of varying management practices.

2. MODEL DESCRIPTION

Environmental fate of pesticides is described in order to calculate predicted environmental concentrations for soil, groundwater and surface water. These are considered in turn below. Site- and practice-specific adjustments are made wherever possible and these are overviewed in Table I. No risk assessment is undertaken for the air compartment to mirror current regulatory practice and gaps in current understanding.

2.1. Pesticide database and input parameters

A pesticide database including a data quality index has been collated to support the software and this is described in an associated paper [18]. The pesticide properties used to calculate predicted environmental concentrations are: soil-water partition coefficient normalised for organic carbon content of the soil (K_{oc}); half-life (normally first-order) for degradation in soil (DT_{50}) determined either in the laboratory or the field (preferred); half-lives for aqueous photolysis, neutral hydrolysis and dissipation from the water phase of a water-sediment system.

The user is required to provide inputs at the level of farm, field and individual application (Tab. II). At the farm level, the user need only enter the postcode which is used to assign the site to broad environmental categories (Sect. 2.3). Farm and field level inputs are held within farm profiles, whereas application level inputs must be entered for each season.

2.2. Concentrations in soil

The risk assessment requires the initial concentration of the pesticide in soil. The amount of chemical hitting the soil surface is calculated from the application rate by correcting for

Table I. Site- and practice-specific factors considered within the fate calculations.

Compartment	Site-specific factors	Practice-specific factors
Soil	Crop type and growth stage	Rate of application
Groundwater	Presence and type of aquifer Soil type Average winter recharge Crop type and growth stage	Rate and timing of application
Input to surface water (drift)	Presence of surface water Width of water body Distance of water from edge of crop	Rate and number of applications Use of a low-drift spray nozzle Implementation of any no-spray buffer
Input to surface water (drains)	Presence and type of drains Soil type Crop type and growth stage	Rate of application
Surface water body	Dimensions of water body	-

Table II. User inputs required to calculate exposure concentrations.

Field level inputs	Application level inputs
Area of field	Product name and formulation type
Broad soil type	Product application rate and date
Presence/type of drains	Incorporation depth
Presence of surface water	Number of treatments with same product
Width and depth of surface water	Crop type and growth stage
Surface water flowing or static	Spray nozzle type
	Distance from the edge of the sprayed area to the field margin
	Distance from the edge of the sprayed area to the near edge of the surface water body

interception by any crop present. The user is asked to input either the fraction of ground covered by crop or the crop growth stage at the time of each application. Crop growth stage is converted to fractional cover and then this information is used to calculate interception of pesticide by the crop on the basis of measured data [2]. In line with current regulatory practice, the initial concentration of pesticide in soil is calculated by assuming that the fraction of pesticide hitting the soil is uniformly distributed within the upper 5 cm of soil which has an assumed bulk density of $1.5 \text{ g}\cdot\text{cm}^{-3}$. For multiple applications, the concentration from each at the time of the final application is calculated and summed based on the rate of degradation in soil:

$$C_t = C_0 \cdot e^{-kt} \quad (1)$$

where for any application prior to the final one: C_t is the concentration at the time of the final application ($\text{mg}\cdot\text{kg}^{-1}$); C_0 is the concentration at the time of the earlier application ($\text{mg}\cdot\text{kg}^{-1}$); k is the first-order rate of degradation ($= \ln 2 / \text{DT50}$) (d^{-1}); and t is the time between the earlier and the final application (d).

2.3. Concentrations in groundwater

Current regulatory practice is to simulate annual average concentrations of a pesticide leaching through soil to 1-m depth and to use this value as a protective surrogate for

concentrations in groundwater. The annual average is compared with the EU groundwater quality criteria of $0.1 \mu\text{g}\cdot\text{L}^{-1}$ to assess regulatory compliance. MACRO is one of the four leaching models recommended for European regulatory use [7]. MACRO (version 4.1) is a physically-based preferential flow model with the total soil porosity divided into two flow domains (macropores and micropores), each characterised by a flow rate and solute concentration [12]. Soil water flow and solute transport in the micropores is modelled using Richards' equation and the convection-dispersion equation, respectively, whilst fluxes in the macropores are based on a simpler capacitance-type approach with mass-flow. Exchange between micropores and macropores is calculated according to approximate, physically-based expressions using an effective aggregate half-width. Pesticide degradation is modelled using first-order kinetics whilst sorption is assumed to be at instantaneous equilibrium and to be described by a Freundlich isotherm. The model has a long running time and it is not feasible to run the model live within p-EMA. Instead, a meta-version of the model was developed by running the model to generate a series of look-up tables.

Inputs to the system need to be kept as simple as possible. The user need only specify the postcode of the farm and a look-up table is accessed to define whether or not the farm overlies a productive aquifer, what soil type is present, and the average volume of winter recharge. The resolution of the database is units of approximately $12 \times 12 \text{ km}$. If there is no

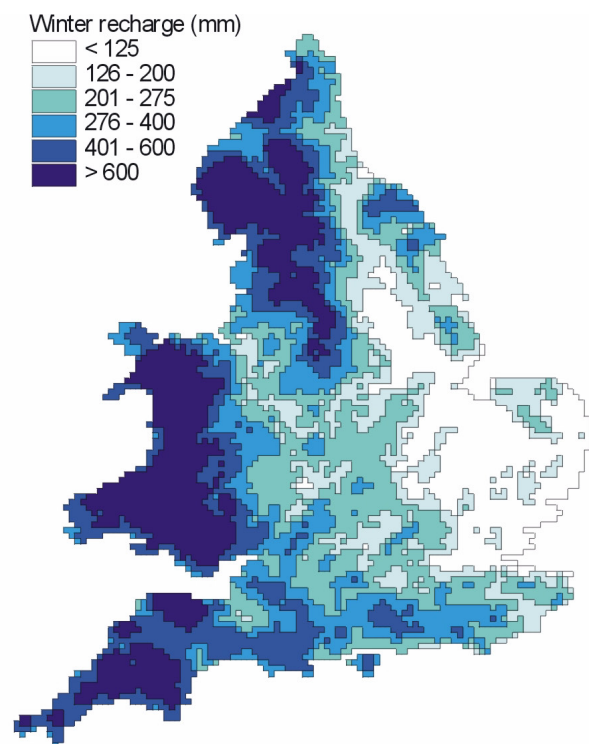


Figure 1. Division of England and Wales into climatic regions based on average winter recharge.

productive aquifer present, then the groundwater concentration is set to zero. Soils overlying aquifers have been divided into six leaching vulnerability classes [6]. Two of these have very low potential to transmit pesticides (again, the

groundwater concentration is then set to zero), leaving four soils to be considered by the system. Winter recharge in the main arable areas of the UK varies from <125 mm to ca. 600 mm [13]. This range was divided into five categories (each accounting for 2.3–3.3 million ha of land (Fig. 1) to give a total of 20 combinations of soil and climate.

Representative soil profiles were defined for each of the four vulnerability classes (Tab. III) and input parameters for the MACRO model were selected using the procedures described by Beulke et al. [3]. Long-term weather datasets were accessed from sites around the UK and single years were selected for each of the five recharge classes to give total recharge at the upper end of the range specified and a roughly even distribution of rainfall across the year (i.e. no significant dry periods). These weather years were repeated within four year model simulations to fully evaluate any long-term leaching of the chemical. The major pesticide properties controlling extent of leaching are Koc and DT50. The model was run for 57 combinations of these two properties with Koc varying from 2 to 1000 mL·g⁻¹ and DT50 varying from 2 to 350 days. Chemicals with Koc >1000 mL·g⁻¹ were assumed to have negligible potential for leaching because of their strong sorption to soil. The model was run to assess leaching following a unit application of 1000 g a.s.·ha⁻¹ in "autumn" (August-January) and "spring" (February-July). This gave a total of 2280 simulations (4 soils × 5 climates × 57 property combinations × 2 application timings). The largest annual average concentration over the course of each simulation was calculated and the 2280 results were held in look-up tables.

For any given pesticide application, the four numbers surrounding the true Koc-DT50 pairing are read from the look-up table and interpolated. The resulting concentration is then corrected to the actual application rate (itself adjusted for any interception by the crop). The concentration is converted

Table III. Representative soil profiles for groundwater and drainflow calculations.

Groundwater vulnerability class ^a	Soil texture group	Representative series	Topsoil organic carbon content (%)	Topsoil clay content (%)	Reason for drains ^b
Groundwater calculation					
H1	Medium loam	Enborne	3.9	39	-
H2	Sand	Cuckney	1.7	10	-
H3	Medium loam	Aberford	2.6	22	-
I1	Light loam	Ludford	2.2	22	-
Drainflow calculation					
-	Sand	Blackwood	2.3	11	1
-	Light loam	Swanwick	2.1	15	1
-	Light silt	Wisbech	1.8	22	1
-	Medium loam	Salop	2.7	24	2
-	Medium silt	Cegin	3.6	29	2
-	Clay	Denchworth ^c	3.6	60	2

^a Environment Agency [6].

^b To control shallow groundwater (1) or because of a slowly permeable subsoil (2).

^c Soil at Brimstone Farm, Oxon.

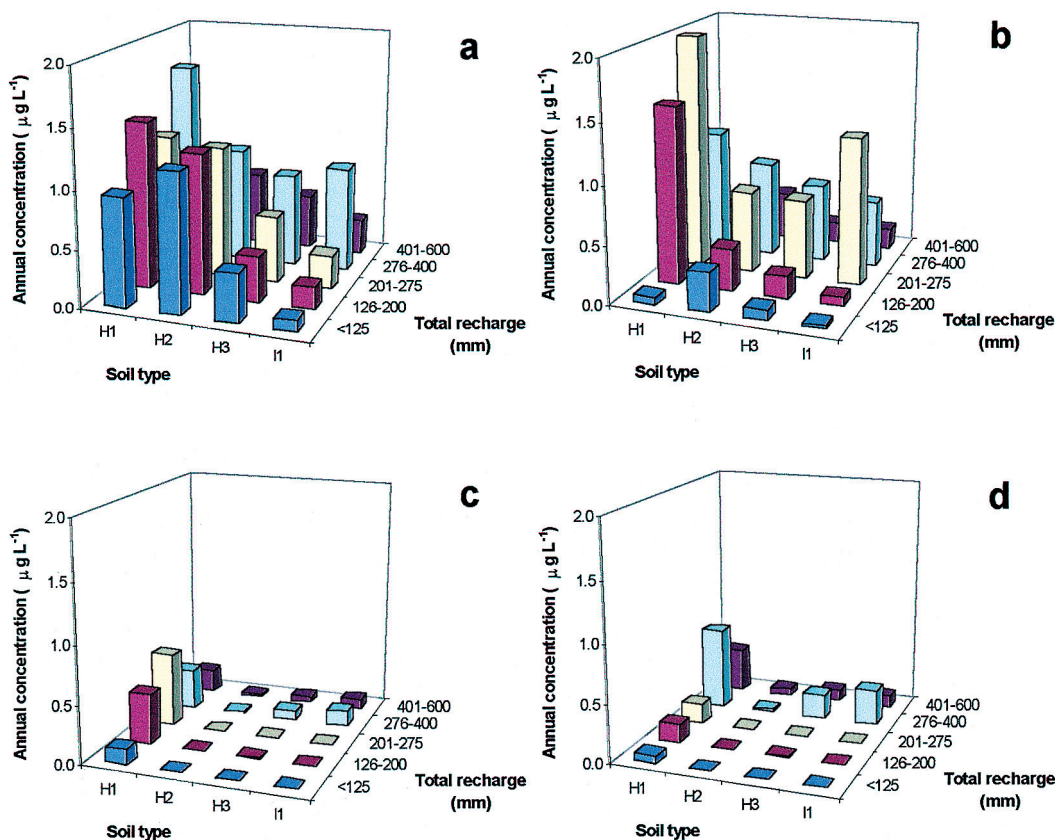


Figure 2. Annual average concentrations of pesticide leaching to 1-m depth for application at 1000 g a.s.·ha⁻¹ of a pesticide with Koc = 20 ml·g⁻¹ and DT50 = 20 days in autumn (a) or spring (b) or a pesticide with Koc = 200 ml·g⁻¹ and DT50 = 50 days in autumn (c) or spring (d).

to an assessment of risk by comparison with the European groundwater quality threshold for pesticides (0.1 μg·L⁻¹). The method to derive the associated risk score is described by Hart et al. [11].

Figure 2 shows output from the groundwater model for contrasting chemicals applied in autumn or spring at 1000 g a.s.·ha⁻¹. The relative vulnerability to leaching of the four soils varies significantly according to the properties of the

pesticide, the timing of leaching and the volume of recharge. The H1 soil generally transmits the largest concentrations. Increasing excess winter rainfall generally gives greater leaching up to a maximum value, above which the greater volume of leaching water carries no extra pesticide but merely dilutes the average concentration. Table IV shows variation in predicted concentration with Koc and DT50 for an example scenario (H1 soil in an area with 126–200 mm average winter

Table IV. Effect of pesticide Koc and DT50 on annual average concentrations (μg·L⁻¹) leaching to 1-m depth for an application at 1000 g a.s.·ha⁻¹ (all concentrations are for H2 soil in an area with 126–200 mm winter recharge).

DT50	Koc (ml·g ⁻¹)								
	2	5	10	20	50	100	200	500	1000
(d)									
2	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001	<0.001
5	0.016	0.015	0.013	0.010	0.005	0.003	<0.001	<0.001	<0.001
10	0.090	0.078	0.065	0.051	0.034	0.019	0.006	<0.001	<0.001
20	0.246	0.214	0.180	0.144	0.096	0.057	0.019	<0.001	<0.001
50	-	-	0.356	0.286	0.193	0.117	0.043	0.004	<0.001
100	-	-	-	-	0.250	0.153	0.059	0.012	0.002
200	-	-	-	-	0.287	0.177	0.070	0.021	0.004
350	-	-	-	-	-	0.189	0.076	0.030	0.007

Table V. Predicted losses of pesticide in 10 mm drainflow according to soil type and sorption category (all values are % of pesticide in soil at application).

Soil texture group	Koc category (ml·g ⁻¹)					
	<15	15-74	75-499	500-999	1000-3999	>4000
Sands	0	0	0	0	0	0
Light loams	0.0012	0	0	0	0	0
Light silts	0.0026	0.0014	0.0001	0	0	0
Medium loams						
- no moles	0.088	0.078	0.066	0.051	0	0
- with moles	0.054	0.090	0.12	0.0064	0	0
Medium silts	0.34	0.47	0.37	0.15	0	0
Clays	1.9	1.9	0.70	0.50	0.020	0.0080

recharge). The sensitivity of the meta-model to the two pesticide parameters is shown and reflects that described for the MACRO model itself [5].

2.4. Concentrations in surface water

Regulatory procedures consider a worst-case surface water body which is static, 30 cm deep, 100 cm wide and runs along the side of a field at a distance of 1 m from the sprayed area. p-EMA takes into account the actual dimensions and distance from the sprayed area of any surface water present. The system calculates inputs to surface water via spray drift and via drainflow after application (for fields where drains are installed). The largest of these inputs is used to calculate concentration in surface water. It is assumed that spray drift and drainflow do not occur at the same time as the farmer is unlikely to apply pesticide under conditions where the drains are flowing. A further assumption is that inputs via surface runoff are small relative to those from drift and drainflow. This is a realistic assumption for most of the UK arable area [14] which is relatively flat and receives mostly low intensity rainfall. However, surface runoff would need to be included as a fate process for many other parts of the world. No assessment is undertaken for fields which are not adjacent to a surface water body.

Spray drift is considered a major route of entry for pesticides to surface waters [1]. Calculation of inputs to surface waters are based on spray drift tables derived from experimental data [8]. Current regulatory procedures to calculate a 90th-percentile drift input were incorporated directly into p-EMA with the addition of reduction factors for the use of low-drift spray nozzles. In setting up the farm profile, the user is asked to specify for each field: whether surface water is present; its width and depth; and the average distance from the edge of the normal sprayed area to the near edge of the water. In addition, the user must specify whether any additional strip alongside the water body has been left unsprayed to comply with regulatory requirements. The amount of pesticide entering the surface water is calculated as a percentage of the field application rate using an equation which integrates drift across the width of the water body:

$$P = a * \left[\frac{(y + z)^{b+1} - (z)^{b+1}}{(b+1) * y} \right] * L \quad (2)$$

where P is drift deposit per unit area as a percentage of the field application rate (-); a and b are drift regression parameters (-); y is the width of the surface water body (m); z is the distance from the edge of the sprayed area to the near edge of the surface water body (m); and L is a reduction factor for the use of low-drift spray nozzles (-).

Parameters a and b take the value 2.7593 and -0.9778, respectively for a single application of pesticide to an arable crop. Separate values are available for multiple applications up to a maximum of eight in a season. Reduction factor L takes a value of 0.25–1.00 for various categories of accredited low-drift nozzles [4].

Inputs to surface water via drainflow are calculated for UK regulation on the basis of a table relating the percentage of applied pesticide lost in 10 mm drainflow to the sorption properties of the compound (Tab. V, clay soil). This is a worst-case, precautionary assessment based on results from a long-term pesticide transport experiment on a heavy clay soil at Brimstone Farm, Oxon, UK [10]. The soil at Brimstone Farm has 60% clay in the topsoil and is highly structured, meaning that there is great potential for water and associated solutes to move rapidly to depth through cracks and along structural faces. Although the method of calculation is appropriate for p-EMA, it was necessary to further develop the look-up table to cover pesticide losses from a range of drained soils most of which will be much more moderate. As there are no UK data for pesticide losses in drainflow from soils other than clays, a modelling approach was adopted. The MACRO model was first used to simulate Brimstone data for pesticides within each of six Koc categories. Comparison with measured values gave correction factors (all within a factor of 3 for compounds with Koc <4000 ml·g⁻¹) to account for model inaccuracy (Fig. 3). Next, standard soil profiles were derived for each of six soil texture categories (Tab. III) and the model was used to predict losses of the various pesticides in drainflow over a year from application. The maximum loss of pesticide in any 10 mm

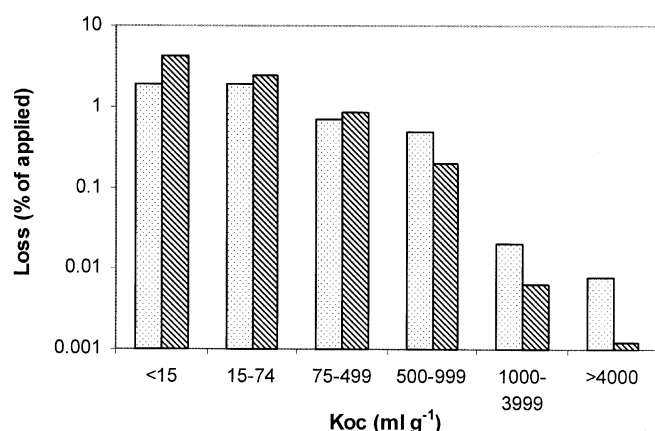


Figure 3. Assessment of the relative accuracy of MACRO for simulating losses of pesticides with a range of properties in drainflow from Brimstone Farm (experimental values open bars, simulated values shaded bars).

flow was derived from the output and these were then adjusted using the correction factors. The system thus predicts percentage of applied loss in 10 mm drainflow according to the Koc of the compound and the soil type (Tab. V).

The loadings to surface water arising from drift and drainflow are used to calculate two initial concentrations in water by dividing the loading into the volume of the water body (plus an additional volume equivalent to 10 mm flow for entry via drains). The larger of the two concentrations is selected and fed into the assessment of acute risk to aquatic organisms. Additive effects from multiple applications of the

same compound are considered for static surface waters only. It is assumed that advective losses will negate any effect for flowing water. Time-weighted average concentrations for chronic assessments are calculated according to first-order kinetics and the most rapid dissipation process from surface water (including partition to sediment).

3. WORKED EXAMPLE

To illustrate the data requirements and output from the exposure model, a simple example is provided comprising a single field sown to sugar beet. The 12 ha field is on a sandy soil in the Bawtry area, near Doncaster, UK. This area has high vulnerability for leaching to groundwater, an average annual rainfall of 680 mm and average winter recharge of <125 mm. A river 2 m wide and 0.6 m deep runs along one side of the field and a further 60% of the field perimeter is hedgerow with no conservation headlands or other special habitats. The river and hedgerow are 1 and 2 m from the edge of the cropped area, respectively. The field receives applications of four pesticides as three products including a seed treatment. A strip of crop 1 m in width around the crop perimeter remains untreated for all spray applications. Details of the application and properties of the active ingredients are provided in Table VI.

Each of the four pesticides applied were run through the exposure model. The resulting predicted environmental concentrations are provided in Table VII. An associated paper [11] describes the combination of these exposure concentrations with ecotoxicity endpoints to generate toxicity-exposure ratios and subsequent conversion to risk indices for communication to the user.

Table VI. Details of properties and example applications of four pesticides to a sugar beet field.

Pesticide	Koc (ml·g ⁻¹)	Half-life in soil (d)	Half-life in water (d)	Date applied	Application rate (g·ha ⁻¹)	Groundcover at application (%)	Interception by the crop (%)	Drift to water (%)	Drift to field margin (%)
Thiram ^a	670	15	0.4	15 March	8.3	0	-	0	0
Lenacil	165	179	30	21 April	176	5	0	0.979	1.40
Carbenda- zim	225	20	60	6 August	82.1	85	80	0.979	1.40
Flusilazole	650	420	1.0	6 August	164.3	85	80	0.979	1.40

^a Applied as a seed treatment; seed sown at 1.0 kg·ha⁻¹ and incorporated to 3 cm depth.

Table VII. Predicted environmental concentrations (PEC's) calculated for applications of four pesticides to a sugar beet field.

Pesticide	PEC for soil in-field (mg·kg ⁻¹)		PEC for soil in the margin (mg·kg ⁻¹)		PEC for surface water (µg·l ⁻¹)		PEC for ground water (µg·l ⁻¹)
	Initial	21-day average	Initial	21-day average	Initial	21-day average	
Thiram	0.0111	0.0071	0.0000	0.0000	0.000	0.000	0.000
Lenacil	0.2347	0.225	0.0033	0.0032	0.287	0.227	0.019
Carbendazim	0.0219	0.0156	0.0015	0.0011	0.134	0.119	0.000
Flusilazole	0.0438	0.0431	0.0031	0.0030	0.268	0.018	0.000

4. CONCLUSIONS

When combined with ecotoxicological information, the exposure assessment model provides a risk-based system which replaces the previous hazard-based approach to pesticide evaluation implemented within EMA. Government policy towards pesticides in the UK is to couple use reduction with risk minimisation. The p-EMA system supports this objective by identifying applications that pose the greatest risk to the environment within the context of local site conditions and farm practices. It is fundamental to the success of the system that the models adopt and build upon current regulatory practice rather than seeking to establish alternative procedures. This ensures that p-EMA delivers a consistent message with respect to regulatory decision-making and controls and industry stewardship activities. Complementarity between regulation and farm-level decision support tools is expected to greatly strengthen initiatives aimed at minimising the risk posed by pesticides to the environment.

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