PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY B BIOLOGICAL SCIENCES

Probability Modelling [and Discussion]

Dennis A. Laskowski, Patti M. Tillotson, Don D. Fontaine and Eric J. Martin

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Probability modelling

DENNIS A. LASKOWSKI, PATTI M. TILLOTSON, DON D. FONTAINE AND ERIC J. MARTIN

DowElanco, Midland, Michigan 48641-1706, U.S.A.

SUMMARY

This paper traces the development of modelling to assess the environmental fate of agricultural chemicals within DowElanco's Environmental Fate Group. Field monitoring of fate was the initial tool for assessment, but inefficiency of the process and poor data interpretability turned the group's attention to benchmarking. This, too, proved to be an inadequate and frustrating process as it evaluated fate only relative to other chemicals and did not allow in an absolute sense the assessment of risk of contamination away from treated locations. It also did not allow the evaluation of management programmes for minimization of environmental impact.

Currently, probability modelling is being evaluated to assess the environmental fate of chemicals and the likelihood of attaining a given concentration at a specified site. It allows the handling of variability and provides estimates of likelihood for environmental events to take place in designated areas of the United States. Through the use of Fourier Amplitude Sensitivity Test and Monte Carlo sampling techniques, ranges of inputs are used to drive environmental models to provide frequency distribution data for output. The process appears useful for assessing environmental impact of chemicals because it allows whole range evaluation with data that are readily available, and provides information appropriate for best management practices.

1. INTRODUCTION

Environmental chemistry has changed considerably over the past 20 years. This relatively new branch of science began to form when it was realized that man must account for the effects his activities have upon the surrounding environment. One aspect of this realization was the dawning that agricultural chemicals used to help feed the world and provide higher quality food had to be understood with regard to their interactions with the surrounding environment. It became clear that the fate of chemicals used in agriculture needed to be known. This paper traces the history of how this process has evolved at DowElanco.

2. USE OF FIELD MONITORING

The initial movement within environmental chemistry dealt with monitoring. Researchers learned of the environmental fate of chemicals through the establishment of monitoring programmes that measured the decline of chemical concentrations in samples of soil, water, or foodstuffs treated with material and then sampled over time. DowElanco did its fair share of monitoring, but it was a frustrating process and soon became obvious from this activity that monitoring alone would not provide answers to the key question emerging from the environmental movement. This was the issue of other life forms being exposed to the same chemicals used to control the presence of pests and disease in agricultural operations. It became clear that simply to monitor the surroundings of an area treated with chemical was not going to show satisfactorily the likelihood of exposure to non-target organisms. There had to be a better and more efficient way of determining whether chemicals were likely to move away from the site of their placement.

An example is provided to show the inadequacies and frustrations encountered when monitoring data are used to determine the movement of chemicals. In 1965 extensive field monitoring of the soil fate of one of DowElanco's weed control chemicals was done. The chemical was picloram and the researchers were J. W. Hamaker, C. R. Youngson and C. A. I. Goring (Hamaker *et al.* 1967). They monitored the soil fate of picloram at 207 locations within the United States and Canada. Picloram had been applied to the sites and then soil from each site was sampled to determine the chemical's movement from the soil surface to lower depths, and to evaluate how rapidly the material would dissipate from the treated areas. The results with regard to movement through the soil profile are summarized in table 1.

The number of positive findings along with relative distribution of picloram with depth of sampling are shown in the table. When chemical was still present in the soil profile, the pattern of distribution suggests bleed from the treated surficial soil layers to those below, but not often beyond 60 cm. The top layers contained most of the material followed by decreasing amounts in the lower depths.

Although patterns of picloram movement through

Table 1. *Pattern of distribution of picloram in soil profiles collected after treatment of 207 field locations with picloram*

(Hamaker *et al.* 1965)

depth (cm)	picloram	
	number of positive findings	% distribution
0–30	100 (48 %)[a]	73–85[b]
31–60	100 (48 %)	15–27
>60	12 (6 %)	Trace-20

[a] This is the percentage of the total number of sites (207) that had positive findings.

[b] This column of values refers to the distribution of picloram within the soil profile for those profiles having picloram present at time of sampling.

soil are apparent from the work, it is not possible from the extensive monitoring to determine climatic and soil situations that had caused greatest movement away from site of application. It is difficult to extrapolate the results to different sites separated geographically and having different combinations of soil and climate. Furthermore, it is not known what might happen the following year at the same locations, but with different patterns of weather. These things must be known if there is to be a successful characterization of the likelihood for contamination by agricultural chemicals moving away from site of placement.

3. BENCHMARKING

The next technique that attention was turned to was the process of benchmarking. This procedure centres around the idea that environmental fate of unknown chemicals can be determined by comparison of key environmental properties to those of chemicals already characterized environmentally. DowElanco developed expressions that combined properties in such a way as to compare relative tendencies for chemicals to leach through soil, vapourize away from site of application, and to persist within the treated area (Laskowski *et al.* 1982). The key properties were soil degradation rate as represented by number of days to degrade 50 % of the initial material, water solubility, vapour pressure, soil/water partition coefficient in the form of K_{oc}, and the octanol/water partition coefficient K_{ow}.

Expressions (table 2) were developed that would combine these properties in such a way as to allow comparison of the relative tendencies for how chemicals behaved environmentally. Table 3 shows how the procedure might work. The table presents a ranking of agricultural chemicals with regard to their relative tendencies to leach through soil, based upon the properties listed above. As shown in the table, it was assumed that leaching away from point of application to soil is directly related to water solubility and time to degrade 50 %; and inversely related to a chemical's vapour pressure and soil adsorption constant. A listing of chemicals is presented in the table, starting with the one most susceptible to movement at the top of the list and ending with the one least likely to move at the bottom. In this manner it is possible to place unknown materials relative to known benchmarks and thus begin to comprehend how the unknown material might behave environmentally.

Table 2. *Expressions used to combine key environmental properties together to compare environmental behaviour of chemicals relative to each other*

(After Laskowski *et al.* 1982)

leaching potential	$S/[(V_p)(K_{oc})]$
leaching index	$[(S)(t/2)]/[(V_p)(K_{oc})]$
volatility potential	$V_p/[(S)(K_{oc})]$
volatility index	$[(V_p)(t/2)]/[(S)(K_{oc})]$
on-site exposure	$[(t/2)(K_{oc})(S)(K_{ow})(F)(R)]/V_p$
off-site exposure	$[(t/2)(V_p)(K_{ow})(V)]/[(K_{oc})(S)]$

Abbreviations used: S, water solubility; V_p, vapour pressure; K_{oc}, soil adsorption constant; $t/2$, soil half-life (in days); K_{ow}, octanol/water partition coefficient; F, frequency of chemical application; R, amount of chemical applied; V, volume of material manufactured.

Table 3. *Relative ranking of potential for chemicals to leach through soil*

(After Laskowski *et al.* 1982)

chemical	leaching index[a]
dicamba	1×10^{10}
picloram	9×10^{9}
monuron	1×10^{9}
carbofuran	2×10^{8}
2,4-D	1×10^{8}
atrazine	1×10^{8}
alachlor	4×10^{5}
propachlor	4×10^{4}
malathion	4×10^{3}
lindane	2×10^{3}
dieldrin	5×10^{2}
chlorpyrifos	2×10^{2}
DDT	1×10^{2}
1,3-D	4×10^{1}
trifluralin	2×10^{1}
heptachlor	8

[a] Leaching index = $[(S)(t/2)]/[(V_p)(K_{oc})]$.

The difficulties and disenchantment that set in after use of the benchmarking process arose from the fact that interpretation was only relative to other chemicals and did not address the key issue of what might happen during actual use of the product. It was not possible to consider exposure levels to non-target organisms, nor was it possible to evaluate the interactions of climate and soil properties with the environmental properties of a chemical and its pattern of usage. It became quite frustrating in that better management practices could not be implemented through the benchmark process, and actual levels of contamination of the surrounding environment could not be determined.

4. PROBABILITY MODELLING

After benchmarking, attention within the Dow-Elanco Environmental Fate Group focused very

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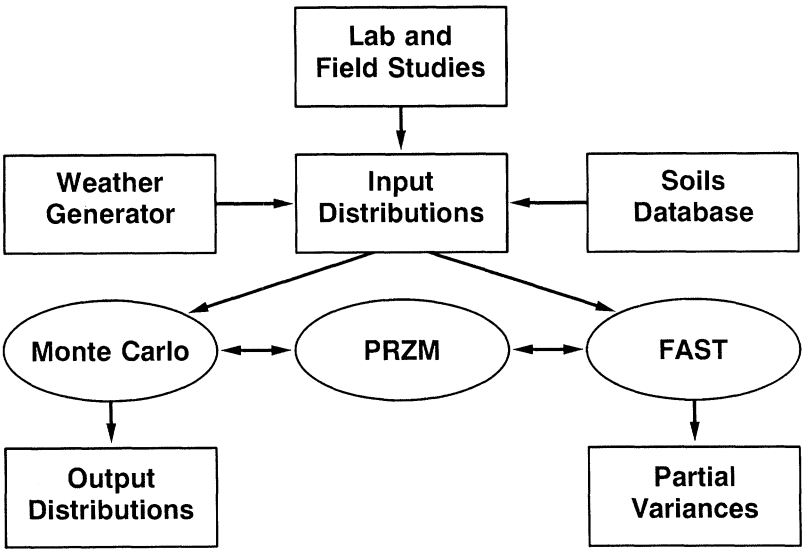

Figure 1. Schematic outline of the probability modelling process.

distinctly upon modelling, and how it might be used to manage DowElanco's products environmentally. It was recognized that only the process of modelling would allow the merger of environmental properties with pattern of use, patterns of climate, and types of soil. But the modelling had to be of a certain kind. It had to deal with variability in the inputs used to drive the models; rainfall, topography, temperature, and soil properties vary considerably according to where and how chemicals are used. It was necessary that the modelling process accepted and propagated the variability of input, and carried it on into the modelling output.

The process selected by DowElanco and now under development is coined 'probability modelling' in this paper. It is a kind of modelling designed to show statistical trends for environmental activities to take place, and was developed through the efforts of E. J. Martin, P. M. Tillotson, and D. D. Fontaine from the Environmental Fate Group at DowElanco, along with G. J. McRae at Carnegie–Mellon University. Figure 1 provides a schematic description of the process.

The procedure begins with lab studies to measure key environmental properties, and field studies to validate their appropriateness as input into a model describing the environmental activity of interest. For purposes of this paper, the likelihood of groundwater contamination is the point of interest. The model describing chemical movement through soil is PRZM, a chemical transport model developed several years ago by EPA scientists (Carsel *et al.* 1984). There is a weather generator (Richardson & Wright 1982) to generate rainfall and temperature distribution patterns specific to distinct areas of the United States, and the USDA Soil Conservation Service's soil survey database for generating the correct soil property distribution patterns (Oliver & Laskowski 1984). Collectively, these serve as input to the model; output is the corresponding distribution of results as dictated by input distributions into PRZM.

Sampling components of the process are Monte Carlo and Fourier Amplitude Sensitivity Test (FAST) techniques. Monte Carlo is a fairly well-known technique that has been used by Carsel *et al.* (1988) recently to provide a similar distribution of output; FAST is not as well known, having been developed by Cukier *et al.* (1973), and expanded upon more recently by McRae at Carnegie–Mellon University (McRae *et al.* 1982). The purpose of FAST is to supplement the Monte Carlo sampling techniques. It is used first to perform sensitivity analysis on the inputs, and then it selects those inputs having the greatest impact on the model's output for further use in Monte Carlo.

Figure 2 shows schematically how the modelling process works. Monte Carlo or FAST analysis is used to develop combinations of input values according to their natural distributions, which are then used by PRZM to generate a corresponding output frequency distribution of maximum depths to which the chemical in question leached. This output frequency distribution then serves as the basis for evaluating the likelihood of a chemical to move deep enough to contaminate groundwater. The risk of groundwater contamination from the use of a chemical in a distinct area of the country, or under a certain management practice, is defined by the area of overlap with the corresponding

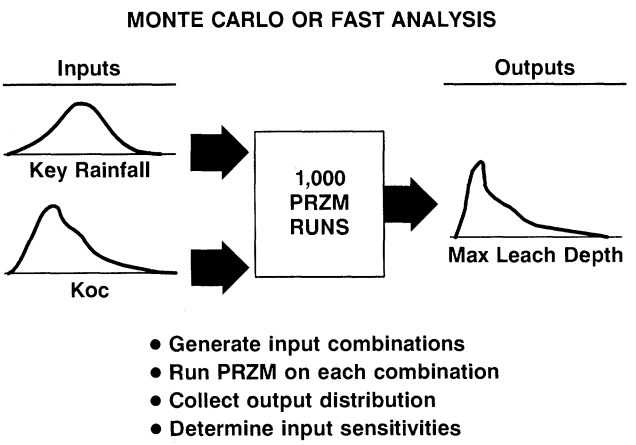

Figure 2. Diagrammatic description of how the probability modelling process works.

frequency distribution of depth to groundwater for that same area, as shown in figure 3.

The reason for using a sampling technique like FAST instead of relying exclusively on Monte Carlo deals with the differences by which the procedures sample input distributions. Figure 4 provides a comparison of the two methods, showing their relative strengths and weaknesses. As shown in the figure, FAST allows the use of many input parameters, provides greater sampling of extremes, and yields the best sensitivity coefficients. But FAST oversamples the extremes and therefore does not maintain the integrity of input distribution in its output. Monte Carlo on the other hand, remains faithful to the distribution of input, and produces accurate distribution of output. However, Monte Carlo is computationally intensive and cannot tolerate as many input parameters, making it more difficult to develop sensitivity coefficients with this procedure.

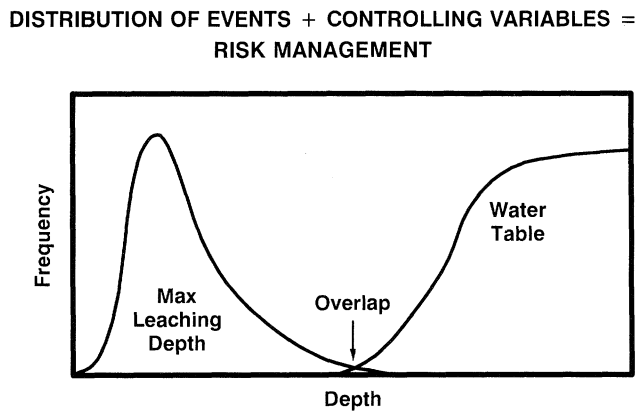

Figure 3. Risk of groundwater contamination as defined by overlap between maximum leaching depth frequency distribution and water table frequency distribution.

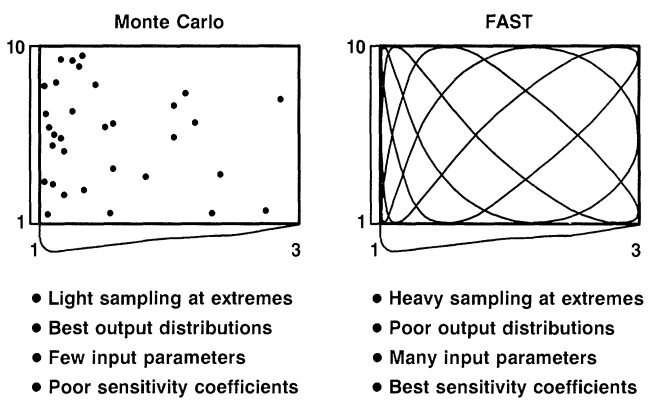

Figure 4. Comparison of Monte Carlo and FAST sampling techniques utilizing two variables. The line below the bottom of each X axis represents the distribution of the variables.

Together the two methods work very well in identifying those parameters most important in influencing the outcome, and then developing the frequency with which an event of interest is likely to happen.

Figure 5 presents an illustration of what the output from the probability modelling might look like. This example is for an agricultural chemical being considered for use by DowElanco in the midwestern corn region of the United States. In the figure, the X axis represents the maximum depth in centimetres at which the chemical would be detected at a detection limit of one part per billion. The Y axis shows the frequency with which the PRZM leaching model predicted a given depth, based upon the ranges for the input parameters: percentage soil organic carbon content, soil adsorption constant L_{oc}, total key rainfall (rain falling within 30 days of application), and soil degradation rate as represented by half-life. FAST was used to select these four parameters as having the greatest impact on the chemical's leaching. (Partial variances in the figure show their importance.) Monte Carlo was then used with these four variables to generate the frequency data shown in the figure. The range used for each variable is also shown.

This type of modelling has definite appeal because it

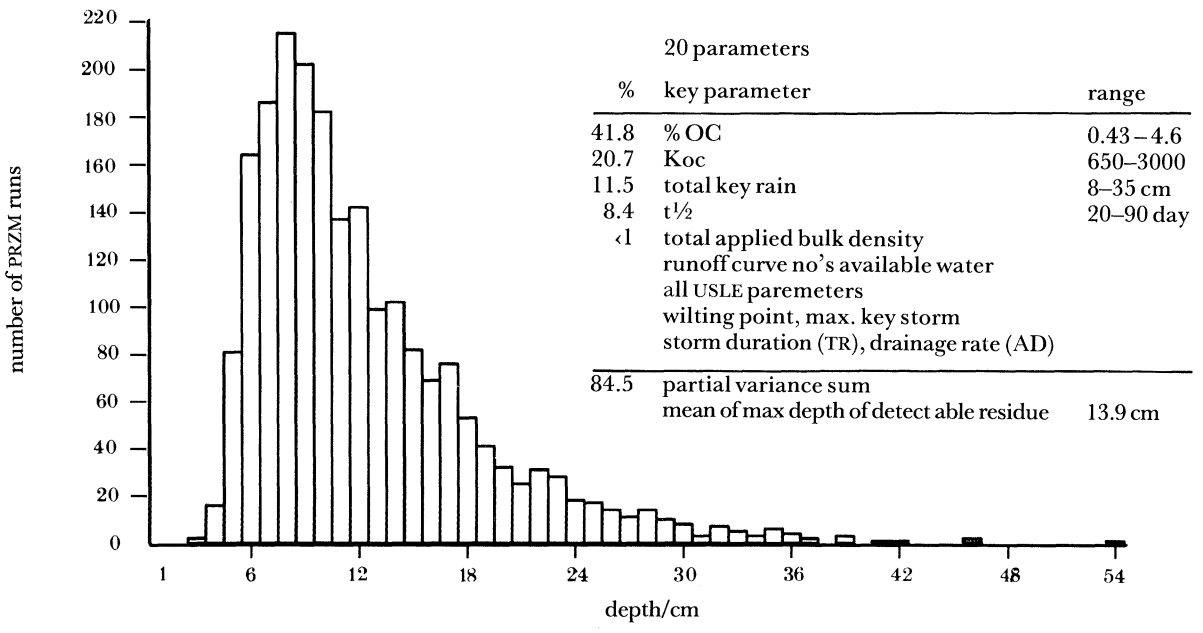

Figure 5. Example of probability modelling output. Frequency distribution of maximum leaching depth for a DowElanco experimental chemical used in the midwest corn market.

propagates variability of input parameters and utilizes data readily available from existing databases. The aspect of variability is of particular interest. Variability has been and continues to be a big issue with researchers involved in environmental modelling. Everyone realizes that nature is full of variation, but debate continues with regard as to how it should enter into the modelling process. The unique thing about probability modelling is the technique's ability to consider the whole range of variability for each input parameter during a modelling exercise. This is of considerable interest because it could allow the debate on environmental impact to move from a shaky foundation of a few field-study results or 'single-modelling-run, worst case situations' to a more meaningful 'most probable event' interpretation. The procedure could provide a mechanism for evaluating real risk of contamination to the environment.

One additional feature that is of interest is the process's ability to identify those input parameters having the greatest impact on output. It is the Environmental Fate Group's intent to utilize this information to focus research effort on the issues deemed most important for assessing the environmental fate of chemicals.

5. THE FUTURE

Future efforts will focus on refinement of the probability modelling process, along with assessment of techniques for disseminating the modelling information to DowElanco's customers and government agency decision makers. The system needs to become more user friendly; and there must be testing to see if predicted frequency distributions relate favourably to actual observed frequency of occurrence. Geographic information systems will be utilized to transform information into more readily understood graphic forms. And expert systems will be examined for their use as friendly 'shells' that allow non-experts to access data bases created by the modelling.

Finally, the group's efforts will be aimed at model improvement. Areas of known weaknesses are the kinetics of sorption/desorption of chemicals, the kinetics of soil degradation, the inability to handle daughter product formation in the models, and inability to describe vapour transport through and from soil.

One area of weakness is the issue of sorption–desorption kinetics. In the environmental arena a concept of two compartments is emerging with regard to the behaviour of chemicals in soil. These compartments (available versus unavailable) relate to changes in availability of a chemical with regard to the residence time of the material within the soil matrix. This availability can deal with aspects of controlling unwanted pests, it may deal with susceptibility to degradation, or it may relate to the ease with which chemicals move through soil profiles during leaching events.

The latter aspect is of considerable interest as much attention is being turned to the pollution of groundwaters from agricultural practices. What is emerging within the scientific community is somewhat of an anomaly. On the one hand there is the suggestion that chemicals can migrate deeper into the soil profile than first thought, because of preferential flow. This is the process by which water flows through large pores and cracks, bypassing much of the soil and thus penetrating deeper than if the flow were uniform throughout the entire matrix. Chemicals dissolved in this water are swept along with the rapid flow without interacting much with the surrounding soil solids. The result is deeper penetration than would be predicted from theory of water movement and soil adsorption partition coefficients.

On the other hand, there is also evidence to indicate less than expected penetration of chemicals after a leaching event. This is thought to occur because of chemical diffusion deep into the organic coatings on soil particles and into the aggregate structure soils naturally possess. This seems to be a normal phenomenon. Once chemical is buried within the coatings or a soil aggregate, it is not as available to leaching, and can no longer exchange as readily back out into the free water moving rapidly through the profile. The result is less than expected movement, and movement characterized more by a slow bleed of material from the surface to the soil layers lying below. The field monitoring data in table 1 dealing with picloram movement support this concept of slow bleed.

Evidence for and discussion of these concepts have been presented by a variety of researchers (Davidson & Chang 1972; Davidson & McDougal 1973; Leistra & Deckkers 1977; McCall & Agin 1985; Rao *et al.* 1974; Van Genuchten & Wierenga 1976; Wu & Geschwend 1986). Experimental evidence for change in availability of one of DowElanco's agricultural chemicals was obtained by P. J. McCall (McCall & Agin 1985), and a portion of the data are summarized in table 4 for purposes of illustration. The data are from an experiment aimed at evaluating the influence of residence time in soil on the rate of desorption of the chemical picloram from soil back into solution. The chemical was incubated in moist soil for periods of 0–300 days. Then desorption was performed by adding water with agitation, and the kinetics of desorption were evaluated by monitoring the release of material into the water. Table 4 summarizes data from a two-minute equilibration period, and one can readily see the change in availability of material by the shift in

Table 4. *Influence of picloram residence time in Holdredge loam on desorption kinetics as shown by K_d after 2 min of desorption equilibration*

(After McCall & Agin 1985)

incubation (days)	apparent K_d
0	2.9
14	4.4
28	5.3
56	6.5
100	8.4
200	10.3
300	12.9

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apparent partition coefficient with time. This was considered to reflect the change in picloram associated with external soil surfaces early in the study to picloram associated with internal surfaces as time of picloram contact with the soil progressed.

Another key issue to be addressed by the Environmental Fate Group in the future is soil degradation kinetics. Models do not handle the kinetics of soil degradation very well, and do not allow the modification of degradation rates during a modelling run. Thus there can be no corrections to degradation rate because of changing climatic conditions such as soil moisture and soil temperature. These are known to have real impact on degradation kinetics, and models must do a better job of describing their interactions. There have been successful modelling exercises that couple soil moisture and temperature to degradation rate; the most notable are the series of elegant studies conducted by Walker (1978). Sensitivity analysis with FAST has shown the importance of degradation rate on transport of chemical through soil, and the Environmental Fate Group will focus its attention on improving models in this general area.

REFERENCES

Carsel, R. F., Jones, R. L., Hansen, J. L., Lamb, R. L. & Anderson, M. P. 1988 A simulation procedure for groundwater quality assessments of pesticides. *J. Contam. Hydrol.* **2**, 125–138.

Carsel, R. F., Smith, C. N., Mulkey, L. A., Dean, D. & Jowise, P. 1984 *User's manual for the pestitide root zone model (PRZM)*. Release 1. Athens, Georgia: U.S. Environmental Protection Agency, Environmental Research Laboratory.

Cukier, R. I., Fortuin, C. M. & Shuler, K. E. 1973 Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. I. Theory. *J. chem. Phys.* **59**, 3873–3888.

Davidson, J. M. & Chang, R. K. 1972 Transport of picloram in relation to soil physical conditions and porwater velocity. *Soil Sci. Soc. Am. Proc.* **36**, 257–261.

Davidson, J. M. & McDougal, J. R. 1973 Experimental and predicted movement of three herbicides in a watersaturated soil. *J. environ. Quality* **2**, 428–433.

Laskowski, D. A., Goring, C. A. I., McCall, P. J. & Swann, R. L. 1982 Terrestrial environment. In *Environmental risk analysis for chemicals* (ed. R. A. Conway), pp. 198–240. New York: Van Nostrand Reingold Company.

Leistra, M. & Deckkers, W. A. 1977 Some models for the adsorption kinetics of pesticides in soil. *J. environ. Sci. Health* **B12**, 85–103.

McCall, P. J. & Agin, G. L. 1985 Desorption kinetics of picloram as affected by residence time in the soil. *Environ. Tox. Chem.* **4**, 37–44.

McRae, G. J., Tilden, J. W. & Seinfeld, J. H. 1982 Global sensitivity analysis – a computational implementation of the Fourier amplitude sensitivity test (FAST). *Computers Chem. Engng.* **6**, 15–25.

Oliver, G. R. & Laskowski, D. A. 1984 Computerized soils information for the agronomic industry. *J. agric. Ed.* **13**, 115–117.

Rao, P. S. C., Green, R. E., Balasubramanian, V. & Kanehiro, Y. 1974 Field study of solute movement in a highly aggregated oxisol with intermittent flooding: II. Picloram. *J. environ. Quality* **3**, 197–202.

Richardson, C. W. & Wright, D. A. 1982 *WGEN: A model for generating daily weather variables*. Temple, Texas: U.S. Department of Agriculture, Agricultural Research Service Grassland Soil and Water Research Laboratory.

Van Genuchten, M. Th. & Wierenga, P. J. 1976 Mass transfer studies in sorbing porous media. I. Analytical solutions. *Soil Sci. Soc. Am. J.* **40**, 473–480.

Walker, A. 1978 Simulation of the persistence of eight soil-applied herbicides. *Weed Res.* **18**, 305–313.

Wu, S. & Geschwend, P. M. 1986 Sorption kinetics of hydrophobic organic compounds to natural sediments and soils. *Environ. Sci. Technol.* **20**, 717–725.

Discussion

D. J. Greenwood (*AFRC, Institute of Horticultural Research, Wellesbourne, U.K.*). Often the inputs into your models must be highly correlated with each other, especially in the case of soil characteristics. For instance, the soil organic matter content must be strongly negatively correlated with adsorption constant. How do you cope with such correlations?

D. A. Laskowski. Correlations among input variables are easily accounted for in the Monte Carlo module of our computerized 'probability modelling' system. The Monte Carlo module consists of a program developed by Iman & Shortencarier (1984) that utilizes a Latin hypercube sampling technique. This program allows users to specify a correlation matrix for input variables in the Monte Carlo analysis. For one particular system, this correlation matrix would include correlations among soil and pesticide properties.

It should be noted that correlations among input variables are not always well defined and are often unknown. The real problem is to define what these correlation matrices should be. In our system, correlations among soil properties are estimated from the USDA Soil Conservation Service's soil survey database (Oliver & Laskowski 1984). However, our limited experience with correlations in this database suggests that it may provide physically unreasonable correlation values in some cases.

References

Iman, R. L. & Shortencarier, M. J. 1984 *A fortran 77 program and user's guide for the generation of Latin hypercube and random samples for use with computer models*. NUREG/CR-3624, SAND83-2365. Albuquerque, New Mexico: Sandia National Laboratories.

Oliver, G. R. & Laskowski, D. A. 1984 Computerized soils information for the agronomic industry. *J. agric. Ed.* **13**, 115–117.

J. H. Ottaway (*Department of Environmental Science, University of Bradford, U.K.*). The technical attraction of the modelling system described by Dr Laskowski is very great, but, as he himself has said, the biological/biochemical component is rather weak, leading to poor results with metabolites. This concentration on physico-chemistry, with respect to biology, is very noticeable if one compares this model with those currently being used for risk assessment of carcinogens (see for instance the Banbury Report **31** (1988)). However, is it possible that the attractiveness of the quantitative outputs provided by the Dow model may lead to its results being incorporated as they now stand,

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quasi-permanently, into the recommendations of regulatory agencies? That is, will once again 'the medium be the message'?

D. A. Laskowski. As Dr Ottaway describes in his question, we presented a system of modelling, which is not really restricted to a specific model. In other words, our focus was on the concept of probability modelling, and how it might be used as a tool for making environmental decisions. The model itself is an integral part of the process, since it provides the actual estimates of environmental concentrations for the exposure side of the exposure/toxicity components of environmental impact.

Models do indeed have strengths and weaknesses, as pointed out by Dr Ottaway, and this is recognized by those who work with them. However, models are tested frequently, represent the current state of knowledge, and therefore are legitimate to that extent. Models are constantly being improved with advancement in knowledge.

It is our perception that regulatory agencies are aware of model limitations and do treat modelling information with caution. They also recognize that processes like probability modelling provide the first real opportunity for agency reviewers to integrate massive amounts of data received as isolated pieces of information into a coherent picture aimed specifically at addressing impact to the surrounding environment. Even though the process may not be without flaw, it certainly is a step ahead for environmental chemistry, and, as in any scientific arena, will continue to be developed and improved as more is learned.

R. Webster (*Centre de Géostatistique, École Nationale Supérieure des Mines de Paris, Fontainbleu, France*). I am pleased that Dr Laskowski and his colleagues are attempting to compute probability distributions of the depths to which agricultural chemicals move in the soil. The distributions from their model depend on the distributions of soil properties among others that enter the model. And so, if they are to represent the underlying distributions faithfully then the input distributions must be derived from a probabilistic sampling of the soil. Otherwise they will almost certainly be more or less biased. So, I should be grateful if Dr Laskowski would say precisely how the soil was sampled over such large regions to provide the data for modelling.

D. A. Laskowski. The U.S.A. has a steadily improving, comprehensive soil inventory database through cooperative soil survey efforts by USDA Soil Conservation Service, State Extension Services, and local governments. The current goal, outlined by Congress, is to completely map and inventory all agricultural lands by the end of 1990. We estimate that more than 90% of the corn belt acreage was included in the database at the time of our study.

Soil survey methods are similar throughout the world, and are dependent upon map scale. At the scale of mapping for primarily agricultural uses (*ca.* 1:200000) an experienced soil scientist will probe relatively few, but well chosen, positions on the landscape to develop the soils map. The mapper uses knowledge of soil formation processes, past experience with soils in the area, and airphoto interpretation skills in developing the map. Map unit composition (expressed as a percentage of soil taxa expected within a map unit) is determined by more intense sampling of random transects located within randomly selected map polygons. This information is summarized for each map unit by acreage in each soil survey area. The national soils database (SOI-6 portion) contains this information, along with reference to acreage of each taxonomic unit within a soil survey area.

Each taxonomic unit (generally classified at the soil series taxonomic level) has an entry in the national soils database (SOI-5 portion) for interpretation of potential soil uses. Ranges of soil properties, some of which are pertinent physicochemical soil characteristics for pesticide transport models, are listed. The range in value for a soil characteristic within a taxon reflects field-observed/laboratory-measured values. Soils are classified by a combination of soil properties; soils observed in the field that fall outside the allowable ranges for an important property (i.e. percentage of clay) necessarily are classified to be within a different soil series.

We view the soils information available to us to be a complete inventory of the population of soils within the region at the commonly used map scale. Model input distributions of soil properties are based upon ranges listed for each soil taxon and known distributions for soil properties from the body of soil science research. We agree that for a less well-characterized population elaborate sampling schemes would be necessary. For regional analysis, however, the existing database allows us to enter data on the 'true' distributions of soil properties to the models without need of probabilistic sampling. The probability of occurrence of a particular soil property value, as seen by the models, is that of the acreage distribution for soils with that property within the region.

S. P. S. Andrew (*The Wynd, Stainton, Middlesbrough, U.K.*). In estimating leaching the solubility has been described as that in pure water. Natural waters, particularly surface water, often contain considerable quantities of plant and microbial decomposition products – humic substances etc. To what extent do these act as solubilizing agents for pesticides which would in pure water have a very low solubility.