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Simulation modelling and soil behaviour

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ABSTRACT

The increasing power and availability of computers has encouraged both the development of computer-based simulation models and their use in making decisions. It has therefore become increasingly important to understand what a model is, when it can be used validly and in what circumstances it can be said to predict. There are also several types of models not all of which are suitable for all purposes. This paper offers some guidelines for soil scientists. Models must be properly validated, particularly when used in decisions, and a recently published validation scheme is summarized. It is suggested that models should be analysed not only for sensitivity to changes in their parameters but in some circumstances to changes in parameter variance, particularly where the model may not be linear with respect to its parameters. Non-linearity may be a problem where parameters are subjected to spatial averaging or interpolation. Models are sometimes developed and validated at one scale and then used at a larger scale. Problems may result, and some questions are suggested that should be asked when a change of scale is envisaged. Some of the modelling challenges implicit in the evolution of sustainable forms of agriculture are discussed.

INTRODUCTION

Twenty-five years ago computer modelling was a rather esoteric activity carried on by a small group of soil scientists to the considerable puzzlement of most of their colleagues. Today's computer modellers could find their activities contributing to decision-making by Governments on environmental and related issues. This change reflects both the enormous advances in the power and availability of computing and the current ubiquity of the computer in everyday life. It is to be welcomed wherever it makes the voice of soil science heard more clearly by those who make decisions, but it also emphasises the essentiality of getting models right — or as nearly right as possible — and of making sure that they are used properly, particularly in any form of decision-making process. It may even necessitate speaking out against inappropriate use of models (e.g. Addiscott and Powlson, 1989).

This paper builds on a review by Addiscott and Wagenet (1985a) that sought to classify leaching models in a framework that distinguished between deterministic and stochastic, mechanistic and functional and rate and capac-

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ity models, and discussed them in terms of their purpose, complexity, flexibility and other measures of practical usefulness. It pursues further several of the issues raised in the previous paper, notably that of validation of models, and also refers to Beven's (1989) thoughtful review of physically-based models in hydrology and to the distinctly astringent review of modelling by Philip (1991). Several definitions are included and the paper discusses in particular what a model is and when a model can be said to "predict". It also makes a suggestion about sensitivity analysis of models that springs from the impact of the spatial variability of a model's parameters on its performance, a topic that emerged as important in the earlier review (Addiscott and Wagenet, 1985a) and which is discussed again here. The paper discusses finally which processes need to be modelled if we are truly to "model soil behaviour".

DEFINITIONS

The following definitions are offered mainly for those not usually involved in modelling. Not all modellers will necessarily agree with them.

Model

A model is a *representation* of reality, albeit a simplified one; this is true of a model of a soil process as it is of a model boat. The difference between the boat and the soil lies in the fact that all relevant details of the boat are known for certain, whereas in the soil there may be some discussion as to which details are important and considerable uncertainty about the values to be given to the details chosen. The soil model is therefore more in the nature of a *hypothesis*. Probably the most useful description (or model) of how scientists work is the *hypothetico-deductive* principle of Popper (1959), also discussed by Medawar (1967). Popper argued that science advances through scientists forming hypotheses about the processes they study and testing them against experiments that can refute the hypothesis. If, as usually happens, the hypothesis is not correct, it is revised and retested until it matches reality sufficiently closely; guidance from statistics is usually helpful at this point. Although hypotheses are often framed in words or single equations, the nature of the soil and the number of processes that can occur in it usually means that a number of equations are needed and that these have to interact with each other; a model that brings together these several equations is probably best described as an *extended hypothesis*. Such a model is almost inevitably formulated in a computer language, most often FORTRAN, and run in a computer. It is, however, important to remember that an extended hypothesis in the form of a computer model must be tested against reality, preferably in a way that enables it to be refuted. The term used by modellers is "validation" and this is a topic to which we shall return.

One question that arises is whether a "model" is in any way different from the much older concept of a "theory". If both develop along the lines suggested by Popper (1959) there seems to be no reason for them to differ and Philip (1975) wrote, "Personally, I have trouble in comprehending how modelling seeks to do anything different from what natural science has been trying to do for at least 300 years. Perhaps, after all, Newton and Einstein were simply "modellers", and it may be that what set them apart is that they were especially wise and especially humble." Philip (1991) quoted Niederer (1990) with approval when the latter suggested that any distinction was one of jargon and said, "In waste management rather than of theories we speak of models, and instead of testing theories we validate our models. But the essential concept and the ultimate goal have always been the same: To find truth." Philip is not an admirer of modelling. He adds rather acidly, after quoting Niederer as above, "I was much heartened by this affirmation that models have to do with truth. That this was a conjunction outside my experience might be construed from what follows." [What does follow (Philip, 1991) is too lengthy to be quoted fully here but is well worth reading.] The key point to remember is that a model is essentially a hypothesis and that no model is perfect; it would presumably cease to be a model if it were. Models are useful usually not because they reproduce reality but because they simplify it and thereby enable the most important aspects to be identified, studied, simulated and, if all is well, predicted in advance. Because of the element of simplification, no model should be used to make predictions outside the context in which it was developed or beyond the range of parameter values from which it has been validated.

Parameters and data

Models need inputs of information, usually in numerical form, which may be parameters or data. These terms overlap to some extent, and the distinction between them is best seen from the dictionary definition of "parameter": quantity constant in case considered but varying between different cases. The quantity of water held at a given hydraulic potential can be a model *parameter*; it is nearly constant for a given soil but varies appreciably between soils. The rainfall that supplies the water is *data* because it does not occur in any consistent way.

Modelling the soil gives an extra dimension to the definition of *parameter*, because soil parameters may vary considerably from point to point within a field. This does not necessarily invalidate the definition because the assembly of values for the site may remain constant. What it does mean, however, is that we need to take account of the variation in the parameter as well as its mean. Failure to do so loses information and can lead to a false result (Rao et al., 1977; Addiscott and Wagenet, 1985b). The problem of variability is

pursued later in the paper. Parameters may also change with time. The definition of the term suggests that they then cease to be parameters, but in practice a parameter that changes in a gradual, regular and definable way remains useable whereas one that changes erratically with time does not.

Simulation and prediction

The word "predict" is used rather loosely in the context of modelling, as can be seen from the dictionary definition, "foretell or prophesy". We obviously need to be quite clear what models do and do not do, which in turn determines the uses to which they should and should not be put. The word "simulate", however, can be used quite safely. A model can be said to simulate a set of experimental data regardless of how the simulation was achieved, provided the simulation fits the data according to some predetermined criterion (see below). With "predict" we have the problem of the time element implicit in its Latin root; "*prae*" translates as "before", which leaves open the question before what? Can a model really be said to "foretell" an event? Much depends on (a) how the parameters of the model are obtained and (b) the timing of the use of the model relative to the events being "predicted" or "foretold". It is not unknown for a modeller to infer the values for some of the parameters of his model from the data to be simulated. The result then is most certainly not a prediction; he needs to know the outcome before he can predict it! Clearly the parameters must be independent of the data to be simulated. This allows the practice of inferring parameter values from one set of experimental data and then using the model to predict another set, although this may not be a simple procedure (Beven, 1989). Because parameters interact with each other, calibrations of equal merit may be given by two or more completely different combinations of parameters, none of which can necessarily be said to be the "right" one. It is far better if parameters can be obtained independently of the model altogether. When models are used, for example, in the practical management of nitrogen in the soil, weather-related events may be simulated from weather data *after* they have happened but before their outcome is known. Here it seems fair to upgrade the "simulation" to a "prediction", but can models ever foretell events?

One answer is that a model should be able to predict from what is already known events not yet observed. Astronomical models, for example, predicted (literally) the existence of the planet Pluto and the ripples at the edge of the universe, both of which were eventually observed. It would be good to be able to record similar predictions in soil science but I am, alas, not aware of any. (I should add, to be fair, that Soil Science has not had the resources devoted to Astronomy.)

What models can do in a more mundane way is to take weather data from the past and use it to predict what is most *likely* to happen in the near future.

An example of this is to be found in a service provided from Rothamsted to farmers and advisors that included assessments of probable leaching after the current date. This was based on rainfall to date in the current year and rainfall in past years on subsequent dates. The median loss and the upper quintile were presented for three generalized soil types (Bland et al., in prep.).

CLASSIFYING MODELS

A scheme for classifying leaching models was suggested by Addiscott and Wagenet (1985a) with the aim of facilitating the choice of appropriate models for particular situations and purposes. This scheme, outlined in Table 1 was for leaching models, and some comments will be made as to its appropriacy for other purposes.

The scheme distinguishes first between *deterministic* and *stochastic* models. A deterministic model presumes that a certain set of events leads to a uniquely definable outcome, while a stochastic model presupposes the outcome to be uncertain and is structured to accommodate this uncertainty. Practically all natural systems have intrinsic uncertainties but these are ignored in a deterministic model, which can only simulate the response to a single set of conditions. Whether the simulations are useful depends on the nature and extent of the variability that has been ignored.

The second distinction is between *mechanistic* and *functional* models, which may in effect be that between more and less mechanistic models. A mechanistic model seeks to describe in the most fundamental way possible the mechanisms of the process, while a functional model aims to give a good general description of the process without going into great detail. A functional model is more likely to simplify the process than a mechanistic one, but this usually means that its parameters are easier to obtain. Despite the simplification, functional models often give simulations that are at least as good as those of mechanistic models (e.g. Nicholls et al., 1982; De Willigen, 1991) while us-

TABLE 1

A classification of models (after Addiscott and Wagenet, 1985a)

(1) Deterministic			
(a) Mechanistic	(usually with rate parameters)		
(b) Functional	(usually with capacity parameters)		
(2) Stochastic			
(a) Mechanistic	(randomly-selected distributed parameters)		
(b) Non-mechanistic	(based on probability density function)		
Other considerations			
Purpose	Complexity	Flexibility	Transferability

ing far less computer time and they seem likely to be increasingly advantageous as the physical scale of the modelling exercise increases (see below).

The classification for leaching models included a distinction between *rate* and *capacity* models which corresponded approximately to that between mechanistic and functional models. "Capacity" refers to the capacity of the soil to hold water, which is important because the more water can be held, the more rain has to fall to displace water and solute downwards. Rate implies the rate at which water is transmitted through the soil carrying solute with it. A capacity model normally computes changes in the amounts of water and solute in the profile without reference to the time during which they occur, while a rate computes rates of change. This distinction refers primarily to the parameters of the model, and there is much to be said for a model that has both rate and capacity parameters. One such model is the SLIM model of Addiscott and Whitmore (1991) which has both a capacity parameter and a much simplified rate parameter. This distinction applied primarily to leaching models but there may be parallels in other areas of modelling.

One very practical distinction between models is that of *purpose*. Some models find their main use in research, where they are used to test the current level of understanding of a process and expose areas in which more needs to be known. Others are used more as management aids to facilitate the efficient use of resources. This is not an unequivocal distinction. Some research models may, with some simplification — usually in the way the parameters are handled, be used in management. The LEACHM family of models (Wagenet and Hutson, 1989) provides an example. Conversely, some management-type models can aid research, particularly in the interpretation of field experiments. I am grateful to G.J.S. Ross (pers. commun., 1992) for the example in Fig. 1. Here we have the results of five notional treatments, one of which is significantly different from the rest. When, however, the results are simulated with a model it appears that this significant difference was to be expected and

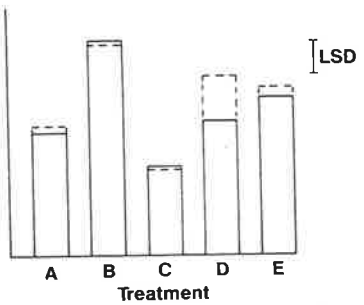

Fig. 1. The notional results of five treatments in an experiment. Treatment *B* is clearly different from the others, but comparison with simulations from a model (dashed line) suggests that it is Treatment *D* that differs from expectation.

it is actually another result which differs from the expectation. It should be added that the model used could well be a statistical model or any other category of model. Models can also help in the design of field experiments and field sampling programmes. Another example lies in what might be described as "value-added" modelling. Simulations from a management-type model were used to extract extra information from field experiments, in one case to determine the depth of soil that needed to be sampled at various times for N fertilizer predictions (Addiscott and Darby, 1991), and in another to partition losses of ^{15}N labelled fertilizer between leaching and denitrification (Addiscott and Powlson, 1992).

Models can also be classified in terms of their *complexity*. This may imply the degree of fundamentality with which a process is treated, but it may also refer to the number of processes included. Related to this is the amount of computing power and computer time needed. Some models run in a few seconds on a PC while others require the services of a Cray for a rather longer time.

The questions of *flexibility* and *transferability* could almost be grouped together under the heading "user-friendliness". With a more mechanistic model the flexibility may depend mainly on the rigidity of the boundary conditions associated with its use. Other questions that may arise include the range of soils for which the model is appropriate and how readily the model can supply different forms of information. The issue of transferability can be summarized in the question, "How easy is it for a person other than the developer to use the model on a computer other than the one on which it was developed?" Problems of transferability can arise from the model's developer, who may, for example, incorporate presuppositions that are not made explicit. They can also arise from the competitive habits of computer manufacturers; a model that will run on one computer may not run on another because of minor differences in input/output procedures or even because certain FORTRAN statements function on the one but not on the other.

Adaptation of the classification to models other than those for leaching

Addiscott et al. (1991) discussed briefly the application of the classification scheme in Table 1 to models for the mineralization of soil organic nitrogen. They concluded that most models for mineralization are *deterministic* but that *stochastic* models were beginning to evolve. Whether or not microbes are perceived to behave in a random manner may depend considerably on the nature of the observations made on them. They found no clear distinction between *mechanistic* and *functional* models, like that for leaching models, mainly because the possibilities for making models of microbial processes more mechanistic seemed almost limitless. Should one consider only the kinetics of the process the microbes are mediating; or should one include the

build-up and decline of the microbial population; or consider rival populations or microbial genetics; or ultimately take account of the new understandings that have come from molecular biology? That being said, there are one or two models, such as the zero-order-kinetic model (Tabatabai and Al-Khafaji, 1980; Addiscott, 1983) and the first-order model (Stanford and Smith, 1972) that fall clearly in the functional group. The *rate/capacity* distinction is not appropriate in this context; the various categories of nitrogen that contribute to the process of mineralization are described as being in "pools" (Jenkinson et al., 1985), but the pools are not of fixed capacity and the quantities of nitrogen in them are dominated by the rates of transformation. These rates vary greatly and most models categorize pools as, for example, "easily decomposable" or "resistant to decomposition" (Parton et al., 1989; Bradbury et al., 1990; Jenkinson, 1990, and references cited therein). The distinction according to *purpose*, however, remains entirely relevant. Research-type models for mineralization may have large numbers of pools and thereby provide useful suggestions on possible flows of nitrogen through the soil but they are unlikely to be useful for practical purposes because of the large number of parameters for which values have to be found. Simpler models with only one or two pools are likely to be of more use for managing nitrogen in the soil.

This review is concerned with modelling soil behaviour and will not therefore consider models for crop growth and nutrient uptake. Information on these can be found, for example, in the book of France and Thornley (1984).

VALIDATION OF MODELS

In the review cited earlier Addiscott and Wagenet (1985a) observed that " ...the quantitative criteria for validating models do not seem to be clearly identified or universally recognised". The closing of this particular gap is important for both philosophical and pragmatic reasons. If we regard a model as part of the hypothetico-deductive process described by Popper (1959) we need the means to test reliably whether or not the hypothesis is refuted, and as models come more and more into the domain of public policy-making it becomes more and more important that they should be properly tested to ensure that they are sound.

The first essential for validating models is reliable data against which to test them. This may seem self-evident but it is a very real problem. So far as solute leaching is concerned the shortage of data sets for this purpose has not abated much since it was noted in the 1985 paper cited above, and I should be surprised if the problem was unique to this topic. It helps greatly if a data set has been obtained with the specific intent of validating a model or models. As Whitmore (1991) noted, the design of the experiment is important; a poor sampling arrangement can lead to the rejection of a good model or the acceptance of a poor one. Replication is usually advisable, and the model must be

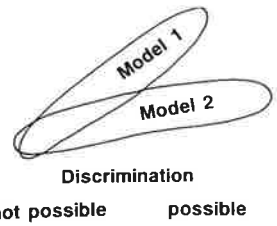

Fig. 2. Discrimination between models. Data for validation must extend into the range in which there is clear discrimination between the models.

tested throughout its intended range of application. When models are compared, attention should be given to the range within which it is feasible to discriminate between the models (G.J.S. Ross, pers. commun., 1992) (Fig. 2).

Whitmore (1991) has taken up the challenge of providing quantitative criteria for validating models. He summarized his procedures for choosing parameters for a computer model or assessing how well it simulated independent data as follows. The exact wording has been changed slightly but the sense has not. In each case he urged that the data should be plotted on a graph.

(1) Where none or few of the measurements were replicated

Choose the best parameters for the model by minimising the sum of squares of the deviations between simulation and measurement (Greenwood et al., 1985). To evaluate a particular model compute the product moment correlation (r) between simulation and measurement and the mean difference (M) between them:

$$M=\frac{1}{N}\sum_{i=1}^{N}(y_i-x_i)$$

where y_i is the ith measurement, x_i its simulation and N the number of such pairs. Specify the acceptable error in the prediction at the outset and use this to compare models that are for giving advice.

(2) Where most or all of the measurements were replicated

Partition the sum of squares of the deviations between simulation and measurement into the components due to lack of fit and pure error.

Choose parameters for a model that minimize the lack of fit ; reduce it to zero if possible. If lack of fit significantly exceeds error, examine the individual experiments. Where lack of fit is generally larger than error the model or its parameters are poor. Where the lack of fit is the greater in just a few experiments inspect the data; note, however, that poor data usually inflate error as well as lack of fit, and that you are more likely to have omitted from the model

some feature common to these experiments. If the latter is so, you must include this feature or restrict the use of the model.

Evaluate a model or compare different models using the ratio of the mean square lack of fit to the mean square error. Keep in mind that only a very good model indeed will give a statistically non-significant result when more than 10 or 20 data are included. With models for giving advice it may be more helpful to compare the simulation with the acceptable error.

(3) For models that simulate changes in a property for which both initial and final measurements were replicated

Compare the error and lack of fit as above. Lack of fit is now a more robust indicator of failings in the model. Minimize lack of fit to find optimum values for parameters and examine lack of fit carefully for signs of systematic bias in the model.

Evaluate or compare models as in (2) above.

The FORTRAN computer programme for calculating the sums of squares due to error and lack of fit is available.*

SENSITIVITY ANALYSIS

Changing the value of one parameter in a model by 10 percent may have a negligible effect on the resulting simulation while making the same percentage change in another may triple the simulated value of one of the model's outputs. We need to know which parameter does which, and this is the reason why publications concerning models frequently include sensitivity analyses. These may take the form of tables or diagrams. One form of sensitivity analysis diagram simply shows the effects on an appropriate output from the model of changing the value of each parameter by (say) 10, 20 or 30 percent in each direction from some central value. One important check to make is whether the percentage change in the output is greater or less than that in the parameter. The ratio of the change in the output to that in the parameter provides a simple measure of sensitivity; ratios appreciably greater or less than unity suggest sensitivity and insensitivity respectively. Problems arise, of course, if the sensitivity changes as we go from the 0–10 percent change to the 20–30 percent change. This makes it important that the sensitivity is assessed across the full range of likely parameter values, and probably a little further.

The diagram shown in Fig. 3a is satisfactory if a model has only two or three parameters, but some models have appreciably more. Sensitivities in such models can be shown by "spider diagrams", (Fig. 3b) in which the "legs"

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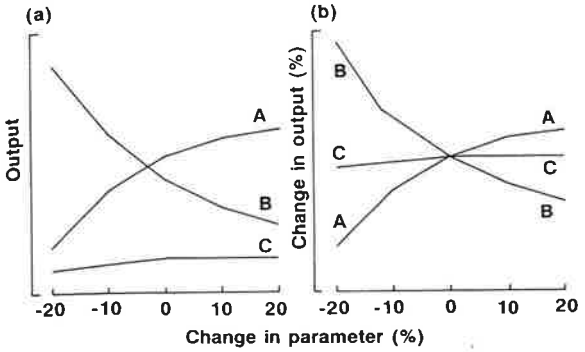

Fig. 3. Sensitivity analysis. (a) Standard diagram. (b) "Spider" diagram. The "legs" show the extent and direction of the effects of changes in the parameters.

of the spider show the extent and direction of the effects of changes in parameters.

Another precaution that may be appropriate is to check the sensitivity of the model to factors that are not specifically parameters but which can influence the model's performance. One such example is the layer thickness in a leaching model (e.g. Addiscott and Whitmore, 1991).

Sensitivity to variance in parameters

Soil parameters, as was noted before, may vary considerably from point to point within a field, and we need to take account of this variation. The reason can be seen in general terms from the equations given by Rao et al. (1977) for a function $f(x, y)$ of x and y, where x and y are distributed normally. The equations relate its mean, $\mu_{f(x,y)}$, and variance, $\sigma^2_{f(x,y)}$, to the means and variances of x and y, μ_x, μ_y, σ^2_x , σ^2_y:

$$\mu_{f(x,y)} = f(\mu_x, \mu_y) + c \tag{1}$$

$$\sigma^2_{f(x,y)} = \left(\frac{\delta f(x,y)}{\delta x}\right)^2 \sigma^2_x + \left(\frac{\delta f(x,y)}{\delta y}\right)^2 \sigma^2_y \tag{2}$$

Equation (1) shows that when the probability distribution representing the value of $f(x, y)$ is calculated from the corresponding distributions for x and y the mean of $f(x, y)$ is not necessarily obtained simply by inserting the mean values of x and y in the function. This point is illustrated in Table 2, which shows a simple worked example in which the mean of the function is certainly not the function of the means. The term c in eq. (1) was shown by Rao et al. (1977) to be:

$$c=\left(\frac{\delta^2 f(x,y)}{\delta x^2}\right)\frac{\sigma_x^2}{2}+\left(\frac{\delta^2 f(x,y)}{\delta y^2}\right)\frac{\sigma_y^2}{2}+\rho\left(\frac{\delta^2 f(x,y)}{\delta x\,\delta y}\right)\frac{\sigma_x\sigma_y}{2} \quad (3)$$

where ρ reflects the degree of correlation between x and y. This means that $\mu_{f(x,y)}$ is equal to $f(\mu_x, \mu_y)$ only if all the second partial differentials are zero, that is, when the function is linear in both x and y, or if the variances of x and y are both zero. If neither of these conditions obtains the correction term c must be calculated from eq. (3) and used to amend the results from eq. (1).

Not every model can be expressed as a simple differentiable function but the problems expressed in eqs. (1), (2) and (3) are potentially inherent in all models (Addiscott and Wagenet, 1985b; Wagenet and Addiscott, 1987). When we are considering sensitivity analysis we need to ask, not only how sensitive the model is to simple percentage changes in the values of its parameters, but also how sensitive it is to changes in the variability of its parameters. This is not a question that I have often seen asked. The equations show that we may be concerned with two aspects of sensitivity.

(a) From eqs. (1) and (3) we see that the mean of a distributed output from a model may be influenced by variability in the parameters of the model (Fig. 4a). The degree of influence depends on the second partial differentials that would be obtained if the model was differentiated.

(b) Equation (2) shows that, as would be expected, the variance of the distributed output depends on the variances of the parameters. Thus ignoring the parameter variances loses information. The dependence of the output variance on the parameter variances is through the squares of the first partial differentials. If the latter are close to unity the variances are more or less ad-

TABLE 2

Simple worked example to illustrate the point that the mean of the function $f(x, y)$ is necessarily not the same as the function of the means

$f(x, y)=e^{2x}/y$

x and y each have the three values shown in the table below, in which $f(x, y)$ is evaluated for each combination of x and y

y	x		
	0.5	0.7	0.9
1.5	1.81	2.70	4.03
2.0	1.36	2.03	3.03
2.5	1.09	1.62	2.42

The mean of the values in the table is 2.23.
The value of the function obtained by inserting the means of x and y is 2.03.

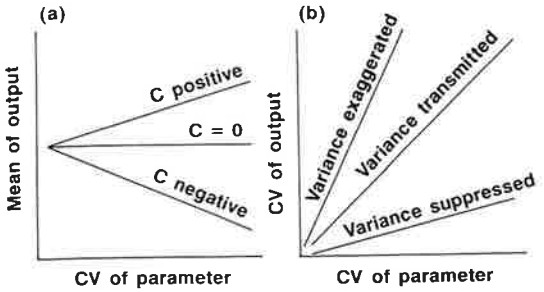

Fig. 4. Analysis for sensitivity to variance in parameters. Plotting (a) the mean and (b) the CV of the output against the CV of the parameter.

ditive, but if a partial differential is appreciably greater or less than unity the contribution from the corresponding variance will be greatly enhanced or diminished. In more general terms, some models will tend to *suppress* the variance of their parameters, so that the variance of the output will be unimportant, while others will *exaggerate* it, possibly to the extent that the standard deviation of the output greatly exceeds its mean. Some models will, of course, suppress the variance of one parameter while exaggerating that of another. A further complication lies in the possibility of interactions within models between the parameter variances such that, for example, a model that tends to suppress the variance of parameter x might cease to do so when the variance of parameter y was also included. Any correlation between parameters would clearly be important.

Analysis for sensitivity to variance in parameters

The discussion above suggests that to assess the sensitivity of a model to variance in its parameters we need in principle to determine the effects of changing the variance of each parameter on each moment of the distribution of values of an appropriate output from the model.

(a) *The mean* of the distribution is usually the moment of which most use is made and it is frequently obtained in a simulation that uses the mean alone to represent the distribution (if any) of parameter values. To avoid error, we clearly need to know in the first instance whether the omission of the variance matters seriously and more generally how much the mean changes as the variance of the parameter changes. For reasons discussed in the next section, it will probably be convenient to plot the mean against the coefficient of variation of the parameter (CV), the ratio of the standard error to the mean, expressed as a percentage (Fig. 4a).

(b) *The variance.* We need to know whether, in the terms suggested above, the model suppresses or exaggerates the effects of the variances of its param-

eters. This means comparing the variance of the output with that of the parameter. A direct comparison of variances, however, tells us little without reference to the mean of the distribution, so the most relevant yardstick seems to be the coefficient of variation (CV). To analyse the model's sensitivity to variance in its parameters we therefore need to plot the change in the CV of the chosen output against the CV of the parameter as the latter is increased (Fig. 4b). If the resulting slope is close to unity the model simply passes on the variability of the parameter to the output. If the slope is appreciably greater or less than one, the model exaggerates or suppresses the variability of the parameter.

(c) *The skew*. It may also be relevant to plot the skew of the output distribution against the CV because it determines whether or not the output needs to be transformed to obtain a normal distribution.

(d) *The kurtosis*, the fourth moment of the distribution, could be plotted similarly, but it is less clear that this would be useful in practice.

There are three ways in which an analysis of sensitivity to variance in parameters could be made, the Taylor Series method of Rao et al. (1977), the "Sectioning method" of Addiscott and Wagenet (1985b) and some form of Monte Carlo simulation. With the Taylor series approach effects on the mean can be assessed using eqs. (1) and (3) and those on the variance using equation (2), but the effects on the skew and kurtosis cannot be evaluated. The sectioning method simply divides the distribution for each parameter into sections, each corresponding to the same number of observations, and uses the section medians to represent the distribution. The model is run with all combinations of parameter and section to yield a distribution of output values whose moments can then be evaluated. A Monte Carlo simulation generates from the distribution of each parameter a random but representative series of values that are used in the model to provide a distribution of output values and thence its moments.

With all three approaches it will be useful to assess the sensitivity of the model to variance in each parameter alone and with the variances of other parameters changed at the same time. This is suggested by the third term in equation (3), which takes account of the interaction of the variances of x and y. It will also be important to make sure that each parameter is transformed to the appropriate distribution before this form of sensitivity analysis is made.

FURTHER ASPECTS OF VARIABILITY

Spatial structure

The discussion in the previous section of the impact of variability in parameters on the performance of models considered the extent of the variability, as measured by the variance, but not its spatial structure. A number of

soil properties that may become parameters in models, particularly hydraulic properties, are not only random but also spatially correlated, so that their statistical properties need to be defined in the terms of the Theory of Regionalized Variables (Matheron, 1965). This theory provides the basis of *kriging*, a form of weighted averaging in which the weights are chosen to avoid bias in the estimates and thereby to minimise the estimation variance (e.g. Journel and Huijbregts, 1978; Webster and Oliver, 1990).

We saw earlier that ignoring the variances of parameters results in loss of information and may result in an incorrect value of an output. This suggests that we possibly need to take account of the spatial structure of parameter variances, but how feasible is this? There is no problem in kriging capacity parameters such as the volumetric moisture content that are additive in nature, but kriging rate parameters presents a much greater problem because of the skewed nature of their distribution (Webster and Addiscott, 1990). This suggests that considering the spatial structure of capacity parameters is more feasible, particularly since Warrick et al. (1990) have shown that a variogram of volumetric moisture content measured on one occasion can be adjusted and used for interpolations on a second occasion. However, doing so may not greatly improve the estimation of the mean; taking account of the variation in a capacity parameter had rather little effect in a study by Addiscott and Bland (1988), and taking account of its structure will presumably have much less effect. The main benefit will come in terms of information, because it will be possible to map the output from the model (e.g. Addiscott and Bailey, 1990), and this could have practical uses with respect, for example, to fertilizer applications.

One interesting question arises by analogy with eqs. (1) and (3). For the function $f(x, y)$ of x and y the mean of the function was not the same as the function of the means unless the function was linear with respect to x and y. If a model has parameters that show marked spatial structure we might wish to determine the variogram of an output from the model and use it for interpolative purposes. This could be done in two ways:

(1) By running the model using the measured but uninterpolated values of the parameters and then determining the variogram of the output and interpolating from it.

(2) By determining the variogram of each parameter and producing interpolated values that are used in the model to give a "pre-interpolated" output.

The analogy with eqs. (1) and (3) suggests that the two procedures will give the same result only if the model is linear with respect to all the parameters. This was shown by Addiscott and Bailey (1990) with respect to the SLIM leaching model. Highly significant differences were found between the results of interpolating before and after the model was run, despite the fact that this model is not particularly sensitive to variance in its parameters. This study used UNIMAP, a commercial package that does not use the kriging technique,

but there is no reason to suspect that using kriging techniques would have altered the overall conclusion very much. In a very recent paper, De Jong et al. (1992) asked a similar question with respect to the Versatile Soil Water Budget model of Baier et al. (1979). They applied a spatial averaging procedure to either the weather inputs to the model or the outputs from the model. They found no difference between the two procedures for temperature-related outputs and only very slight differences, not likely to be of practical importance, for outputs related to moisture. Although these authors did not give full details, it seems that the model is concerned with gains and losses of water and is therefore effectively linear with respect to the moisture inputs. Presumably the same is true of the temperature inputs. The differences between the SLIM model and the Versatile Soil Water Budget model emphasize how important it will be to consider the linearities of the model with respect to its parameters in any spatial averaging or interpolation exercise of this nature.

THE PROBLEM OF SCALE

When a model is developed for a process in the soil there is usually an underlying assumption, which may or may not be made explicit, about the scale on which the model is to be applied. We need to ask, but often do not, whether the model is applicable at other scales. Is a model that is developed and validated with respect to one kilogram of soil in a laboratory appropriate to the several million kilograms of soil found in a hectare of farmland or moorland hillslope? This question has been raised very eloquently in the paper of Beven (1989) cited previously. Beven was concerned about the application of "*physically-based* models" (presumably *mechanistic* models in the parlance of this paper) to catchment-scale modelling. He asked whether models based on the small-scale physics of homogenous systems could be applied realistically to grids that might have 250 m$\times$250 m grid squares. Could any real meaning be given, for example, to the capillary potential gradients in depth increments of 0.05 m computed for a grid square of 62,500 m^2, particularly when the relief may vary by much more than 0.05 m within the square? Using "effective" parameter values for each grid square carries the implicit assumption that the grid square is homogenous, but we know very well that both the hydraulic gradient and the hydraulic conductivity vary greatly so that the fluxes of water, and any solutes carried in it, are not only very variable but also, bearing in mind eqs. (1) and (3), uncertain too. Beven was discussing the relative value, at a catchment scale, of physically-based (mechanistic) and "*lumped-parameter*" models; the latter may in some cases correspond with the *functional* models discussed earlier. He concluded that the physically-based models used with "effective" parameters on a grid-square basis were, in effect, lumped-parameter models. Could the physically-based models,

he went on to ask, be redeemed by increasing the scale of averaging to decrease the variances of the model's parameters? Beven himself concluded that the necessary spatial averaging carried inherent problems, and it is clear from the behaviour of the SLIM and Versatile Soil Water Budget models discussed above that there would be problems unless the physically-based models were linear with respect to their parameters, which they are not.

Beven's concerns were with catchment-scale modelling of water flows. We need to discuss now how the issues he raised relate to the modelling of soil processes at other scales.

Implications for other modelling efforts

Solute and water flow in the Vadose zone

Mechanistic models for flows of water and solute in unsaturated soil use the Richards Equation in combination with the Convection–Dispersion Equation (e.g. Wagenet, 1990, and references cited therein). The "physically-based" models to which Beven (1989) referred almost certainly use the Richards Equation, so Beven's comments could be strongly applicable to the modelling of these processes. The approach involves computing a water flux from the Richards equation which is used in two ways in the Convection–Dispersion Equation, to compute the convective flux of solute and to evaluate the dispersivity which is a function of the volumetric moisture content and the water flux. Let us ask a question analogous to that of Beven; can any real meaning be given to single-valued fluxes and dispersivities in grid-squares of 100 m^2 in a 250 m $\times$ 250 m *field* (the size of one of the grid-squares to which Beven referred)? Surely the answer is still no, even when the grid-square is 62.5 times smaller than that discussed by Beven? Despite the much decreased scale, the smaller grid-square probably encompasses practically as much variability in transport parameters as the larger square because much of this variance is likely to be "nugget" variance and the rest at short lags or, in less geostatistical terms, variability that is contained within a small area (e.g. Webster and Addiscott, 1990). If we seek to redeem the models by applying spatial averaging to their parameters, in concept if not in practice, we return to the problem of non-linearity. The analogy with eqs. (1) and (3) discussed above suggests that the result of running the models with spatially-averaged parameters will be the same as the result of running the models with the unaveraged parameters and applying spatial averaging to the output only if the models are linear with respect to their parameters, which these models are not. Thus "effective" parameters cannot truly represent the spatially variable grid squares, and these mechanistic models run with "effective" parameters on grid squares seem to me to cease to be fully mechanistic. That is, the conclusion about these models is the same as that reached by Beven (1989) about the physically based water flux model.

The discussion above suggests that if we wish to use models at a large scale on a grid basis with validly averaged parameters we need to look for models that are linear with respect to their parameters and whose parameters are not too variable in space. Some simple capacity models (e.g. Burns, 1974; Addiscott, 1977) probably fulfil both these conditions. The more recent SLIM model (Addiscott and Whitmore, 1991) has a simplified rate parameter as well as a capacity parameter. The rate parameter should be an asset for discriminating between soils of differing permeabilities but it is several times more variable than the capacity parameter and preliminary tests suggest that it introduces a detectable degree of non-linearity into the model, so it may be less of an asset in this context. It may be that a straight capacity model will be appropriate when we wish to model sandy and other relatively unstructured soils at a large scale, but that structured soils, especially those that crack will necessitate an extra parameter to take account of rapid macropore flow. As far as possible, the latter should be defined so that its variance is minimised and the problem of non-linearity is avoided. The outcome of this endeavour should be a model that is *functional with respect to scale.*

Mineralization

Models of mineralization, like those for the leaching process, need to be appropriate to the scale on which they are applied, but far less is known about the spatial variability of mineralization parameters than about those for leaching. Studies by White et al. (1987), Bramley and White (1991) and Whitmore et al. (in prep.) suggest that mineralization and nitrification show considerable variability with a short range of spatial dependence. Once again we need models that are linear with respect to their parameters and otherwise tolerant of variance in them, if we wish to have valid "effective" values of parameters. The simplest mineralization model of all, the zero-order model, may be as useful as any, because models with exponential terms will be non-linear.

Increasing the scale at which a model is used

It is clear from Beven's (1989) paper and from the above discussion that there can be problems in using a model at a scale greater than the scale at which it has been validated or used previously. The following questions are suggested as an aid to determining whether use at the larger scale is advisable:

As we translate a model from one scale to an appreciably larger one:
(1) Does the underlying hypothesis of the model remain the same?
(2) Do the mechanisms of the model retain their meaning in a descriptive sense?

(3) Is the model still being used within a range of parameter values for which it has been validated?

(4) Can realistic, independently-derived values still be assigned to the model's parameters?

(5) Is the scale of the modelling commensurate with the scale of the measurements from which the parameters were derived?

(6) Do the parameters at the larger scale differ appreciably from those at the smaller? If so, why?

(7) Has the sensitivity of the model to its parameters changed? If so, why?

(8) Has the classification of the model changed *de facto*? For example, from *physically-based* to *lumped-parameter*, or from *mechanistic* to *functional*?

(9) Is there anything in the use of the model at the larger scale that offends common sense?

MODELLING SOIL BEHAVIOUR: KEY ASPECTS

Choosing a list of key aspects of soil behaviour inevitably involves adopting a particular standpoint. The greatest challenge currently facing the world is that of feeding an ever-increasing world population without polluting the environment or degrading the soil; in short, the challenge of sustainable agriculture. Our part lies in promoting, through modelling, good stewardship of the soil.

Key aspects of good stewardship of the soil

No group of soil scientists will necessarily be unanimous about the keys of good soil stewardship, but I suspect that most lists would include at least some of the following items. It would not be possible, or indeed desirable, to give an in-depth review of the models relating to each aspect. Where I have felt competent to provide a brief review of available models I have done so, and where I have not I have suggested an appropriate review by someone else. In some instances I have done both.

Water in the soil

Water was the subject of the earliest experiments made on the soil and also the earliest theoretical study. The French meteorologist de la Hire established the first lysimeters in 1688, and Buckingham published the first quantitative theory of the behaviour of water in the soil in 1907. The well-known law of Darcy (1856) antedates Buckingham's work by 51 years but this theory was for *saturated* flow in porous media (filter beds of sand); the soil is usually unsaturated. Because of this early start, soil water has a voluminous literature, both experimental and theoretical, attached to it, and this is needed be-

cause many of the most challenging problems in sustaining agricultural production still lie in the efficient use of water. Not only can we not waste water, we also have to ensure that excessive use of water does not cause pollution of groundwater. Among the many reference works on the theory of soil water are those of Childs (1969), Hillel (1980) and Baver et al. (1972). Towner (1989) has provided a useful concise account of this theory and of the problems of implementing it. Some of the references cited include solute leaching and reviews specific to this topic were provided by Wagenet (1983, 1990). Two other reviews by this author deserve attention; one (Wagenet, 1986) discusses methods of measuring fluxes of water and solutes together with the associated theory, and the other (Wagenet and Rao, 1990) deals with the increasingly important topic of modelling pesticide leaching.

Organic matter in the soil

Organic matter plays an important part in the supply of nutrients, the retention of water and the maintenance of good soil structure. Sound stewardship of soil organic matter is therefore a key part of sustainable agriculture. The turn-over of carbon and nitrogen through organic matter provides a good example of a process that is so complicated that any model, however sophisticated, is bound to be an oversimplification. Changes in the quantity and composition of organic matter are slow, so that the time scales of models tend to be in decades and the number of sets of data for validation rather limited. Transformations of organic matter are usually subjected to the simplifying assumption that the conversion of one form of organic matter to another proceeds with first-order kinetics and that the degree of complexity is determined by the number of compartments, or categories, of organic matter considered. The Rothamsted organic matter model (Jenkinson, 1990, and papers cited therein) takes account of decomposable and resistant plant material from crop residues, biomass, humus and inert organic matter. Another notable multi-compartment model is the Century Model (Parton et al., 1989). There are also a number of simpler models that exist in the form of equations; these are described by Jenkinson in the paper cited above.

Soil pH

Many processes in the soil, both chemical and biological are affected by the pH of the soil. The problem of acidification has led to the evolution of a few models of this phenomenon of which the MAGIC model (Cosby et al., 1985) is possibly the best known. This model and the MIDAS, SAFE and SMART models were described briefly and tested in a study by Wright et al. (1991).

Adsorption, ion exchange and speciation

The processes that control the concentrations of ions in the soil solution play an important role in soil fertility and therefore in sustainable agriculture. Their role is a dual one in that fertility, in the broadest sense, can be diminished not only by the under-supply of some ions but also by the over-supply of others, notably the heavy metal ions. Adsorption has traditionally been modelled using the Freundlich and Langmuir isotherms but it is becoming increasingly clear that the kinetic aspects of adsorption need to be considered, as in the model of Barrow (1983). The modelling of ion exchange and speciation is a very complex problem because of the large variety of interactions that may occur between different ionic species, both inorganic and organic, particularly when complexes are formed in solution. The best known model of this assembly of interactions is the GEOCHEM model of Mattigod and Sposito (1979).

Diffusion

Diffusion in the soil is important in the supply of some nutrients to plants. In this context we are interested in diffusion in the whole soil, but within aggregates, diffusion of oxygen may influence denitrification and diffusion of nitrate transfers it to or from the relative safety of intra-aggregate water when flow of water between aggregates makes leaching a risk. At an even smaller scale the release of non-exchangeable potassium from clay minerals is usually treated as a diffusional process. Nye and Tinker's (1977) book remains one of the best texts on diffusion and related processes.

Nutrient supply to plants

A large all-embracing model for the supply of nutrients to plants, though arguably desirable, is probably about as achievable as a global environmental policy. The main problem is that the various nutrients are supplied by completely different processes. The supply of nitrogen and sulphur is strongly influenced by the cycling of these nutrients through the soil's organic matter, while the supply of cationic nutrients is influenced by ion exchange. Speciation is studied mainly for the trace elements but is not restricted to these; mineral nitrogen divides between ammonium and nitrate. Adsorption is important with respect to phosphate and sulphate. Diffusion is important for all nutrients whose concentration in the soil solution is too small to maintain an adequate supply in water drawn to the root by transpiration, notably phosphate and potassium.

Soil structure

The structure of the soil plays a part in several of the processes discussed above. notably leaching, and is itself influenced by changes in the amount and nature of organic matter in the soil. It may be changed by natural agents such as roots and worms, by the weather, particularly frost, and by human cultivation. Everyone knows that structure can be improved by thoughtful cultivation and management and damaged by careless or untimely cultivation, but exactly what it is that is improved or damaged is less clear. Although progress has been made in characterising soil structure (Dexter, 1988), we still lack the means of quantifying and modelling it, and this is one of the more interesting challenges for soil modellers.

Soil genesis

Another interesting challenge for modellers lies in soil genesis, which is again the result of a variety of natural and anthropogenic influences. Hoosbeek and Bryant (1992) reviewed previous efforts at modelling this process and made some suggestions for future progress.

Weeds and pathogens

The soil plays a part in the transfer of weeds and pathogens from crop to crop. This problem lies outside the main core of this paper, but reviews of models have been given by Cousens et al. (1987) for weeds and Gilligan (1983) for pathogens.

Erosion

All efforts at practising good stewardship of the soil come to nought if the soil is washed or blown away. Models should be able to help those who manage the soil to minimise erosion, and a number of such models have been published. Morgan (1986) has provided a review of them.

"EUPHORIC MODEL-MAKERS"?

Philip (1972) (quoted by Towner, 1989) wrote after commenting on the problems caused by soil heterogeneity to the application of classical soil water physics, "One must hope that soil physicists will attempt to come to grips with this problem. It is not good enough to leave it to the euphoric model-makers." The word "euphoria" means "a feeling of well being" and carries the implication that the feeling is unjustified. The tone of Philip's other comments about modelling leaves little doubt that he used the word "euphoric"

with perjorative intent, but the passage of 20 years has left his jibe looking rather wet. Classical soil-water physics is still in trouble with heterogeneity, and if Beven (1989) is correct the physically-based model is in effect a lumped-parameter model when used on a large scale, surely itself a target for Philip's rumblings of disapproval. Perhaps too, "it is not good enough to leave it" to the fundamentalists of soil physics. We need a *via media* between euphoria and fundamentalism. "Good scientists", wrote Medawar (1967), "study the most important problems they think they can solve. It is, after all, their professional business to solve problems, not merely to grapple with them." Our professional business as soil modellers is surely to seek the most mechanistic model that is appropriate to, and has been validated for, the scale and the purpose of the project in hand. "If politics is the art of the possible", suggested Medawar, "research is surely the art of the soluble." Is modelling perhaps the art of the applicable?

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