Modelling Soil Productivity and Pollution [and Discussion]

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Modelling soil productivity and pollution

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SUMMARY

Predictive models of soil and plant processes should be of much benefit both in developing and developed countries. They can assist in enabling agronomic practices to be better adjusted for differences in conditions; in avoiding disasters that can accompany change in land use; in minimizing waste and environmental pollution, and in modifying and implementing legislation. These views are discussed in the light of recent advances. Particular attention is drawn to (i) the excellent relationships linking average national yields, nutrient uptakes, etc. to single factors such as average fertilizer application; (ii) equations for predicting the behaviour of added chemicals and water in soil that have been obtained by rigorous deduction from physical and chemical laws; (iii) the discovery of semi-empirical, but nevertheless widely applicable quantitative relations for key soil and plant processes, and (iv) the formulation and use of computer models for field situations. There is a pressing need to find ways of presenting the outcome of this work so that it can be more widely applied in practice.

INTRODUCTION

Agronomic, fertilizer, pesticide and soil and water management practices are at the centre of some of the most pressing problems facing mankind. Many nations must increase food and fuel-wood production if they are to avert starvation. There is a need to reduce costs, waste and pollution in agriculture almost everywhere.

The benefits from a given practice vary greatly from one situation to another but it is quite impractical to carry out experiments that cover more than a fraction of the conditions that exist. Some form or other of prediction is essential so that the available resources can be used in the most effective way in any country. Methods of prediction aimed at solving these problems can be divided into three groups. Those concerned with national data; those concerned with deduction from well-known chemical and physical laws, and those concerned with developing equations for key soil and plant processes and combining them into computer simulation models. The main purpose of this paper is to discuss the merits and limitations of the various approaches that have been used, and to identify opportunities for future advances.

THE NEED FOR PREDICTIVE MODELS

A large proportion of the world's population is primarily concerned with getting enough food to eat and fuel-wood with which to cook it. Food and fuel-wood shortages are becoming more serious. The Food and Agriculture Organization (FAO 1984) predicts that by the end of the century, 64 countries will be unable to meet their population's need for food even if all the tillable land is cropped by using current agricultural techniques. If starvation of up to 450 million people is to be avoided (Cochrane 1986), it is essential to increase production of food in those areas of the world in need.

Although the 'green revolution' enables yields to be increased where soils are ideal and there is ample water, nutrients and pesticides, these conditions do not prevail in many areas where people must grow food. Serious problems of acidity, salinity, nutrient and water stresses and risk of erosion are widespread. Also, most people cannot afford appreciable quantities of fertilizer or crop protection chemicals. Man has not learned how to recycle nutrients when he grows the crops he needs (see, for example, Greenwood 1989), so fertilizer application is indispensable for improved productivity in most of the world. Fertilizer requirements, however, vary greatly from field to field, for every crop in every country. Therefore, it is essential to modify practice for differences in conditions and there is an urgent need to forecast how best to make these adjustments.

New minimum-input methods of growing crops are essential to improve productivity in many countries. Conditions, however, vary greatly and it is impossible to carry out experiments to cover more than a small fraction of them. Some means is needed to forecast how to adapt such practices for differences in conditions.

Changes in land use, even the introduction of new cultural practices, all too often result in an irreversible decline in soil fertility. For instance, cutting down forests resulted in unexpected salinization of valley soils in western Australia (Marshall & Holmes 1988), irrigation resulted in salinization in many arid areas of the world (Stanhill 1986), and other modifications in land use have resulted in irreversible loss of soil productivity and even in the disappearance of whole civilizations (McCracken 1987; Sinclair & Fryxell 1985). It is therefore of considerable importance to forecast the consequences of any change in practice if serious damage to soils and harm to human well-being is to be avoided.

The more affluent parts of the world are becoming increasingly concerned about the effects of agricultural practices on the environment. There is special concern that nitrate and pesticides may be polluting water and food to such an extent that they are harmful to the health of animals and humans. There is concern that they are disturbing the balance of nature, and in the case of nitrate, causing eutrophication in the sea and inland waters; some even believe that they may be inducing the formation of greenhouse gases. So great are these pressures that they are prompting several rich nations to introduce legislation to control the use of chemicals in agriculture. Unless such legislation is considered with great care, it may be ineffective in controlling pollution and may also have, unintended, but very harmful side effects. For instance, it has been argued that the proposed European Community (EC) legislation to control nitrate in water could reduce arable production in the U.K. by about one third (House of Lords 1989). In addition, the proposed EC limit of 0.1 $\mu g\,l^{-1}$ of any individual crop protection chemical in potable water supplies may, in the future, also severely restrict agricultural practices. In the case of nitrates, legislators have been considering various alternative control strategies, and have been asking for predictions of the effects of the various proposals on the extent of nitrate leaching and on crop yields throughout the nation. We foresee that scientific prediction will become increasingly important in law making, especially when concerned with control of pollution.

LEVEL OF ORGANIZATION

Before discussing the various approaches to prediction, it is worth drawing attention to the fact that agronomic studies cover a wide range of levels of organization of phenomena as is shown by the scheme in figure 1 adapted from Thornley (1980). On the left hand of the scheme, three levels are labelled by indices $i+1$, i and $i-1$. Hierarchical systems such as this have a number of features; each level has its own concepts and principles; discoveries made at a given level may be explained in terms of phenomena at the next lower level (Thornley 1980). Thus a description at level i can provide explanation phenomena at level $i+1$. On the other hand, it is often difficult, to deduce phenomena at a higher level of organization, e.g. $i=1$ from studies of a lower level of organization as was vividly shown by Passioura (1979). He presented an array of dots and invited people to identify features in their arrangement, one relative to another. Most people note that the dots form a square array where rows are at 45° to the horizontal, that there is a bimodal distribution of sizes of dots and that the dots at the given size tend to be clustered together. All this is correct. What people fail to realize is that by looking at the details of the arrangement, they have failed to grasp the overall pattern. This is clearly revealed by standing back so that the individual dots are blurred when it is seen that the dots represent a man with glasses, smoking a pipe. It was only possible to get the overall picture by study at a high level of organization; it could not be deduced from the detailed relations governing individual dots.

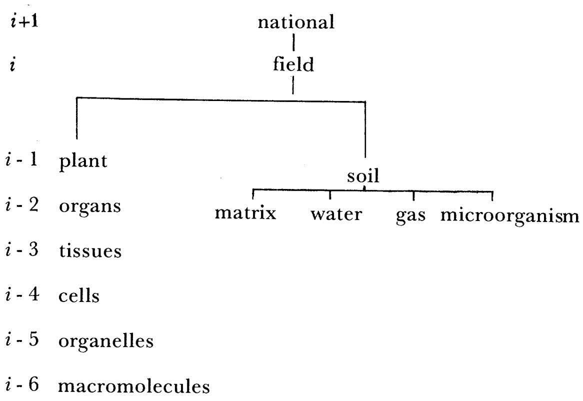

Figure 1. Level of organization in soil plant processes.

QUANTITATIVE RELATIONS AT THE NATIONAL LEVEL

This view suggests that the main factors influencing variation in yield between nations might be identified by correlation of average national yields with other factors. Indeed many good relations have been found and some are summarized in table 1. They include such unlikely ones as the very good negative relation between agricultural productivity per worker and the percentage of the total workforce in a nation engaged in agriculture (Hoffman & Stoner 1986). Also, over the period 1945–74, the energy content of the maize crop per unit area, grown in the U.S.A. is well correlated with the energy concerned with its production (Evans 1986). Even more significant is the fact that the average national grain yield per ha† is strongly correlated with the sum of fertilizer $N+P_2O_5+K_2O$ applied to permanent arable crops in different nations. Of course, this relationship does not mean that simply applying more fertilizer will increase yield, but what it does mean is that no nation gets high yields without heavy applications of fertilizer. There is also a good correlation between grain yield per hectare and the average rates of fertilizer-N applied in each nation, when these are less than 160 kg N ha^{-1} (table 1). In Britain yields of winter wheat have increased almost in proportion to increase in fertilizer-N over the past 40 years. Moreover there is a strong correlation with the yields of the different types of U.K. cereals and the fertilizer-N applied to each. What is remarkable about all these relations concerning fertilizer-N, is that the values of the regression coefficients are roughly the same; those of the intercept 'a' vary between 1.55 and 1.99 t ha^{-1} and those of the gradient 'b' between 0.023 and 0.027 tonnes of grain per kilogram of fertilizer-N. Although all correlations have to be treated with caution, the indications are that if N-fertilizers are withheld, then in the long term, grain yields will fall to between 1.5 and 2 t ha^{-1} in most nations of the world, and that yields of grain will fall by abut 0.025 t ha^{-1} or

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† 1 hectare = 10^4 m^2.

Table 1. *Some linear relations of the type $y = a + bx$ for national yields and* N-*uptakes*

Equation	comment	y	x	average values a	b	% removal of variance	reference
1	covers all countries with more than 1 million inhabitants for which appropriate information for 1985 could be deduced	average national grain yield ($\mathrm{t\ ha^{-1}}$)	Average sum of fertilizer ($N+P_2O_5+K_2O$) in $\mathrm{kg\ ha^{-1}}$ applied to arable and permanent crops (excluding grass)	1.83	0.088	82 (14)	derived from FAO 1986, 1987
2	as above, but figures from countries where average N-fertilizer application greater than 160 $\mathrm{kg\ N\ ha^{-1}}$ excluded	average national grain yield ($\mathrm{t\ ha^{-1}}$)	average fertilizer-N ($\mathrm{kg\ ha^{-1}}$) applied to arable and permanent crops (excluding grass)	1.50	0.023	75 (11)	derived from FAO 1986, 1987
3	average 3-year wheat grain yields regressed against 3-year average fertilizer-N in U.K. over period 1950–88	average U.K. wheat yield ($\mathrm{t\ ha^{-1}}$)	average fertilizer-N ($\mathrm{kg\ ha^{-1}}$)	1.99	0.025	97.2 (10)	derived from Hood (1982) and data supplied by Home Grown Cereal Authority
4	average yield of three main U.K. cereals regressed against average fertilizer-N for each crop. Data for 1986	average cereal yield ($\mathrm{t\ ha^{-1}}$)	average fertilizer-N ($\mathrm{kg\ ha^{-1}}$)	1.66	0.027	97.5 (1)	derived from data supplied by Home Grown Cereal Authority
5	N-uptakes of U.K. winter wheat grain and rates of fertilizer-N (2-year averages) regressed against each other for the period 1975–88	N-uptake of grain ($\mathrm{kg\ N\ ha^{-1}}$)	average fertilizer-N ($\mathrm{kg\ ha^{-1}}$)	27	0.51	93 (6)	derived from data supplied by Home Grown Cereal Authority

25 kg ha^{-1} for every kilogram of fertilizer-N per hectare that is withheld. These coefficients are remarkably constant despite the differences in conditions and their values are consistent with the results of British field experiments. Indeed, such relations have been used in conjunction with other evidence to estimate the effects of proposed legislation which would reduce fertilizer use on the yields in the U.K. (House of Lords 1989).

In this connection it is also notable that a good relation is obtained between the increase in nitrogen uptake in U.K. wheat grain brought abut by the increase in fertilizer-N in recent years (table 1). According to this relation, 51% (s.e. 5.6%) of the fertilizer-N is recovered in the grain. If allowance is made for nitrogen absorbed in straw, the figure for recovery of nitrogen by the crop is about 75%.

(*a*) ***Fertilizer responses***

Simple relations have been found to define the general shape of fertilizer response curves obtained in nationwide fertilizer trials. Constancy in the values of some of the coefficients in many different conditions has been found, whereas the values of others have sometimes been related to easily measurable properties of the soil.

The first significant use of these findings in Britain was at the beginning of the 1939–45 war when there was a pressing need to devise a way of estimating how best to use limited supplies of fertilizer (Crowther & Yates 1941). The results of all past experiments were interpreted with the Mitscherlich equation:

$$Y = A(1-\mathrm{e}^{-c(X_S+X_F)}) \tag{1}$$

where Y is the yield with X_F (applied as fertilizer); A is the potential maximum yield obtainable with X_F in the circumstances of the experiment, X_S is the amount of nutrient provided by the soil and c is a coefficient. It was found that the value of c was remarkably constant for a given nutrient in different situations. These findings enabled the results of the previous 40 years experiments to be summarized and used to estimate average response curves of the major arable crops to nitrogen, phosphorus and potassium fertilizers throughout the country. The work permitted a much better use of fertilizer than had hitherto been possible.

Other workers (for example Scaife 1968) found that, in some areas at least, the coefficients X_S could be related to soil analysis. Thus in nationwide fertilizer experiments with maize in Tanzania, X_S for nitrogen was related to the total nitrogen concentration in the soil and X_S for phosphate was correlated with the amount extracted from soil with weak acid. This work enabled adjustments in fertilizer practice to be made for differences in nutrient status of the soil.

The development and use of somewhat similar models facilitated the prediction of the response curves of 19 vegetable crops to nitrogen, phosphorus and potassium fertilizers from a small programme of field experiments. The predictions were in terms of the standard U.K. advisory methods of assessing soil nutrient status. They were shown to be in approximate agreement with the results of nationwide field experiments that were independent of those used for making the predictions (Greenwood & Collier 1979). They have formed the basis of much practical advice on the use of fertilizers for vegetables over the past 15 years.

A major breakthrough in the notoriously difficult problem of forecasting how to adjust fertilizer-N for differences in conditions was the discovery in field experiments that some crops can extract most of the mineral-N in soil to depths of at least a metre. The amounts of mineral-N to this depth in spring varies greatly from site to site and are measured routinely in some parts of western Europe for advisory purposes. This method of adjusting fertilizer practice is most useful when the soil is uniform, deep and does not vary much from field to field and the crops are deep rooted (Greenwood 1986).

Nevertheless, there are many situations where no such correlations have been found between any feature of the response curves and an easily measurable soil property. Presumably this is a reflection of fertilizer response depending on a range of different factors, the relative importance of each varies from one situation to another. Simple correlative techniques have not enabled these complexities to be unravelled.

Studies at the national level have therefore revealed robust relations that govern complex phenomena. They have given results that have improved agricultural practice and proved to be of value in developing legislation. The basic problem, however, is deducing causality from such relationships. It has not been generally possible to develop relations involving more than a very few dependent variables.

APPLICATION OF PHYSICAL AND CHEMICAL LAWS

At the other extreme to nationwide studies, physicists and chemists have attempted to make predictions about agronomic practice and chemical fate from well-established physical and chemical laws.

(*a*) ***Drainage***

Especially notable is the development of drainage theory. Excellent reviews on the topic include those of Childs (1970); Hillel (1980); Marshall & Holmes (1988) and Youngs (1983). Drainage is important in temperate regions to minimize yield loss from soil anaerobiosis and to increase the number of days on which traffic can get on the land without causing damage to soil structure. It is especially important in arid regions to obtain through percolation of salts so as to avoid salt accumulation near the soil surface and yield loss.

Flow of water through soil is governed by Darcy's law which states that it is proportional to the hydraulic potential gradient. From this law and the continuity equation, differential equations have been derived to define drainage in many idealized situations. Numerous solutions of these equations, differing in the approximations that are made, have been derived. But as the conditions in the field are generally complex, the available equations are approximations to the real situation and have to be used with caution. Analogue and numerical techniques are also used for the solution of land drainage problems. The drainage engineer has thus been provided with a sound theory on which to make broad conclusions about drainage problems in general and especially about large-scale reclamation projects such as those that occur on more or less uniform alluvial plains in some developing countries. Experience has, however, shown that the cost of making the necessary measurements for the application of the theory can be prohibitively expensive. Improved methods of measuring key input parameters in the field appear to be the major need to ensure more widespread application of the theory.

(*b*) *Solute leaching*

Darcy's law has also been used in estimating the transport of solute through soil and the basic equation describing solute movement under steady-state one-dimensional flow in a homogeneous soil is (Addiscott & Waganet 1985):

$$J_s = [\theta D_m(q) + D_p(\theta)]\, dc/dz + qc \qquad (2)$$

where J_s is the steady-state flux, θ is the volumetric water content, q is the volumetric water flux, c is solute concentration and z is depth. The effects of mechanical dispersion due to variations in flow paths and velocities is considered in D_m, and the process of chemical diffusion complicated by a consideration of partially water-filled porous medium is represented by an effective diffusion coefficient D_p.

Equation (2) is applicable to either adsorbed or non-adsorbed solutes provided that the due allowance for the adsorption–solution equilibrium is made in the values of appropriate parameters (Jury *et al.* 1983; Hutson & Wagenet 1989). One of the main problems with modelling movement of adsorbed solutes is that the rate of equilibration between adsorbed and solution phases may be slow relative to the rates of water movement and accurate descriptions of the kinetics of adsorption and desorption may be difficult to achieve (see, for example, Van Genuchten *et al.* 1974).

In practice, in field soils there is seldom a steady state and the total mass of solute defined as θc at any position changes with time; the equation must be modified with the continuity equation and used in conjunction with Darcy's law. These models have been well reviewed by Addiscott & Wagenet (1985). Most of the experimental work testing their validity has been in the laboratory rather than in the field, and has confirmed their theoretical base. The models do, however, have a number of drawbacks, especially when they are used with field soils. Values of the coefficients needed in the models for characterizing soils are very difficult to obtain and appear to be very variable over a given field. The validity of the models does not seem to have been tested, as have the capacity type models referred to later, against the results of numerous multi-site field experiments.

(*c*) *Dissolution of added materials*

Models have been developed from fundamental chemical laws to calculate the effects of various nutrient sources on the concentrations of nutrients in soil and thus on their availability to crops (Nye 1990). One set of models concerns rock phosphate. It is cheap, exists in different forms, and its dissolution and thus availability to crops varies considerably depending on the form of phosphate and on soil conditions. The models take account of the solubility product at the particle surfaces, the equality of fluxes of each ionic component from the particles (required for continuous dissolution), the diffusion of the various ions through the surrounding soil, the adsorption of phosphate on soil, and the maintenance of electrical neutrality (Kirk & Nye 1985, 1986*a*, *b*). The models require inputs that, in general, can be measured easily and their validity has been confirmed by experiments. A somewhat similar approach has been used successfully to calculate the dissolution of other rock phosphates and in particular, the carbonate-apatites. A similar model has also been used to forecast the time change in pH after the application of lime and other alkaline materials, which is important because many soils are acidic and in areas remote from sources of lime (Nye & Ameloko 1986, 1987).

(*d*) *Urea behaviour in soils*

Urea is an inexpensive and widely used N fertilizer, but a substantial proportion of the nitrogen it contains can be lost to the atmosphere as ammonia gas. A wide range of factors affect these losses and it is important to predict how they do so to provide a basis for improving efficiency of use. A model aimed at meeting this objective has been derived from chemical laws (Rachhpal-Singh & Nye 1984*a*, *b*, 1986, 1988). Urea on addition to soil is hydrolysed by the enzyme urease to ammonia and carbon dioxide; some of the ammonia dissolves in the aqueous phase and is in equilibrium with ammonium ions in solution and ammonia gas in the adjacent gas phase. In the model, there is an equation for the dependence of urease activity on urea concentrations and there are continuity equations for urea, ammoniacal-N, soil alkalinity and CO_2, which are solved numerically subject to the relevant initial and boundary conditions. Excellent agreement has been obtained between predictions of the model and the results of experiment.

(*e*) *Volatilization of pesticides*

Diffusion theory has been applied to predict the volatilization of pesticides from soils under conditions where mass transfer caused by water movement was minimal (Mayer *et al.* 1974). Models covering a range of initial boundary conditions gave accurate predictions of vapour fluxes in well-controlled laboratory studies. Extension of such models to take account of upward water movement and hence mass transfer of pesticide to the soil surface was described by Jury *et al.* (1980) and, once more, excellent agreement between observed and predicted vapour fluxes was obtained in laboratory tests. The main problem in extending such models to the field is to obtain an accurate definition of boundary conditions.

These fundamental mechanistic models for the fate of important chemicals in soil appear to have two great merits.

1. They are based on fundamental laws, involve the minimum of assumption and thus should be of wide applicability.
2. They can predict the effects of numerous factors influencing the fate of added chemicals to soil, provided that consideration has been given to each of the important processes in developing the model. Indeed, if one could be certain that no such omission had taken place there would be no need to test the validity of the models experimentally before they were applied in practice.

The potential value of the models could be enormous if the inputs are readily available.

SEMI-EMPIRICAL QUANTITATIVE RELATIONS

Relations have been found for many of the phenomena governing soil productivity and pollution. Some have been deduced by calibrating well-established theoretical relations, some by developing equations that mimic existing concepts, and yet others by fitting empirical equations to data. They include relations linking volumetric soil water content and soil suction (Marshall & Holmes 1988); erosive loss of soil and slope and the length of the slope (Williams & Renard 1985); release of mineral-N and C:N ratio of decomposing organic matter in soil (Jenkinson 1984); the critical %N in plants and plant mass (Greenwood *et al.* 1985; Lemaire *et al.* 1985); the rate of plant nitrogen uptake and the mineral nitrogen in soil (Burns 1980); the potential maximum growth rate and interception of radiation (Monteith 1986); potential evapotranspiration and meteorological parameters (Penman 1948); or simply temperature (Thornthwaite 1948) and growth rate and transpiration rate when water stress limits growth (Hanks & Ashcroft 1980). These relations usually give good fits, often with remarkable constancy in coefficient values, to widely different sets of data. They can be used both directly and indirectly for a wide range of predictive purposes.

COMPUTER SIMULATION MODELS

Relations of the type described in the previous section are often major components of simulation models. Such models vary in complexity from ones that are little more than algorithms to those that include hundreds of relations (see, for example, Williams & Renard 1985). We show some developments by reference to forecasting fertilizer-N requirements and the fate of pesticides in soil.

(*a*) *Behaviour of fertilizer-N*

One set of models was prompted by the discovery, previously referred to that mineral-N in the top metre of soil, measured in February, was useful in forecasting the fertilizer-N requirements of some crops on some soils. The need to extend the sampling period and thus achieve a more even work load, prompted the development of simulation models to calculate the distribution of soil mineral-N in February from measurements made on soil samples taken in the previous year. Several such models (Addiscott & Whitmore 1987; Richter *et al.* 1988; Zandt *et al.* 1986) have readily available inputs and have been tested against large numbers of field measurements. Nevertheless, all these models predicted the soil mineral-N to a depth of one metre within ±20 kg N ha^{-1} of those measured experimentally in at least 70 % of instances, which is remarkably good because differences of this order of magnitude could be attributed to measurement errors. For many situations the inputs to the models did not include a measurement of soil mineral-N done at any time and some of the testing of the models was carried out by different workers from those who had developed the model. All the models are used to some extent for advisory purposes. They are essentially capacity models that have evolved by expressing a physical conception of the processes in terms of semi-empirical equations.

Factors other than soil mineral-N to a depth of one metre in February often influence the fertilizer-N requirement. Attempts have therefore been made (see, for example, Aslyng & Hansen 1985; Barnes *et al.* 1976; Van Keulen 1981; Whitmore & Parry 1988) to develop simulation models to take account of these factors. They are also used to calculate, for each day during the growing period, the distributions of roots water and mineral-N down the soil profile, the increments in N-uptake and dry weight by the crop, and the nitrate lost by leaching. One such model, (Greenwood & Draycott 1989*a*) covers 18 crops. The inputs are potential maximum dry mass, mineralization rate (under defined conditions), soil textural class and the distribution of soil water down the profile at field capacity. The initial nitrate distributions are also required in some situations but often in the U.K. they are not needed, because if simulations are started in November, the values of the soil nitrate and water input often have little effect on the prediction of nitrogen response made for crops sown during the following spring and summer. This insensitivity results from most of the residual nitrate being leached out over winter. The other inputs to the model are daily rainfall, potential evaporation from an open water surface and temperature.

The validity of the model has been tested against the results of numerous experiments on different vegetable crops, potatoes and cereals in western Europe (see, for example, Greenwood & Draycott 1989*b*; Neeteson *et al.* 1987). The degree of agreement has been good in experiments on research stations where the history and properties of soils are well known. They have been less satisfactory for predicting responses on growers' fields, but in these predictions no account was taken of inter-site variations in the mineralization rate or in differences in residues from previous crops both of which can greatly influence nitrogen supply. Even so, the model did predict some unexpected relations that have been subsequently confirmed experimentally. They include the prediction that when different crops are grown on a low nitrogen-status soil, in the absence of added fertilizer-N, the percentage of nitrogen at harvest of the crop will be dominated by plant mass and hardly effected by species (Greenwood & Draycott 1989*b*); another prediction is that when crops are grown on a wide range of soils, the following relation should hold:

$$\frac{\%\text{N in dry matter in absence of fertilizer}}{\text{critical }\%\text{N}} = \frac{\text{mass of dry matter in absence of fertilizer}}{\text{maximum weight of dry matter with any level of fertilizer}}.$$

Evidence that it does hold has been obtained for vegetables in fertilizer experiments on growers' holdings (ADAS, unpublished data) and in herbage (Lemaire *et al.* 1989).

(*b*) *Behaviour of pesticides*

Numerous simulation models of the environmental behaviour of pesticides have been described in recent years. Some have been developed to evaluate just one of the components of the dissipation process such as degradation (Walker & Barnes 1981) or leaching (Leistra 1978). Others aim to describe the interactions between several processes such as leaching and degradation (Leistra *et al.* 1976; Nicholls *et al.* 1982); volatilization, degradation and leaching (Jury *et al.* 1983); leaching, degradation and plant uptake (Waganet & Hutson 1986); or volatilization, leaching, surface run-off and degradation (Troester *et al.* 1984). The main objective of all of them is to provide a basis for forecasting the likely behaviour of a chemical under a wide range of use conditions, data that would be very time consuming and costly to obtain by standard experimental procedures. The statistical approach to evaluation of data output from environmental fate models is discussed further by Laskowski *et al.* this symposium. One important consideration is that valid models can help to identify where detailed confirmatory experimental work would be most profitable.

A relatively simple model that has been widely used is that of Walker & Barnes (1981). It uses detailed laboratory measurements of the effects of soil moisture and soil temperature on pesticide degradation rates in conjunction with readily available weather data and soil properties to simulate persistence of residues in soil in the field. The model has been tested with over 20 different pesticides in 16 countries and its predictive ability is generally acceptable for compounds that are neither volatile nor appreciably mobile in the soil. Although the model is specific for those soil-pesticide combinations for which degradation data are available, it can be used to give a first approximation to the variations in field persistence that will result from variations in weather patterns irrespective of soil type. The United Kingdom Agricultural Development and Advisory Service routinely uses a system based on this model to forecast whether the climate in a particular season is likely to give rise to unusually long or short persistence when compared with long-term average predictions. The calculations are updated every month for different 'persistence category' pesticides using weather data from 50 sites in England and Wales and the model predictions are checked by soil analysis when necessary. It is in making generalized predictions of this type that models can be most useful. Often it is inappropriate to expect specific predictions for other than a relatively restricted range of situations.

In general, as models become more complex, more input data are required and they often become more specific to the pesticide–soil combination for which appropriate input parameters are available. Troester *et al.* (1984) argued that the ideal model would require simple data inputs, be applicable to a wide range of pesticides, soils and weather patterns, and should be based on sound theoretical concepts thus requiring a minimum of empirical calibration. Their attempts to construct such a model led to the conclusion that there are too many limitations in present knowledge for these objectives to be met, and that the best models currently available are either restrictive in their applicability or semi-empirical in nature. One aspect of pesticide behaviour that has so far proved impossible to model satisfactorily is the variability in degradation rate between different soils. Clearly the variability in populations of degrading microorganisms between different soils will be important in this respect. Aspects of this are discussed by Soulas (this symposium).

As already mentioned, one important use of a valid simulation model is to gain a first approximation to the likely behaviour of a chemical in a much wider range of situations than it is possible to examine experimentally. A related use is to provide estimates of behaviour in situations where it is difficult, if not impossible, to make suitable experimental measurements. An example of this was discussed recently by Waganet *et al.* (1989). Results from a field experiment to measure DBCP (1,2-dibromo-3-chloropropane) distribution during leaching through unsaturated soil were interpreted by using an appropriate mathematical model. The model gave accurate predictions of water flux in the soil suggesting that solute flow should also be predicted accurately. Measured concentrations of the pesticide in the soil water were, however, much lower than those predicted. The authors suggested that substantial quantities of the highly volatile DBCP would be lost during vacuum extraction of soil solution and that the model probably provided more accurate estimates of DBCP fate in soils than could be made by field sampling techniques. This conclusion may also be true when considering deep movement of trace quantities of pesticide sufficient to contaminate subsoils and possibly enter drainage waters at concentrations close to the EC limit of $0.1\ \mu g\ l^{-1}$. Standard soil analytical techniques would rarely be sensitive enough to measure residues at this level unless direct measurements could be made on the soil solution which is both difficult and expensive to extract. Few research workers have access to equipment capable of removing sufficient soil solution from depth. Simple calculations using the leaching model of Nichols *et al.* (1982) as modified by Walker (1987) show clearly that significant concentrations in the water phase may well be present at depth in soils when normal soil sampling procedures followed by residue estimation would indicate an absence of measured residues. This once more shows the ability of a model to estimate behaviour that it is not possible to measure by standard experimental methods and to indicate where investment in more complex experimentation would be justified.

VALIDATION OF SIMULATION MODELS

Validation is a major problem with all simulation models. As already mentioned, one difficulty is that experiments are expensive and can be time consuming. It is generally only feasible to make a few measurements on any one experiment and few data sets are available that allow multi-input models to be tested experimentally on more than a few sites.

A major problem with many of the more complex simulation models is that they involve numerous relations and interactions. As Passioura (1973) has argued, it is often difficult to test the validity of the simplest equation so it should be virtually impossible to test the validity of a complex simulation model. Yet it does appear that such simulation models have provided estimates of the effects of quite different variables on a factor of considerable interest that appear to be in agreement with experiments and had not been derived in other ways. Examples have been given in this paper and other fields (Evans 1977). Perhaps we should consider simulation models simply in terms of:

(i) whether they can improve the predictability of a factor in question and thus can improve practice;

(ii) whether they can suggest any new relations or principles that are subsequently confirmed by experiments.

Several computer simulations models have satisfied these criteria and some examples have been discussed above. Although simulation models may never do justice to the subtleties of the various feedback mechanisms, they clearly show promise of being of help in improving practice, especially if they are simple and in terms of readily available inputs.

DISCUSSION

It appears from the foregoing analysis that various processes relevant to the production of field crops can be defined in terms of their level of organization (Thornley 1980). General rules and equations which are of wide applicability govern phenomena at each level of organization. All these relations have been obtained empirically as a result of experiment, but some of those concerning processes at a low level of organization (figure 1) have, as a result of frequent confirmation, become embedded in scientific thought and are now regarded as fundamental (Nelder 1982). It might seem that the best method of prediction for the field is to make deductions from fundamental laws because of their firm foundation. There is, however, little evidence that this procedure has been any more successful in soils work than deduction from some less well established relations. The reasons for the apparent anomaly appear to lie in the facts that fundamental laws govern processes at a much more detailed level than is required in practice, they are in terms of coefficients that can be difficult to measure in the field, and they govern only a few of the factors required to make useful predictions in the field.

The foregoing analysis, however, also suggests that it is possible to deduce relations that govern processes at a high level of organization from those obtained at a lower level of organization, provided that the gulf between the two levels is not large, that the number of relations is small and that the overall size of the model is also small.

There are many relations that govern phenomena at various levels of detail and which appear of wide applicability. It would seem that they should be applied more widely than at present in solving some of the more pressing international agricultural and environment problems. A major obstacle to their wider application is the inaccessibility to the user of many of the relations. They are often embedded in difficult-to-use computer programs and are published in scientific journals covering a wide range of disciplines. There is a notorious inter-disciplinary communication barrier. Maybe there is a need to bring these relations together and to produce an 'engineering' type handbook containing them.

In the past, predictions from various models have been presented to users in the form of tables, graphs and slide rule-type calculators. We believe this practice will continue to be the major role of presentation in much of the world for many years to come, but improvements in layout are essential to facilitate understanding and use. Microcomputers are, however, being increasingly introduced and these open up a new dimension in prediction in agriculture. Among other things, computer programs provide very rapid means of communicating models between research workers and users. We believe that in some areas, simulation models will be used routinely for optimizing fertilizer, pesticide, irrigation and cultivation practices on individual fields. Models for making these calculations that can run on IBM compatible microcomputers are readily available. The inputs in the main are standard soil characteristics which are usually measured in soil surveys, easy-to-get weather data and the normal field records that are often kept at individual farms for each field on a microcomputer. It should thus be possible to run the models almost automatically on the farm. If the input weather data are confined to past records, the methods should be used to estimate the distribution of nitrate to a depth of one or two metres, as described earlier, has been shown to have a decisive influence on fertilizer requirements but is difficult and often costly to obtain by direct measurement, especially on stony soils. The models could also estimate soil-water status and they could estimate residual levels of herbicide that could be important in deciding what future crops could be grown. If the models are run with past weather records, together with the best estimates of future weather they can be used to forecast such things as how much fertilizer and pesticide needs to be applied; when leaching is likely to have removed nitrate beyond the depths of the rooting zone and thus when top dressings are needed to avert loss of yield; when irrigation is needed; and when the land is going to be sufficiently dry to permit harvesting and cultivation without damage to soil structure. If more precise relations concerning the effects of an aerial environment on growth and development are incorporated, the models could also be used for forecasting yields and harvest dates. The models therefore could be used to optimize inputs; to avert restricted growth through transient deficiencies of nutrients and water; and to enable better planning and thus make more efficient use of resources. If this may seem rather far fetched, it is worth mentioning that models are widely used in the western European glasshouse industry to provide a basis for automatic computer control of carbon dioxide concentration, temperature, humidity and lighting according to weather conditions.

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Discussion

S. P. S. ANDREW (*The Wynd, Stainton, Middlesbrough, TS8 9BP, U.K.*). The future computer-borne farmer in your cartoon appears to be wearing a blindfold. May I suggest that this shows a regrettable tendency of using a model to calculate the present from the past when the present is immediately open to observation. The chief use for such a procedure should surely be as a check on the validity of the model before using it to predict the future which is otherwise inaccessible.

D. J. GREENWOOD. I think the problem is that it is often too time-consuming and expensive to monitor the soil parameters in a way that is most needed to improve the efficiency of agricultural practice. For instance, the amount of nitrate at a metre deep has a strong bearing on the crop's requirement for nitrogen fertilizer. The only way at present of measuring nitrate at that depth is to take soil samples, which is costly, especially if the soil is stony, extract these samples and analyse the extracts, all of which takes time. The estimation of herbicide residues requires sophisticated analytical techniques that are costly to use. On the other hand, computer simulation offers the opportunity for estimating soil nitrate and herbicide residues cheaply and quickly so that a rapid response can be made.

Nevertheless, I agree with Professor Andrew, in so far that I do see considerable opportunity for devising novel sensor techniques for measuring key parameters in soil and plants. I also agree about the need to test the validity of models in the field and of their value for forecasting what is likely to happen in the future.

J. BINGHAM (*Plant Breeding International Cambridge Ltd., Maris Lane, Trumpington, Cambridge, CB2 2LQ, U.K.*). Although not much more than half the nitrogen applied as fertilizer to cereal crops is to be found in the above-ground parts of the crop in the year of application, it does appear that winter wheat in particular uses and conserves available nitrogen very efficiently. For the past five years the average rate of application of nitrogen fertilizer to U.K. winter wheat has been relatively constant at about 195 kg N ha^{-1}. In 1989 the average grain yield of wheat in the U.K. was 6.7 ha^{-1} at 11.3% protein (14% moisture basis). At harvest the N content of the crop per hectare amounted to 132 kg in the grain plus about 55 kg in the straw. Although more difficult to quantify, the roots also contain some N at the time of harvest, probably about 20 kg ha^{-1}. Thus the uptake of N by the crop is at least equal in amount to that applied as fertilizer. For the now common situation of sowing in late September, with the straw ploughed in, it may be taken that some 75 kg N ha^{-1} is added to the soil organic matter by the wheat crop, much of which will become available to succeeding crops.

D. J. **Greenwood**. I fully accept Mr Bingham's figures for 1989, but I believe they are consistent with the view that there is still an opportunity for improving efficiency of the use of fertilizer-N for winter wheat. You rightly point out that on average, in the U.K., 132 kg N ha^{-1} are in the grain and this is removed from the field. The remaining 55 kg N ha^{-1} are in the straw and say *ca.* 20 kg N ha^{-1} are in the roots, both of which are returned to the soil. Eventually therefore, when equilibrium is reached, it should be possible to grow a grain crop with 132 kg nitrogen in the grain by applying only sufficient nitrogen to compensate for that removed by the crop. Some of this nitrogen is deposited from the atmosphere and some also is applied as farmyard manure. The total from both sources will be about 50 kg N ha^{-1} in the U.K. as a whole. So it should be possible to grow cereal crop removing 132 kg N ha^{-1} with an input of 132 less 50 kg N ha^{-1}, which equals 82 kg N ha^{-1} each year. We add 195 kg N ha^{-1} as fertilizer. What happens to the remaining 110 kg N ha^{-1}?

I think the explanation for this deficit in nitrogen may lie in the changes that take place in the soil organic matter, as small changes can make a big difference to nitrogen balances in the soil plant system. Some of the incoming nitrogen fertilizer may also be lost by denitrification.

I do, of course, recognize that very little mineral-N remains in soil after a crop of winter wheat grown in field experiments, even when very different levels of fertilizer-N are applied. But the possibility exists that the rate of mineralization of nitrogen from the organic matter increases with increasing fertilizer-N at least when fertilizer has been applied for long periods of time (e.g. *New Scient.* 1989, **1662**, 28–29). This increase in release of mineral-N may be in excess of that which can be absorbed by the autumn crop, at least in certain circumstances, before winter leaching. Also in practical agriculture, as opposed to carefully controlled experiment, there is uncertainty about how fertilizer levels should be adjusted for differences in conditions, there is uncertainty about how the requirement of fertilizer varies across the field, there is unevenness in fertilizer application and crops are not always planted when planned and, on occasion, accidents occur so there are bare patches in the field. It may be for these reasons that research workers at the Water Research Centre and elsewhere have deduced, from measurements of nitrate in underground aquifiers, that nitrate leaching has increased with increase of fertilizer-N application (see, for example, Whitehead, this symposium). Indeed some go as far as saying that the equivalent of between 20% and 40% of fertilizer-N applied is leached from cereal soils each year (House of Lords' Select Committee on the European Communities, 1989, 16th Report, p. 120 and pp. 154–158).

I. J. **Graham-Bryce** (*Shell Internationale Petroleum Maatschappij B.V., The Hague, Netherlands.*). Professor Greenwood referred to different hierarchical levels in considering soil productivity and environmental pollution and outlined the type of model appropriate for each level. Does Professor Greenwood believe that there should be greater attempts to relate the models at different levels, for example, to use information obtained at lower levels to help construct higher models, possibly using probabilistic approaches? Does Professor Greenwood see this as a gap in our approaches, or would he argue that we should simply accept that we need distinct types of model at each level, appropriate for the questions being asked? If Professor Greenwood adopts the latter position, where would he put the emphasis in relation to current needs?

D. J. **Greenwood**. I certainly believe that phenomena can be regarded as existing at different levels of organization and that there are general theories, relations and rules that hold at each of the different levels. I believe also that it is possible to deduce what happens at one level of organization from theories gained at a more detailed level provided the gap is only about one level in the hierarchial system given in my figure. Thus it should be possible to deduce, at least to some extent, what happens at the national level from relations gained in the field, or to deduce useful information about what happens at the field level from what happens in the laboratory on the whole soil. I do not believe, however, that it is generally possible to deduce much from phenomena separated by two or more levels in the hierarchial system. Then the subtleties of all the various interactions and feed-back mechanisms become just too numerous and too difficult to unravel or to simulate.

In the past, tremendous scientific prestige has been attached to logical deduction from fundamental laws. And indeed such deduction has been fruitful in soil productivity studies as will be shown in subsequent papers at this meeting. Obviously this work is of much importance. But my feeling is that the emphasis on logical deduction has tended to obscure the need to develop relations at higher levels of organization. It is essential to be very clear about the level of organization that is necessary for the problem in hand and to concentrate on work at that level of organization.

Dr Graham-Bryce asks where I would put emphasis in relation to current needs. The answer must depend on one's personal perception of the current problems. Probably the most pressing problem that faces mankind will be shortage of food and the fuel wood with which to cook it. This is caused by increasing population and by diminishing areas of land available for growing crops, caused by erosion, desertification and the use of stored waters for irrigation at rates faster than they are replenished. I believe therefore that improving soil productivity is the greatest need, and this should be studied primarily at the field level.