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A Review of Models of Investigating the Behaviour of Nitrogen in Soil

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A review of models for investigating the behaviour of nitrogen in soil

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An efficient way to integrate knowledge on the behaviour of nitrogen in soil is by the development of mathematical models. Models are developed for several aims, such as prediction, management or scientific understanding. Prediction and management models are mainly based on a statistical treatment of data series from preceding years. Models that have been made to obtain a better understanding of the nitrogen cycle are usually based on a mechanistic description of processes such as leaching, volatilization of ammonia, mineralization, immobilization, nitrification, denitrification and uptake by the roots. Differences between models occur because these processes are described with varying degrees of sophistication; often, the description of one or two of the processes dominate the entire model. Thus, a classification of models can be based on the processes that are emphasized. A useful categorization distinguishes between transport models, organic matter models and soil–plant relation models.

1. Introduction

The only N inputs and outputs of a soil that can be observed without the use of sophisticated analytical methods are fresh vegetation and the gradual disappearance of old plant material or litter. By means of chemical analysis we can observe leaching of N as well as inputs and outputs to and from the atmosphere. We are also able to determine that N in the soil is distributed among a few inorganic and many organic compounds. Owing to all kinds of transformations, this distribution changes continuously; these changes are important because they have a considerable effect on crop production, leaching and volatilization. Microscopic studies indicate that numerous microorganisms are involved in these transfer processes. Intuitively, we feel that the only way to integrate knowledge on all these phenomena with sufficient detail is the development of a 'parent' model. Zeigler (1976) calls such a model a *base* model. However, it is obvious that such a model can never be made; it would be too complex and the computational resources required would be too large. Zeigler (1976) assumes, however, that 'given an experimental frame of current interest, a modeller is likely to find it possible to construct a relatively simple model that will be valid in that frame. This is the *lumped* model. It is the experimenter's image of the real system with components lumped together and interactions simplified.' When the existing models for the behaviour of N in soil are reviewed it appears that the actual situation is far from Zeigler's ideal. One should expect one simplified, generally accepted model as a basis for the derivation of other models for special applications. This has not been realized; in fact there is a confusing wealth of models in which one or two processes dominate and in which other processes are treated superficially or even completely neglected. This is because most models are based on data from experimental work on one or two processes. To place the results of such work in a wider context and to make them more generally applicable, the model is expanded. Often, this expansion is not based on one's own study – a complete study of the nitrogen cycle is indeed impossible within one man's

lifespan – and sometimes processes are included on which the model builder has insufficient knowledge.

Perhaps one of the oldest models (Beek & Frissel 1973) is also one of the most balanced ones. This model is, however, not directly applicable. Changes have been made by simplifying the water and heat transport and by expanding the description of the decomposition of organic matter, which has led to an unbalanced model (Van Veen & Frissel 1981).

2. Classification

A major problem arising when selecting a certain model for a specific purpose is that the included processes are always clearly indicated, but the oversimplified and excluded processes are usually not. Also, the objective of the model is often not clear. Many models are said to have been developed for predictive purposes, but in fact they were not; they were developed to gain a better understanding of the system by organizing existing knowledge, to understand process interactions and to identify critical feedback mechanisms. This possibility of integrating knowledge is one of the most powerful advantages of modelling, but it is not the same as prediction. Models mainly developed for better scientific understanding are called here 'scientific models.'

Criteria

The following criteria are helpful in evaluating models.

(i) *Purpose*

The purpose of a model may be prediction, management or scientific understanding. Typical of predictive models is their input–output character. As Brockington (1978) says, the mathematical equations 'represent such relationships as x kg of nitrogen and/or y mm of rain IN, leading to z kg of grass or wheat grain etc. OUT'. Such models are of great value; they allow optimization of fertilizer use and crop production. The models are based on statistical treatment of data of foregoing years and are, as such, site and crop specific (see, for example, Jackson & Sims 1977).

Management models are based on predictive models, but they include various options and may consider different types of crops, rainfall and irrigation patterns, fertilizer levels and prices (see, for example, Zentner *et al.* 1978). They allow economic optimization and may indicate risks due to misfortunes such as water shortage or falling prices.

Scientific models could, in principle, provide the same information (with the exception of the economic aspects), but often they do not. These models are much closer to Zeigler's *base* model (§1), and therefore require an enormous amount of detailed input data. All these details impede practical application.

(ii) *Timespan*

Although the timespan of different models varies enormously, it is probably the criterion that provides least problems. Timespans vary from hours for models of processes such as denitrification, gaseous diffusion and transport of heat and water to hundreds of years for models on soil organic matter transformations and levels. Changing the timespan of a model by a factor of ten or more usually requires reconceptualization. For instance, the description of microbiological activity is a key point in models with a timespan of up to 1 year (Van Veen *et al.* 1981), in models that cover periods of up to 100 years or more the role of the soil microflora

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can be implicitly included in the rate kinetics of the process (see, for example, Van Veen & Paul (1981) and Russell (1981)). An exact calculation of the position of the waterfront during irrigation is of extreme importance for irrigation schedules; for long duration models such calculations are undesirable because the computational resources required are too great.

(iii) *Dynamics*

Models can be divided into budgeting or interactive models. Budgeting models usually consider a complete growing season, i.e. they contain data for annual fertilizer application, manure, biological N_2-fixation as input, and leaching of N, volatilization of NH_3, denitrification losses and N in the harvested products as output (West & Skujiņš 1977; Frissel 1977). Despite their simplicity, it is often difficult to obtain reliable data; data on denitrification losses are mainly determined by balancing the budget. For fertilizer efficiency studies, these types of balances are extremely useful. Interactive or dynamic models are based on a description of the system by rate equations, usually in the form of differential equations. The processes considered are similar to those of budgeting models, but rates are continuously adjusted via feedback relations. The differential equations are almost always numerically integrated. Only interactive models are discussed here.

(iv) *Concept*

As already mentioned, there is a big difference between predictive and management models and scientific models. To the former belong many crop-productivity models. The construction of these models is a 'top down' process, i.e. the model is constructed by analysing results such as the crop production of earlier years, and not by a conceptual consideration of the processes.

Scientific models are developed by a 'bottom up' process. All processes and mechanisms that might be important are studied in detail and the mathematical expressions describing these details are mounted in a larger framework, *the simulation model*. It is this difference in approach that makes it so difficult to couple predictive and management models with scientific models.

Within the scientific models three or four groups can be distinguished:

models in which transport processes such as leaching of N and volatilization of NH_3 dominate (transport models);

models in which the availability of mineral N for plants and the build-up and decomposition of soil organic matter dominates (organic matter models);

models in which N uptake, dry matter production and production limitations dominate (soil–plant relation models);

models for erosion (not considered here).

Each group is characterized by a relatively detailed description of the dominating process(es) and a relatively oversimplified description of the other processes. Many leaching models consist of a sophisticated description of the flow of water in a soil. It is the only group of models in which geometry (one-, two- or three-dimensional) is considered. The transfer of N is then calculated by multiplying the N concentration of the soil water by the water flux. The calculation of the N concentration is already simplified. In many of these models all biological transformations are only represented by one simple source term (Tanji *et al.* 1981; Wagenet 1981; Rao *et al.* 1981; Selim & Iskandar 1981; Kruh & Segall 1981). Other leaching models consider only the vertical flow of water but specify a phase for mobile and stagnant water with an exchange of N compounds between both phases (Addiscott 1981; Frissel & Van Veen 1981*a*).

The organic matter models, however, are oriented towards the fate of mineral N. Often

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they include descriptions of microbiological processes in which the carbon and nitrogen cycles are interrelated. In these models (which are often developed by microbiologists), the biomass is the key variable (Van Veen & Frissel 1981; McGill *et al.* 1981).

In another type of soil organic matter model, the C:N ratios of the various soil organic compounds control the mineralization and N immobilization processes (Bosatta 1981; Parnas 1975). The transport equations are rather simple in almost all organic matter models. In the third group of models, the soil–plant relation models, the N uptake and dry matter production are emphasized. The models concentrate on aerial dry matter production, on photosynthesis and on respiration. Moreover, in some of these models evapotranspiration is a key variable. Uptake of N is controlled by the demand of the crop and sometimes by mass flow and diffusion. Soil water and N may be rather simple growth-limiting factors; the processes that make N available are seldom, if ever, included (Barnes *et al.* 1976; Greenwood *et al.* 1977; Seligman & Van Keulen 1981).

3. Status of modelling

Status reports on modelling of nitrogen processes in soils are presented by Frissel & Van Veen (1981*b*). Many of the conclusions in this section are based on these reports (Addiscott *et al.* 1981; Bosatta *et al.* 1981; Breteler *et al.* 1981).

General conclusions

Our mathematical skill exceeds our knowledge of biological systems. Modern computers have removed many of the mathematical limitations that existed only 10 or 20 years ago. Nevertheless, severe limitations still remain, of which the most important is probably the impossibility of describing the heterogeneity of the soil system in detail. A three-dimensional description of the development of cracks and pores in a soil to calculate details of the water flux or the development of anaerobic zones in soil aggregates is not yet feasible.

Another problem is that it is very difficult to achieve identical levels of precisions in describing processes and in determining input parameters. As explained in §1, Zeigler's *base* model is not feasible, but even a general *lumped parameter* model has not yet been developed. Even when we succeed in developing such a model we have no data sets available to test it. All input parameters need to be known and verifiable variables should be measured. Only a well organized group of scientists is able to collect such data. Such a model is no better than the input data. When certain parameters are determined for a 10 cm layer the model can calculate what will occur in a 1 cm layer, but the results cannot be verified.

Within the sequence *transport models*, *organic matter models*, *soil–plant relation models*, the type of input data tends to vary from parameters that can be determined from independent measurements to parameters that have to be determined from data of preceding years. The leaching of nitrate can be calculated from independent observations, but the uptake of nitrogen by wheat cannot; in this case data from foregoing years are essential.

Part of the descriptions of microbially mediated processes are also based on data collected during previous years, e.g. decomposition of organic matter. In these models, therefore, 'top down' elements dominate (Kruh & Segall 1981; Van Veen & Paul 1981), and in others the 'bottom up' approach (Beek & Frissel 1973; Van Veen & Frissel 1981; Laudelout *et al.* 1977; Juma & Paul 1981).

The type of a model is important with respect to its validation. For statistically based models,

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validation is superfluous, but for models based on independently determined parameters validation is peremptory. This validation is possible as long as small sections of the models or submodels are tested. For the larger models, in which different submodels are integrated, validation is difficult. Because almost all models contain both statistical and conceptual elements, the validation procedure that has to be used is often not sharply defined.

Another problem is the mathematical correctness of the model. In principle, it could be tested by comparing the results of two similar programs with a standard set of data. But a certain data set, suitable for the one program, would require elaborate modification, including many small arbitrary assumptions, to be applicable to the other program, even when the differences are only small. This impedes comparisons between similar programs.

Specific conclusions

(i) *Movement of nitrate and ammonium ions*

In all models the movement of solutes is calculated by multiplying the water flux by the solute concentration. The calculation of water movement in non-swelling soils poses no problems as long as the spatial variability is small (Tanji *et al.* 1981; Wagenet 1981; Selim & Iskandar 1981; Rao *et al.* 1981; Kruh & Segall 1981; Ferrari & Cuperus 1973). Models based on capacity terms such as bulk density, soil water content, tension at a particular depth, and granular distribution, are less sensitive to spatial variability than models based on intensity parameters such as hydraulic conductivity, diffusivity and soil water flux. Capacity terms tend towards a normal distribution. Intensity parameters do not exhibit normal distributions; they are usually log–normal. Well structured and swelling soils are more difficult to model: the formation of cracks and migration of water through cracks and wide pores is particularly difficult (Addiscott *et al.* 1981; Leffelaar 1981; Smith 1981; Edwards *et al.* 1979; Bouma 1981). Solute movement is then calculated by assuming that part of the water flux is immobile or passes through the soil without transport of solutes (Addiscott 1981; Frissel & Van Veen 1981*a*). The transport of NH_4^+ is complicated because NH_4^+ is adsorbed onto soil particles. In systems with two groups of cations, i.e. NH_4^+ and other cations, Gapon-type or Vanselov-type equations are adequate to describe the exchange process. With multi-cation systems this becomes more difficult, mainly because of the large number of parameters required to describe the system. This can be solved, without losing significant information, by using simpler adsorption models, i.e. linear isotherms or a saturation-type isotherm. Ammonium fixation, i.e. almost irreversible adsorption, is easier to handle, although parameter data are missing (Van Veen & Frissel 1981).

(ii) *Gas diffusion and volatilization*

Diffusion is a well known process and its mathematics is well described in many textbooks. The difficulty is in defining the physical environment: its geometry, spatial variability and three-phase composition of microelements. This is especially true for wet soils in which anaerobiosis occurs within aggregates (Addiscott *et al.* 1981). It is not yet possible to calculate the oxygen diffusion rate accurately enough to ascertain anaerobic zones. This limits the possibilities of modelling denitrification. A correlation model for N_2O production, explicitly based on the relative soil moisture content and NH_4^+ and NO_3^- concentration, has recently been developed by Mosier *et al.* (1982). The organic matter content could not yet be included, but the model accounts for N_2O production during nitrification and transport of NH_3 through soil is included. A typical ammonia volatilization model is described by Dawson (1977).

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(iii) *Biological* N_2 *fixation*

Despite the utmost importance of this process, it has hardly ever been modelled. If included it is usually as a constant N_2 fixation rate that does not depend on other system variables (Bosatta 1981).

(iv) *Nitrification*

This appears to be the best-described process of the nitrogen cycle. The most common description is based on Monod kinetics, which considers the process as a two-step one (Laudelout *et al.* 1977; Van Veen & Frissel 1981). In other models it is considered as a one-step process (McGill *et al.* 1981) and sometimes the description is simplified to zero-order or first-order kinetics (Tanji *et al.* 1981).

(v) *Denitrification*

The biological part of this microbiological process in which nitrate is converted into N_2 has been described by single (see, for example, Requa & Schroeder (1973) and McGill *et al.* (1981)) or double (Bowman & Focht 1979) Monod kinetics with the use of the nitrate concentration or the nitrate and soluble organic carbon as rate-determining variables. Models with zero-order and first-order kinetics also exist (Mehran & Tanji 1974; Focht 1974). The physical part of the process, i.e. the development of anaerobic conditions, is, however, difficult to model. Oxygen is supplied by diffusion and consumed by microorganisms. It is extremely difficult to calculate both oxygen diffusion and oxygen removal with sufficient accuracy (Van Veen & Frissel 1981; Leffelaar 1981; Smith 1981).

Some model-builders therefore explicitly allow denitrification to occur whenever specified conditions are fulfilled, e.g. pressure head of soil water 15 cm or less, or water content exceeding 80% of the saturation water content (Selim & Iskandar 1981).

(vi) *Hydrolysis of urea*

This is a well documented enzymatic process. Modelling of this rather fast process offers no special problems (Parton *et al.* 1981).

(vii) *Mineralization and immobilization*

Differences between models are usually caused by assuming that more than one type of biomass (e.g. fungi and bacteria and actinomycetes) (McGill *et al.* 1981) and different types of organic compounds account for differences in availability of organic matter components as substrate for microbes. Juma & Paul (1981) consider eight different soil organic compounds: rapidly decomposable fresh material, slowly decomposable fresh material, biomass, carbon-containing metabolites, carbon- and nitrogen-containing metabolites, active fraction, stabilized fraction, and old organic matter. Van Veen & Frissel (1981) follow the same approach but consider only seven different organic fractions. Van Veen & Paul (1981) differentiate between six forms, but divide two of the pools into protected and unprotected material. Bosatta (1981) considers only two organic fractions. It is remarkable that existing separations of organic compounds, for example separation into amides and α-amino compounds (Söchtig & Salfeld 1977) have not been used by model-builders. Further differences between the models are the use of Monod (McGill *et al.* 1981; Van Veen & Frissel 1981) or first-order (Bunnell *et al.* 1977; Juma & Paul 1981) kinetics and the ways in which the C:N ratios of the different soil organic compounds are handled.

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(viii) *Root growth*

Most root models rely on empirical relations for specific sites and types of plants. There is an urgent need for better and more generally applicable models. Lack of root growth models is a major limitation to developing models for investigating the behaviour of nitrogen in soil (Breteler *et al.* 1981; Barnes *et al.* 1976).

(ix) *Uptake of water and nitrogen*

If the actual transpiration rate of a plant is similar to the potential transpiration rate, almost all models use Darcy-type equations to describe the water flux to plants. The model of the structure of the root system is the only weak point in this approach. For plants where actual transpiration is less than the potential transpiration, empirical relations are preferred. There is a need for models that use the water potential within a plant as a key feature. Models on the uptake of N are less sophisticated. In some models, the uptake is governed by the N demand of the plant. In others, the N content at the root surface is the key variable. The actual uptake is thus assumed to be controlled by mass flow and diffusion, but enzymatic processes are also assumed to be involved, and are expressed by the use of Michaelis–Menten equations. The uptake of N often depends on the presence of ammonia. Although this approach is rather universal, the input parameters are again plant-specific. In conclusion, better conceptual models could be developed if more knowledge were available on the following processes:

the dependence of N uptake by crop roots on the N status and the physiological condition of the plant;

the transport of nitrate through the soil and especially how it is affected by soil water content and properties of the root–soil interface;

the proportion of roots that need to take up N to satisfy the needs of the whole crop.

(x) *Root debris and exudation*

There are scarcely any models for the calculation of root debris and exudates, although it is clearly understood that these materials play an important role in the mineralization–immobilization processes as described under (vii). One exception is the model of Newman & Watson (1977), which describes the abundance of microorganisms in the rhizosphere in relation to its distance to the root and the time required for root exudation to start.

(xi) *Environmental conditions*

The most common way of considering environmental conditions such as temperature, moisture content and pH is to multiply the rates for optimal conditions by reduction factors. Experimental data to evaluate the several possibilities to combine these factors are lacking, and this is considered to be a serious drawback in agro-ecosystem modelling (Frissel & Van Veen 1978).

4. Conclusion

Models have been advertised as a means to organize knowledge. Even during development they should indicate gaps in our knowledge, and, by means of parameter analysis, should identify the most important problems. This is all true. Other researchers have noticed the problems that exist with validation, although they sometimes overlook the fact that statistically based models or parts of models do not need validation. Only parameters of models that are entirely based on conceptual or mechanistic approaches should and can, in principle, be derived

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from independent experiments. The development of mechanistic models is lagging behind that of statistically based models. The combination of both types is difficult. Despite this, the progress made in modelling is enormous. Only 10 years ago, models for soil N hardly existed; at present we are confronted with a sometimes confusing wealth of models. It is only logical that difficulties should have been encountered during this development.

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