LEACHING MODELS OF THE UNSATURATED ZONE: THEIR POTENTIAL USE FOR MANAGEMENT AND PLANNING

P. De Willigen[1], L. Bergström[2], R.G.Gerritse[3]
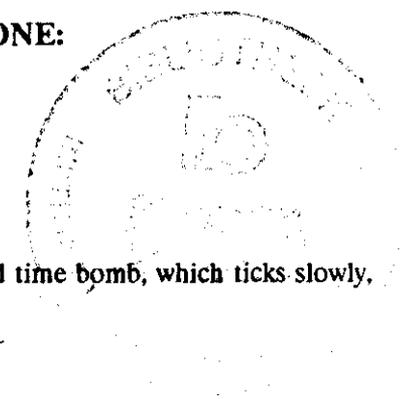
"Thus one can think of the unsaturated zone as a pollutant-filled time bomb, which ticks slowly, but which will eventually explode." (Goldshmid, 1984)

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ABSTRACT

This paper gives a review of models in use outside the USA dealing with leaching of pollutants in the unsaturated zone. An inventory of such models is presented in a table. It is concluded that only a few are suitable as such for application in management and planning. Three case studies pertaining to leaching of nitrate, phosphate and herbicides are discussed.

INTRODUCTION

Input of fertilizers and pesticides can be a highly effective means to increase crop yields. Unfortunately, the increasing use of agrochemicals has also created environmental problems of which degraded water quality is considered one of the most serious. Fertilizers or heavy metals not taken up, or pesticides not volatilized or decomposed are potential pollutants of groundwater. Before any such pollutant can reach the groundwater it has to pass through the unsaturated (vadose) zone, which can be said to be "the buffer between human activity and the groundwater sources" (Goldshmid 1984). In order to control agricultural pollution, a better quantitative understanding is needed of the effects of different soils, climatic conditions and combination of crops on the cycling of agrochemicals in, and leaching out of, the vadose zone. Therefore, interest in using mathematical models has rapidly increased, for the purpose of analyzing the behavior of water and chemicals in agricultural soils, and for policy evaluation and management.

A large number of nonpoint-source models have been devised and are available for planners dealing with agriculture and water quality (see table 1 and reviews by Frissel and Van Veen 1981, Haith 1982). The differences between these models usually concern structure, underlying assumptions and general purpose. The complexity can range from relatively simple models of solute transport which are used for estimating fertilizer movement (Burns and Greenwood 1982) and for making regional estimates of leaching losses (Burns and Greenwood 1982; Bergström et al. 1987) to more comprehensive models used as research tools (Van Veen and Frissel 1981). The simpler, empirically-based models are more suited for widespread use since they require considerably fewer input data than complex, multi-process models. However, a number of complex models have also been developed with a view to widespread application (Johnsson et al. 1987). The applicability of a model is more often limited by the need for calibration rather than by complexity, since models requiring calibration have limited use for sites which lack monitoring programs.

[1] P. De Willigen, Research Scientist, Institute for Soil Fertility, Haren, The Netherlands.

[2] L. Bergström, Research Scientist, Swedish University Agricultural Science, Uppsala, Sweden.

[3] R.G. Gerritse, Research Scientist, CSIRO, Perth, Australia.

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This paper summarizes and discusses model characteristics of interest to potential users, and presents a state-of-the-art review of experience with leaching models developed outside the USA. Case histories of a selection of leaching models dealing with nitrogen, phosphorus, and pesticides are presented.

AVAILABLE NONPOINT-SOURCE MODELS

A list of leaching models in use outside the USA is presented in table 1. This list is based on information collected by Vachaud et al. (1988). Although all are intended for leaching problems, the models listed are quite different in terms of complexity and general purpose.

The majority of the models (18 of 29) deal with linearly-adsorbed or nonadsorbed pollutants. Because the classical convection-dispersion transport equation (see equation 1 below) with steady flow and linear production/consumption term applies here, many analytical solutions are known, for widely divergent boundary conditions. Van Genuchten and Alves (1982) made a catalogue of such solutions. In addition to nonsteady flow, an important reason for solving the equation numerically is the fact that the production/consumption term is nonlinear and/or is a complicated function of environmental conditions (temperature, water content). Most of the nitrate leaching models include a description of nitrogen transformations (mineralization, (de)nitrification).

Nonlinear adsorption is considered in two models (ONZAT, and model 10), one (ONZAT) treating generally nonlinearly sorbed solutes, whereas the other specifically deals with cadmium. Ion exchange is included also in two models (MITM and IMPACT). Such models are particularly intended for use in descriptions of transport of cations (e.g. Ca, Mg, and K).

The models previously mentioned assume that instantaneous chemical equilibrium exists. Nonequilibrium in adsorption or in other chemical reactions is taken into account in the models dealing with phosphate (models 14 and 27) and pesticides (models 8 and 21).

The major transport mechanism for pollutants is transport with water. Leaching in a field situation generally occurs under nonsteady conditions, and flow of water for such circumstances should in principle be calculated fundamentally, i.e., using Richards' equation. This is usually quite time-consuming, and does not necessarily lead to better results as far as solute leaching is concerned (Wierenga (1977), Richter et al. (1978), Beese and Wierenga (1980), De Willigen and Neeteson (1984)). Of the models in table 1, 11 solve Richards' equation; the others either describe time-variable waterflow in a simplified way, or assume steady conditions. Five models partition the soil water into mobile and immobile parts; transport is limited to the mobile part only, whereas there is an exchange of solute between the mobile and immobile parts. As shown by Nkedi-Kizza et al. (1984), this description is equivalent to that where chemical nonequilibrium is considered.

Only one model deals with spatial variability (model 28), but it should be mentioned that De Haan et al. (1987) and Van der Zee and Van Riemsdijk (1987) considered spatial variability of cadmium sorption parameters using a simplified version of model 10.

Few of the models are at present suitable for solving problems related to management and regulation. Of the 29 models listed in table 1, only two were specifically designed for management purposes: PULSE (Bergström, 1987) and MORELN (Geng et al., pers. commun.). Model 24 was originally set up as a simple transport model for nitrate, but has evolved into a model for the complete nitrogen regime, to be used for advisory purposes. As opposed to the situation in the USA, in Europe and elsewhere little emphasis has been put on the development of management-oriented models. However, simulation models designed primarily for research in principle do have the potential to be used for management and planning. One of the reasons for the limited practical use of such models is the lack of thorough validation of the models. Sixteen

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of the models in table 1 have been validated against field data; still fewer (viz. 13) have been used for sites other than those for which they were originally validated. Moreover, in many cases too many site-specific parameters are used that are not readily available or very difficult to obtain. In order for models to be used as management tools, a prerequisite is that proper documentation is available and that the model code is easy to understand for users other than the model designer. Only about one third of the models cited in table 1, can, in the opinion of their designers, be used without author supervision or advice. As one tends to overrate the lucidity of one's own work, this is probably an overestimation of the accessibility of these models.

Table 1. List of leaching models discussed in this paper.

Model name	Authors	Country	Pollutant	Remarks
1.SLIM	Addiscott,T.M.	UK	Nitrate	Mobile/immobile phases
2.____	Ackerer,P. 1/	France	Nitrate	Major N-transformations, plant uptake, heat transport
3.____	Ammentorp,H.C. Refsgaard,J.C.	Denmark	Any ions	Ion exchange, oxygen transport 1988)
4.NITCROS	Aslyng,H.C. Hansen,S. (1984)	Denmark	Nitrate	Major N-transformations, plant uptake
5.GAMON	Barraclough,D. (1988)	UK	Nitrate	Mobile/immobile phases
6.ANIMO	Berghuijs,J.T. Rijtema, P.E. Roest,C.W.J (1985)	Netherlands	Nitrogen	N-transformations, oxygen demand, heat transport
7.PULSE	Bergström,S. Brandt,M. Gustafson,A. (1987)	Sweden	Nitrate	Major N-transformations, plant uptake
8.____	Boesten,J.J.T.I (1986)	Netherlands	Pesticides	Instantaneous and time-dependent adsorption and decay
9.____	Burns,I. (1975)	UK	Nitrate	
10.TRANS.CSM	Chardon,W.J. (1984)	Netherlands	Cadmium	Nonlinea adsorptioa

1/ no publication available, see list of addresses

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Table 1. continued.

Model name	Authors	Country	Pollutant	Remarks
11.MITM	Chen,W., 1/ Li, I.	China	Any ions	Ion exchange
12.____	Dautrebande,S. (1985)	Belgium	Linearly adsorbed solutes	Mobile/immobile phases, originally developed by Van Genuchten & Dalton (1986).
13.TRANS	De Smedt,F. Wierenga,P.J. Van der Beken,A. (1981)	Belgium	Linearly adsorbed solutes	Mobile/immobile phases
14.____	De Willigen,P. Raats,P.A.C. Gerritse, R.G. (1982)	Netherlands	Phosphate	Instantaneous adsorption, time-dependent fixation
15.____	Ferrari,Th. Cuperus,J.L. (1973)	Netherlands	Nitrate	
16.MORELN	Geng,Q.Z. Girard,G. Ledoux,E. (1987)	France	Nitrate	Major N-transformations, management-oriented
17.SOILN	Johnsson,H. Bergström,L. Jansson,P.-E. Paustian,K. (1987)	Sweden	Nitrate	Major N-transformations, heat transport
18.____	Kirda,C. Nielsen,D.R. Biggar,J.W. (1973)	Turkey	Chloride	
19.MONO	Lafolie,F. 1/ Habib,R.	France	Nitrate	Mobile/immobile phases, plant uptake
20a.SWATRZ 20b.SMMC	Maciejewski,S. 1/ Zaradny,H.	Poland	Linearly-adsorbed solutes	SMMC considers two-dimensional transport

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Table 1. continued.

Model name	Authors	Country	Pollutant	Remarks
21.CALF	Nicholls,P.H. Walker,A. Walker,R.J. (1982)	UK	Pesticides	
22.FAUST	Pachepski,J.A. Mironenko,E.V. Ponizovski,A.A. (1988)	USSR	Any ions	Ion exchange
23.EPIC	Piehler,H.	BRD	Nitrate	Includes erosion originally developed by Williams et al. (1983).
24.____	Richter,J. Kersebaum,K.Chr. Utermann,J. (1988)	BRD	Nitrate	
25.IMPACT	Schweich,D. Sardin,M. Jauzein,M. (Sardin et al., 1986)	France	Any ions	Non-linear adsorption
26.ONZAT	Van Drecht,G. (1986)	Netherlands	Non-linear adsorbed solutes	
27.____	Van Der Zee,S. Van Riemsdijk,W.H. (1986)	Netherlands	Phosphate	Non-linear adsorption, time dependent fixation considers spatial variability
28.SIMP	Vogel,T.1/ Cislerova,M. Simunek,J.	CSSR	Linearly adsorbed solutes	
29.____	Zandt, P.A. Willigen, P.de (1981)	Netherlands	Nitrate	Includes major N-transformations

1/ no publication available, see list of addresses

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CASE STUDIES

From the models listed in table 1, we selected three models dealing with leaching of nitrate, pesticides and phosphate, respectively, which we will discuss in case studies. The models are well documented, have been tested and validated against field data, and are suitable for use in management,regulation and planning.

General Transport Equation

All models discussed in this section numerically or analytically solve the general one-dimensional equation of transport by diffusion/dispersion and convection:

$$\frac{\partial}{\partial t} (\rho F + \theta c) = \frac{\partial}{\partial z} D \frac{\partial c}{\partial z} - \frac{\partial}{\partial z} vc + S \qquad [1]$$

where
ρ = the bulk density of the soil [ML^{-3}],
F = the amount of sorbed pollutant per unit soil mass [1],
θ = the volumetric water content [1],
c = the concentration of the pollutant in the soil solution [ML^{-3}],
D = the diffusion/dispersion coefficient [L^2T^{-1}],
v = the flux of the soil solution [LT^{-1}],
z = the vertical coordinate [L], and
S = the production/consumption of the pollutant in the soil [$ML^{-3}T^{-1}$].

It is assumed that transport only takes place in the liquid phase.

Case Study 1: Leaching of Nitrogen

Models dealing with nitrate leaching and nitrogen transformations in agricultural soils vary widely in scope, but their main structures usually show distinct similarities. The biological, chemical, and physical processes included in these models are either described in a mechanistic way or by empirically-based relations. Quite often combinations of the two also occur. In the model chosen for the case histories described here (SOILN, see table 1) both mechanistic and empirically-based submodels are included (Johnsson et al. 1987). This model was applied to several sites and data sets: sites where the information on processes included was extensive (Johnsson et al. 1987; Bergström and Johnsson 1988), and data sets describing relatively long-time series, comprising several crops (Jansson et al. 1987, Gustafson 1988). It has also been used to evaluate long-term trends in nitrate leaching in a whole watershed where information was very sparse (Jansson and Andersson 1988). These various applications, with completely different prerequisites concerning input data, suggest that relatively comprehensive models can also be useful for applications-oriented problems related to planning, management and regulation.

Only an overview of model structure and basic assumptions underlying important processes are given here.

Structure of the Model
The model consists of two parts which are used in sequence. First, soil moisture and temperature conditions are simulated in a water and heat submodel. Its outputs are utilized as driving variables for the nitrogen submodel. Common to both submodels is the vertical structure that facilitates division of the soil into different layers depending on the resolution requested and information available on basic physical and biological characteristics.

Water and Heat Transport

The water and heat submodel has been described earlier by Jansson and Halldin (1980). It is based on two coupled differential equations describing heat and water transport (derived from Fourier's and Darcy's laws, respectively) in a one-dimensional soil profile. Snow dynamics, frost, evapotranspiration, precipitation, groundwater flow, water uptake by the plant, and drainage flow are included. The model predicts daily values for soil temperature and soil water content at any level in the soil profile using standard meteorological data as driving variables.

The model also deals with water transport in the saturated zone. The flow rate from each saturated layer above the depth of the drainage tiles is calculated, taking into account the thickness of the layer, the saturated conductivity, the depth of the drainage tiles, the depth of the groundwater table and the distance between drainage tiles. In addition to the water flow drained via the drainage tiles, the saturated water flow directed toward a stream or ditch is calculated with an empirical equation.

Surface runoff can occur due to limited infiltration capacity or limited permeability of the soil.

Nitrogen Transformations and Plant N-Uptake

A detailed description of the nitrogen model is given by Johnsson et al. (1987). Biological N-transformations in the model (fig. 1) apply to each layer. Mineral-N pools include ammonium and nitrate. Organic-N is distributed over litter, feces, and humus. The carbon pools for litter and feces are included to control nitrogen mineralization and immobilization rates.

Undecomposed material (e.g., crop residues, dead roots, microbial biomass) constitutes the litter component, while the humus component consists of stabilized decomposition products.

Mineralization of humus-N (denoted as N_h) is calculated as a first-order rate process:

$$N_{h \to NH4} = k_h \, e_t \, e_m \, N_h \tag{2}$$

where k_h = the specific mineralization constant $[T^{-1}]$,
          e = response function, subscripted to denote temperature and moisture [1], and
         N_h = the mass of humus-N [M].

Similarly, decomposition of the organic carbon pools of litter and feces are calculated as first-order rate processes controlled by specific mineralization constants and by response functions for soil moisture and temperature (the same as those used for mineralization of humus-N). Of the decomposed carbon in the litter and feces pools, one fraction $(1-f_e)$ is lost to the atmosphere as CO_2, the fraction $f_e(1-f_h)$ is recycled within the pools, and the fraction $f_e \, f_h$ is stabilized as humus. The parameters f_e and f_h represent an efficiency constant and a humification fraction, respectively. Corresponding nitrogen flows are calculated assuming a constant C/N ratio of decomposing biomass and humification products (r_o). The net mineralization or immobilization in the litter pool is calculated as:

$$N_{l \to NH4} = (N_l/C_l - f_e/r_o)C_{ld} \tag{3}$$

where N_l and C_l are the masses of nitrogen and carbon in the litter pool, and C_{ld} is the decomposition rate of litter carbon. The same equation is valid for the feces pool. When net immobilization occurs (i.e., $N_l/C_l < f_e/r_o$) the immobilization is limited to a maximum available fraction in the soil. Both ammonium and nitrate can be immobilized, with preference for available ammonium.

Nitrification of ammonium to nitrate is calculated from the excess of ammonium present when the ammonium/nitrate ratio exceeds an assumed equilibrium. The calculation employs a specific rate constant and abiotic response functions.
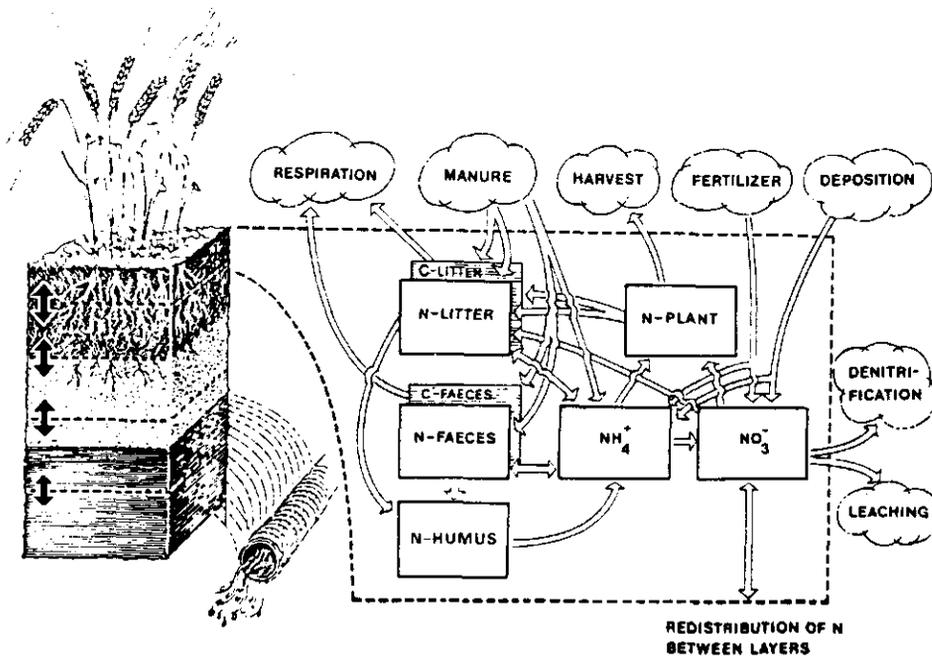
Figure 1.
Structure of the nitrogen model (SOILN). Components within the dotted
line represent the uppermost soil layer. Subsurface layers have the same
structure but do not receive any direct inputs from fertilizer and deposition
(from Johnsson et al. 1987).

The abiotic response functions regulating decomposition, mineralization, and nitrification are
functions of soil temperature and soil water content. An exponential expression is used for
temperature, where the response increases by a factor 2 for a rise in temperature of 10°C. An
empirical relationship is used for volumetric water content, based on the assumption that the
range within which water content is optimum is defined by two thresholds representing dry and
very wet soil.

Denitrification is calculated as a zero-order process based on a potential rate and on response
functions of temperature, water content, and nitrate concentration. The temperature response
function is the same as that used for other microbial processes, while the response to water
content is zero up to a value close to saturation, from where the response increases with increased
water content to an optimum level at saturation. The nitrate concentration response is calculated
with a Michaelis-Menten expression with a half-saturation constant (cf Burns 1978).

Plant uptake of nitrogen is controlled by an assumed root distribution and a potential logistic
growth curve. Nitrogen uptake is reduced when the demand exceeds a maximum availability
fraction of mineral-N in the soil, similar to the situation described for immobilization. The ratio of
ammonium uptake to nitrate uptake was taken to be the same as the ratio of ammonium to
nitrate in the soil solution.

Agricultural management characteristics and different crop characteristics can be used to estimate
most model parameters controlling inputs and outputs of nitrogen. The most important
information requirements for determining model parameters are those describing different
nitrogen transformations in the soil. Some of the parameters are well known from laboratory
studies while others are only qualitatively known and have to be estimated (Johnsson et al. 1987)

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Transport of Nitrogen

Only nitrate is considered to be mobile, and nitrate flows are calculated as the product of water flow and nitrate concentration in the soil layer from which the water flow originates. Diffusion and dispersion are not explicitly accounted for, but due to the division of the soil profile into layers of finite thickness, numerical dispersion sometimes occurs.

Site Description

To test the applicability of the model to different field data sets, two extreme applications concerning available information for validation of the various parts of the model were chosen.

First, the model was applied to a field for which extremely detailed information was available. This field in central Sweden, Kjettslinge, was the experimental site for the project "Ecology of Arable Land" (Persson and Rosswall 1983, Steen et al. 1984). Data were collected on decomposition, denitrification, leaching, mineralization, mineral-N profiles, primary production, and soil abiotic conditions. The climate is cold-temperate and humid with annual precipitation of 520 mm and mean annual temperature of and 5°C. The topsoil, 30-cm thick, contains 15-20% clay, 2.2% organic carbon and has a pH of 6.0-6.5. The topsoil is underlain by a layer of fine sand with average thickness of 25 cm, underlain by an oxidized clay layer down to a depth of about 75 cm, and finally an non-oxidized clay layer down to 100 cm. Simulated and measured nitrate leaching and mineral-N profiles were compared in two treatments with barley (with and without N-fertilization (120 kg N/(ha·yr)) (Johnsson et al. 1987) and a fertilized (200 kg N/(ha·yr)) grass ley (Bergström and Johnsson 1988). The simulated periods were 3 and 4 years, respectively, on each 0.36-ha plot size.

Secondly, the model was tested on a 202-km^2 watershed in southern Sweden. Simulated values of nitrate leaching were compared with measurements for a 20-year period (Jansson and Andersson 1988). More than 2/3 of the total flow of nitrogen in the river draining the basin originated from agricultural nonpoint sources (Andersson 1986). The proportion of the area under perennial leys decreased from 16 to 3% during the 20-year period, whereas that under cereals increased from 44 to 57%. On the remaining part sugar beets and oilseed rape were grown. The predominant soil type in the area is clay till with a well-developed structure, well aerated, and with favorable water-holding characteristics. In the simulation, a grain field was chosen to represent arable land in the area. Most of the parameter values in this application had to be estimated from the literature or from agricultural statistics for the region. This, in combination with the problems of analyzing field measurements from watersheds integrating many biologically and physically different subareas, made a detailed analysis of the simulated results difficult.

Results

The main objectives of the simulations with Kjettslinge data were to obtain a thorough test of the different model components and to evaluate the usefulness of the model for studying nitrate leaching in annual and perennial crops. In the watershed simulation, efforts were made to elucidate trends in nitrate leaching over the 20-year period as indicated by measurements. The relative importance of labile and stable organic matter (litter and humus) in supplying mineral N to the soil and thus affecting leaching losses, was tested. Therefore, two sets of parameters were used, one representing a fast turnover of organic matter (because the major part of the litter-N was assumed to move directly to the soil) and one in which litter-N was largely directed to the humus pool, representing a slow turnover of organic matter.

The detailed field simulation. Since simulation of nitrate leaching depends on model output both of nitrate concentration and of drainage water flow, three time series of cumulative leaching were compared: (1) calculated from measured nitrate concentrations and simulated drainage (i.e., "partly simulated") (2) calculated from simulation of both nitrate concentrations and drainage flow, and (3) measured. Figure 2 shows this comparison. In this way deviations in leaching pattern caused by

either poor predictions of drainage water flows or of nitrate levels could be isolated; however, this was only done in the simulations with barley as test crop. Cumulative nitrate leaching was similar in all time series. The greatest differences between measurements and simulations occurred during the initial year (1981) and were largely due to underestimated drainage water flows in the simulations.

Similar results were obtained for the grass ley, as shown in figure 3. In this case a substantial difference between simulated and measured nitrate leaching also occurred at the end of 1984; in this case, the reason can also be found in deviations in drainage behavior. The earlier start and short duration of measured drainage and leaching at the end of 1984, compared with the corresponding simulated values, can be accounted for by soil physical conditions. Macropore flow and lateral water flow in layers with high hydraulic conductivity are the most plausible causes of the earlier start. Once vertical flow becomes dominant in the field, the groundwater table, which had fallen considerably during the dry years 1982 and 1983 (Alvenäs et al. 1986), had to rise again before any water flow through the drainage tiles could be expected. This explains the absence of measurable nitrate leaching after the initial, rapid tile-drainage flow. Neither flow through macropores in dry soil directly to drainage tiles nor lateral water flow above the groundwater table are considered in the model, which explains the discrepancy between simulated and measured nitrate leaching in the grass ley during 1984. In that year, however, simulated leaching was in good agreement with measurements in lysimeters at the Kjettslinge field (Bergström 1987) in which percolation to deeper groundwater did not occur. This test indicates that the model considerably underestimates nitrate leaching from tile-drained plots.

In both simulations with Kjettslinge data the nitrogen part of the model was adapted to obtain reasonable agreement between simulated and measured values for soil mineral-N content. The simulated values for nitrate leaching were arrived at independently. The fairly good agreement between simulated and measured values of leaching in these two Kjettslinge applications indicates that good leaching predictions can be obtained with a simulation model if data on soil mineral-N content are available (cf. Jansson et al. 1987).
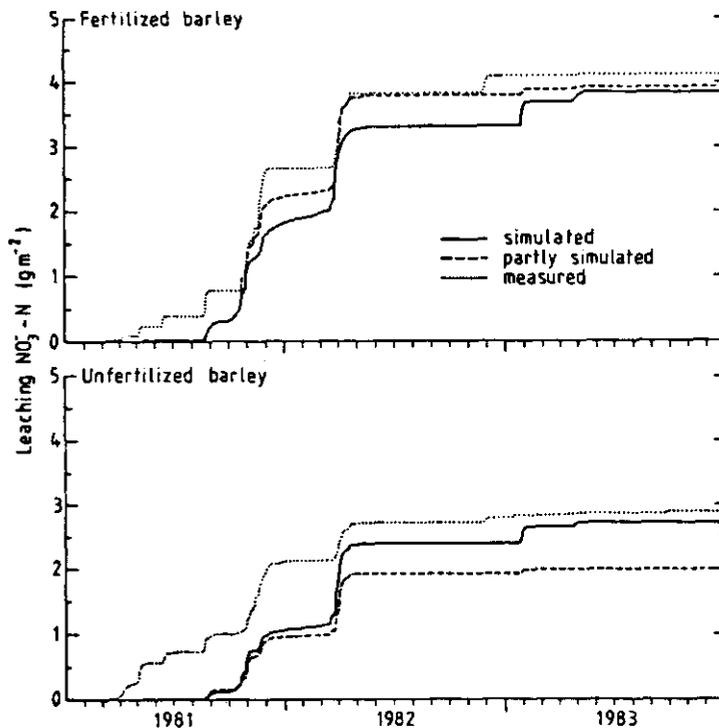

Figure 2.
Simulated, "partly" simulated, and measured cumulative nitrate leaching from the barley crops at Kjettslinge (from Johnsson et al. 1987).
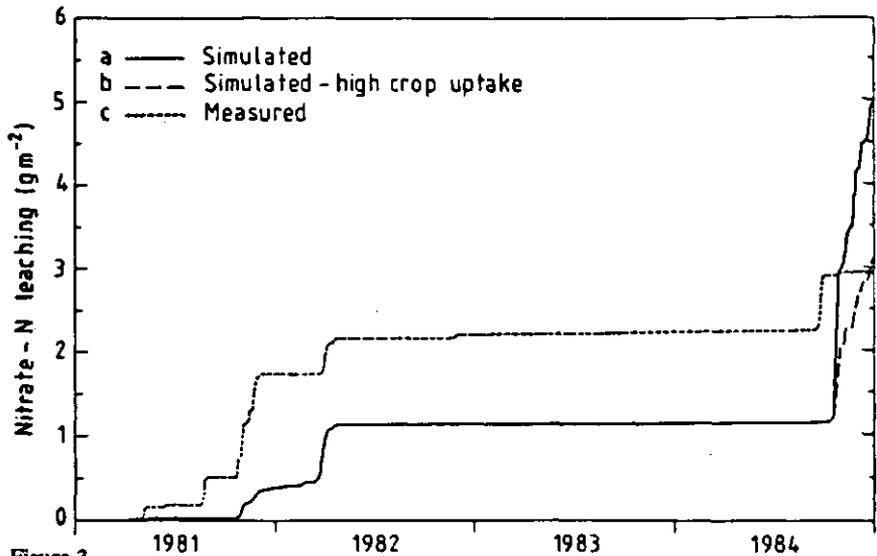
Figure 3.
Simulated and measured cumulative nitrate leaching from the grass ley
at Kjettslinge (From Bergström and Johnsson 1988).

The watershed simulation. Over the 20-year period, N-fertilization rate in this area has increased from 90 kg N/(ha•yr) during the first 10 years to 120 kg N/(ha•yr) during the following period. The higher amount of N-fertilizer used during the second 10-year period caused a distinct increase in simulated nitrate leaching, mainly when turnover of organic matter was assumed to be rapid (fig. 4). Observations showed a pattern similar to that simulated by the fast-turnover approach, while the simulation assuming a slow turnover of organic matter led to an obvious underestimation of nitrate leaching during the final years.
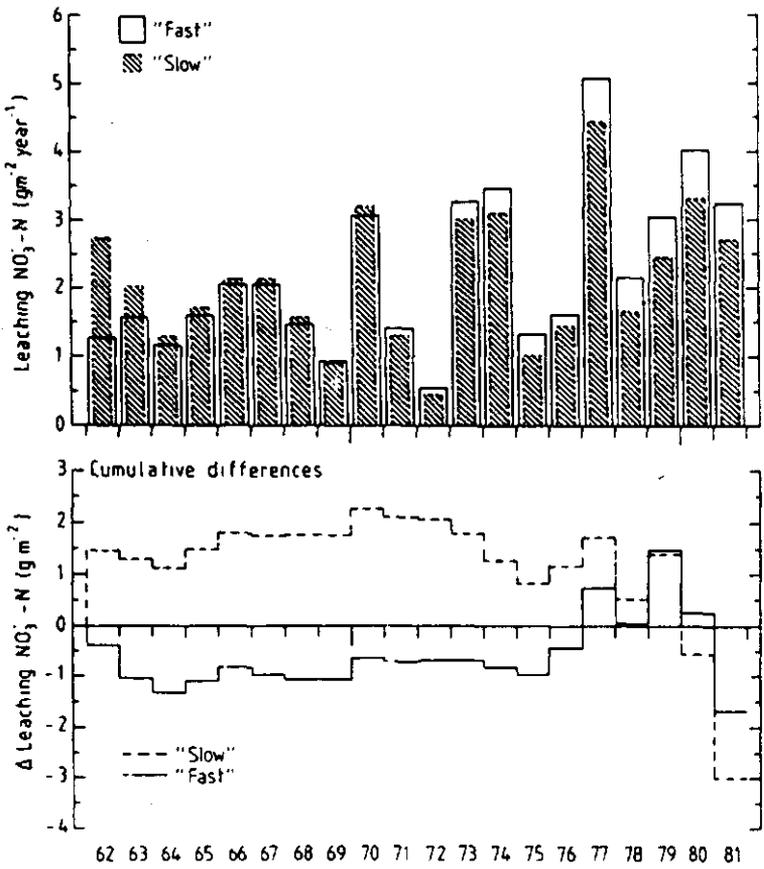

Figure 4.
Annual amounts of simulated leaching
with two different parameter sets
and cumulative differences between
simulated and measured leaching.

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The increased N-fertilization resulted in higher crop yields and thus also in a larger crop-residue input in the model. In the fast-turnover approach this led to an increased net mineralization. However, the slow turnover of organic matter increased immobilization and therefore decreased net mineralization compared to the first 10-year period. In both simulations the model predicted that the additional N-fertilizer input was mainly taken up by the crop, and only a small fraction was lost directly from the system due to leaching.

Although there was a general lack of detailed information from the watershed, the results showed that both organic-N fractions in the soil contributed to the simulated change in leaching associated with increased N-fertilization. The question remains if a higher rate of net mineralization, following increased crop residue input, will occur within a couple of years or will require decades after incorporation of residues.

Perspectives
Since the model described here is representative of a whole group of simulation models dealing with nitrate leaching and nitrogen transformations in agricultural soils, comments and suggestions for model improvements are also applicable to many other nitrogen models.

Characteristic of most of these models, despite similarities in structure, is that they usually emphasize certain processes while treating others more superficially. To be suitable for management and regulation, models should be balanced. The use of a fixed potential uptake curve to control plant N-uptake is one example of a crude simplification in the model described here. No climatic factors, such as drought stress, are considered, which is a shortcoming when nitrate leaching during longer periods is simulated. Another example is the oversimplified treatment of denitrification, which is a common problem with models dealing with nitrogen transformations in agricultural soils. However, the simulated annual amounts of N denitrified in the Kjettslinge applications were similar to preliminary estimates, based on field measurements (Klemedtsson 1986), which is satisfactory for a model intended for use in management. Further experimental studies are needed to make a critical test of the denitrification part of any model possible.

Some processes and parameters were identified, in the applications cited above, as being crucial for accurate simulation of nitrate leaching from agricultural soils. Assumptions concerning N-flows between organic-N pools were shown to play an important role in the watershed simulation, when leaching trends are investigated. It is still difficult, however, to predict how changes in agricultural practices in the model will affect soil organic matter and the flows between the organic pools. Another example is crop N-uptake and parameters associated with this process. Common both in decomposition/mineralization of nitrogen and plant N-uptake is the high magnitude of these N-flows. For example, simulated annual N-uptake by the grass ley at Kjettslinge was about 400 kg N/ha and simulated mineralization was about 200 kg N/ha. This is in contrast with simulated leaching (fig. 3) and denitrification, which averaged only 10 and 5 kg N/(ha•yr), respectively. Thus even small variations in plant N-uptake and/or N-mineralization can easily overshadow changes in mineral-N content and N-leaching. Consequently, it is very important to accurately simulate these large N-flows in order to get good estimates of nitrate leaching. This is especially important when dealing with management and regulation, for which accurate quantification is crucial.

Discrepancies between simulated and measured leaching in the Kjettslinge applications were mainly explained by uncertainties in hydrological flow paths rather than by uncertainties in biological processes. This suggests that it would be a substantial improvement to add a mechanism for water flow in macropores to the model, similar to that described by Jarvis and Leeds-Harrison (1987). However, their model does not, at present, include solutes. A bypass mechanism in structured soil is also considered in a model described by Addiscott (1977, see table 1) which includes solute transport; it is simple to use and suited for management purposes. This model, however, is not based on soil physical theory, which somewhat limits its general applicability.

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An obvious advantage of the physically-based water and heat model described here is that it can be adapted to different sites by using available texture information (cf. Jansson et al. 1987). Moreover, driving variables are derived from standard meteorological variables. Both these factors make more widespread use possible.

Case Study 2: Leaching of Phosphate

Phosphate is considered the limiting nutrient as far as eutrophication of surface waters is concerned. Although agriculture is certainly not the only source of phosphate pollution, it is nevertheless a major one, perhaps the most important nonpoint source. The problem is most serious in those regions where a very intensive form of agriculture is practiced on soils with a limited capacity to hold phosphorus, e.g. in pig-breeding areas on light soils in The Netherlands, Belgium and West Germany. In some of these regions, disposal of large amounts of animal slurry on a relative small area has created a situation where the phosphorus sorption capacity of the soil is almost reached.

The Dutch government has enacted legislation that limits application of animal slurry on soils. Because additional future regulations will be based on studies done by Van der Zee and Van Riemsdijk (1986), we decided to use their work in our case study on phosphorus. The specific paper we will discuss deals with transport of phosphate on a column scale and in a field situation. The model considers non-calcareous sandy soils.

Structure of the Model

First transport in a single column is treated. In principle, here the basic transport equation 1 without the production/consumption term applies. Because of the nature of phosphate sorption by the soil, one can expect a relatively sharp front to develop, so it was considered justified to neglect dispersion and diffusion. The governing equation then is:

$$\rho \frac{\partial F}{\partial t} + \theta \frac{\partial c}{\partial t} = v \frac{\partial c}{\partial z} \qquad [4]$$

where F is the sum of adsorbed and precipitated phosphate. The field is supposed to consist of an ensemble of such columns.

Sorption

Sorption is modeled as two processes: a short-term Langmuir-type adsorption (equilibrium reached in about one day) and a long-term diffusion-controlled precipitation (pseudo-equilibrium reached after several months). This description of phosphate behavior in soil is based on numerous earlier publications (Beek (1979), Lexmond et al.(1982), Van Riemsdijk and De Haan (1981), Van Riemsdijk and Van der Linden (1984)) dealing with the different aspects of the physico-chemical interaction between phosphate and the soil matrix.

Transport

Column scale. When slurry is applied to the soil surface the concentration there will be buffered at a particular value, c_o, until all solid phosphate in the slurry has dissolved. Accordingly the boundary condition at the soil surface in the case of such a slurry application can be approximated by a Heaviside step function:

$$z = 0; \qquad c = c_o H(t^* - t), \qquad [5]$$

where t^* is the period in which all solid phosphate is dissolved and the step function H(x) is defined as: $H(x) = 0$ for $x < 0$, and $H(x) = 1$ for $x > 0$. Solving equation 4 then yields:

$$F = F(c_o)H \left\{ \frac{vt^*}{R} - z \right\},$$ [6]

where $R = 1 + \rho F(c_o)/\theta c_o$. For a sequence of M applications of slurry the P-front can be approximated by:

$$F = F(c_o)H \left\{ \frac{v\Sigma t_i^*}{R} - z \right\}$$ [7]

$F(c_o)$ can be approximated by the sorption capacity, evaluated at the buffering concentration, $F_m(c_o)$. One calculates F_m from the content of amorphous aluminum and iron oxides in the soil, which can be assessed by extracting the soil with acid ammonium oxalate. With this extraction, almost all soil phosphate is also extracted.

Equation 7 can be rewritten as:

$$F = F_m H \left\{ \frac{P_{ox}}{F_m} - \varsigma \right\}$$ [8]

where P_{ox} is the oxalate-extractable quantity of soil P. Because P_{ox} and F_m are depth-averaged quantities (averaged over a depth of L m), the ratio P_{ox}/F_m gives the degree of saturation of a column of length L, at the time of sampling. The dimensionless depth ς is defined as :

$$\varsigma = {}_0\!\int^z (Fe + Al)_{ox} \, dz \, / \, {}_0\!\int^L (Fe + Al)_{ox} \, dz$$ [9]

In equation 9, $(Fe + Al)_{ox}$ is the sum of the oxalate-extractable amounts of Fe and Al, which are generally a function of depth z. From equation 8 it follows that the dimensionless concentration of P in the solid phase is:

$$\Gamma = F/F_m = H \left\{ \frac{P_{ox}}{F_m} - \varsigma \right\}$$ [10]

Results
Field scale. The field is assumed to consist of an ensemble of columns, each with its own P_{ox} and F_m, both of which are considered to be randomly distributed.

In a field experiment, on a sandy soil, the soil profile was sampled shortly after the harvest of the crop (corn) at 67 locations. In each of these samples P_{ox} and $(Fe + Al)_{ox}$ were determined. Both P_{ox} and $(Fe + Al)_{ox}$ were found to be normally distributed. With the computed statistics of P_{ox} and F_m the field-averaged profile may be calculated, assuming that P_{ox} and F_m are independent. This can be compared with the field-averaged experimental profile, as is done in figure 5. Experimental and computed profiles are in reasonably good agreement, although the former follows a somewhat steeper course.

Perspectives
The model is relatively simple and is reasonably accurate, when a particular situation is described. However, to use it for predictive purposes the spatial nature of the random variables should be known, e.g., the occurrence of a certain trend in the spatial variables and the correlation between variables. As yet this appears to limit a routine application of the model.
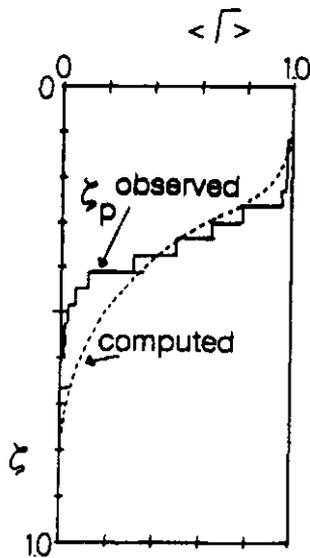
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Figure 5.
Average dimensionless concentration of P in the solid phase $<\Gamma>$ (see equation 10) as a function of dimensionless depth ζ (equation 9).

Despite model limitations, the insights gained with the model have made it possible to formulate a protocol (Van Der Zee 1988) for phosphate-saturated soils. The protocol is a set of procedures for the details of soil sampling, soil sample treatment and laboratory analysis, and data evaluation, to which (in principle) each field is subjected in a region suspected of harboring many phosphate-saturated fields. It will be used to estimate the maximum permissible thickness of the phosphate-saturated topsoil, as a function of adsorption and fixation (precipitation) parameters and the depth of the groundwater table. As such it will be used to extend and supplement existing regulations.

Case Study 3: Leaching of Pesticides

Although simulation models for transport of pesticides have been designed for more than a decade in Europe (Leistra 1972), apparently they have not been used specifically for planning, management and regulation (Leistra and Boesten, pers. comm.). In The Netherlands, admission of new pesticides is, among other things, based on studies of Leistra (1975), Leistra and Dekkers (1976) on adsorption, decay, and transport of such substances. Boesten (1986), elaborating on Leistra's work, presented an extensive and detailed study on simulation models for the behavior of herbicides in soil. Although his model has not yet been used for management purposes, in our opinion it offers sufficient possibilities to do so. Therefore we selected the thesis of Boesten as a case study. In this thesis both instantaneous and time-dependent nonlinear sorption of the herbicide are taken into account, in addition to transformation and transport.

Structure of the Model
The numerical solution of equation 1 is obtained by a finite-difference approach. The 40-cm soil profile is divided (from top to bottom) into 10 0.05-m thick layers, 15 0.01-m thick, and 10 0.02-m thick. The calculations pertain to a non-cropped soil.

Sorption and Decay
From both short- and long-term batch experiments it was found that for the herbicides in question three classes of sorption sites had to be distinguished. The total bulk density of the herbicide in soil can thus be given as:

$$C = \theta c + X_1 + X_2 + X_3 \qquad [11]$$

where θ = the volumetric water content, and
X_i = the amount sorbed on sites of class i in mass per unit soil volume.

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Sorption on sites of class 1 was found to proceed so fast that instantaneous equilibrium can be assumed, whereas sorption to, or desorption from, class 2 and 3 sites was found to proceed at finite rate:

$$X_1 = K_1 c^{(1/n)} \tag{12}$$

$$dX_2/dt = k_2 \{K_2 c^{(1/n)} - X_2\} \tag{13}$$

$$dX_3/dt = k_3 (K_3 c - X_3). \tag{14}$$

Equilibrium for class 1 and 2 sites is described by a Freundlich isotherm (with parameters K_1, K_2 and n), and for class 3 by a linear isotherm (with parameter K_3). Rate constants are given by k_2 and k_3, the latter being one order smaller than the former (values are about 0.5 day^{-1} and 0.02 day^{-1}, respectively).

Decay of the herbicide was described according to first-order kinetics:

$$S = k_1 \theta c \tag{15}$$

Transport

Transport by water is an important component of total transport, so the model contains a routine by which flow of water is calculated. The flow of water is described by a "functional" model (Addiscott and Wagenet 1985), i.e., instead of calculating fluxes of water in a fundamental way a simpler approximation is used. This approximation is for downward flow (e.g., when rainfall exceeds evaporation) similar to the method proposed or used earlier by Terkeltoub and Babcock (1971), Burns (1975), Van Keulen (1975), and Stroosnijder (1982). Precipitation in excess of evaporation fills the soil layers from top to bottom to water content at field capacity. The resulting flux to the next lower layer can thus be estimated.

Evaporation is estimated as 90% of the Penman evaporation as long as the cumulative potential evaporation is less than a soil specific value, β^2. If cumulative potential evaporation (counting from the first day that evaporation exceeds rainfall) exceeds this value, actual cumulative evaporation is taken to be the product of β and the square root of the cumulative potential evaporation. From the cumulative actual evaporation, the actual evaporation rate (the flux of water leaving the soil surface) is calculated. A withdrawal function, giving the fraction of the surface flux withdrawn from a specific layer as a function of its depth below the soil surface, is employed to estimate the fluxes of water between neighboring layers. The water flow model has been validated with results from two years' field experiments. Figure 6 shows a comparison of calculated and measured water content for a particular year (1981), and demonstrates the good agreement between simulation and measurement.

In addition to transport by flow of water, transport by diffusion and dispersion are also considered (see equation 1). The diffusion coefficient D_{dif} for the herbicide was taken from the literature, whereas the dispersion coefficient D_{dis} was calculated as:

$$D_{dis} = |v| \ell \tag{16}$$

where ℓ is the dispersion length, which was estimated from field experiments with bromide as a tracer.

Results

The performance of the simulation model was tested with results of field experiments, where the values of the necessary parameters had been determined in independent batch and field
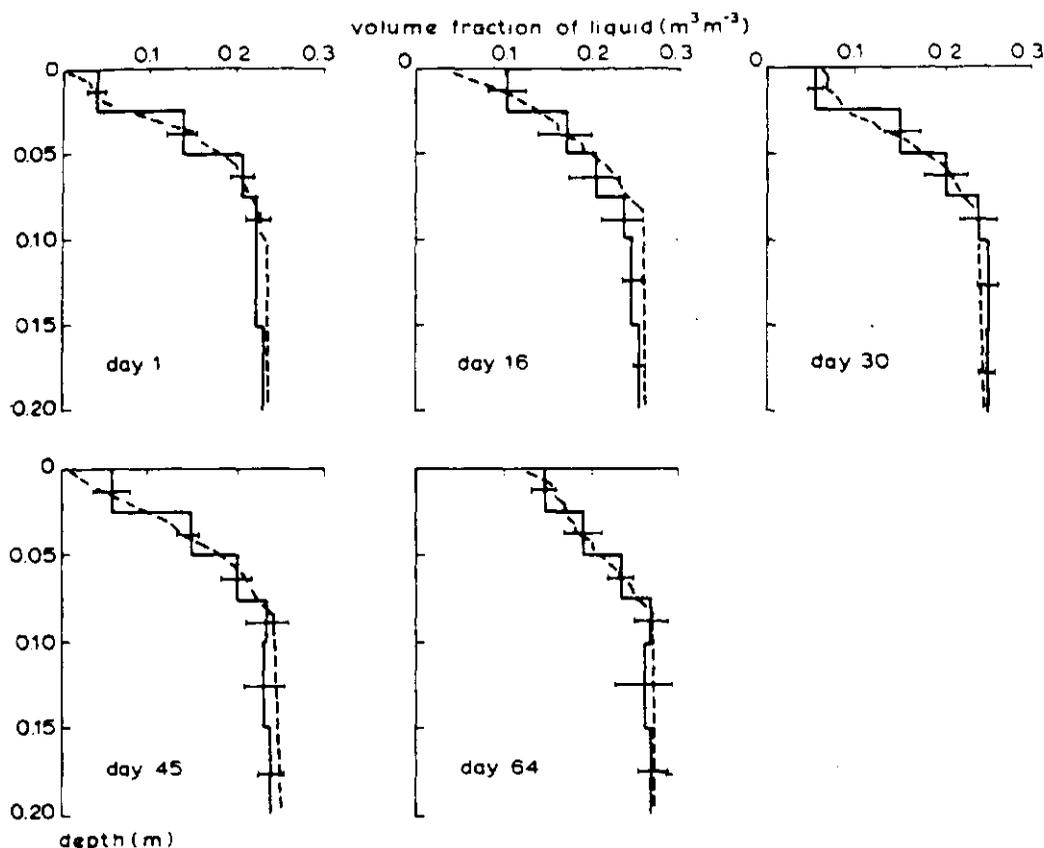
Figure 6.
Profiles of water content on 1981 sampling dates in a field experiment.
Vertical solid line segments are averages of 5 measured profiles; horizontal
bars are standard deviations; and dashed lines are simulated profiles.

experiments. The soil simulated was a loamy sand, containing 1.8% organic matter, 3.6% $CaCO_3$ (pH 7.4 in 1 N KCl), and was fallow during the 64-day experimental period. Figure 7 compares measured and predicted soil profile concentrations of metribuzin at five times during the simulation period. The model results are in good agreement with the experimental results.

Perspectives

This model appears to be well balanced. It includes the processes relevant for the phenomenon studied. Although simplicity was an objective (e.g., the calculation of water flow), no process description was simplified for the sake of simplicity alone.

The model has been properly validated with independent experiments. The results of the validation, which appear to be quite good, therefore give a fair impression of the reliability of the model. The model thus seems applicable on other sites.

The model demands quite a few parameters: i.e., seven for the physico-chemical part, to which the number of parameters governing transport, also seven, has to be added. Some of these parameters (e.g., water content at field capacity or soil bulk density) are relatively easy to estimate or can be obtained by simple standard measuring routines. Others (the parameter β governing evaporation, or especially the parameters connected to sorption to class-3 sites) call for rather complicated or time-consuming experimental estimation methods.
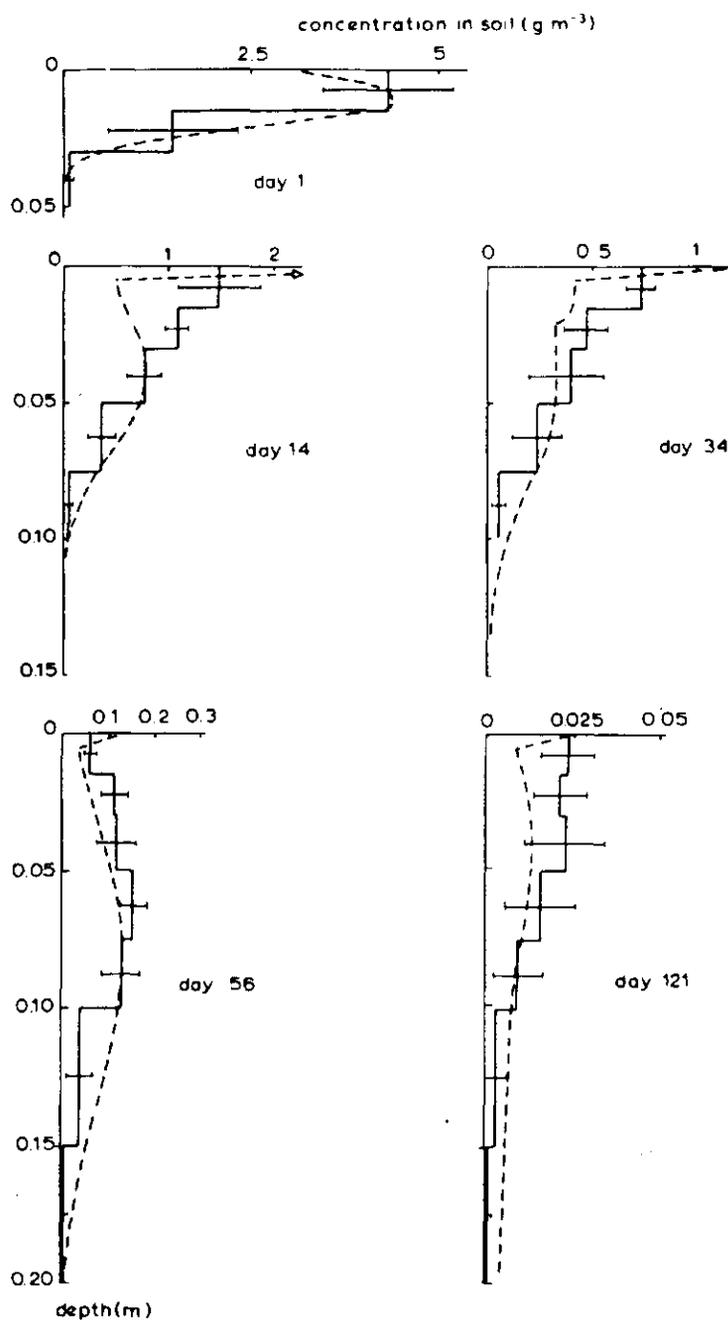
Figure 7.
Comparison of calculated and measured profiles of the herbicide metribuzin. Vertical solid line segments are averages of measured concentrations; horizontal bars are standard deviations; dashed lines are calculated.

An obvious extension of the model is to consider also the period in which the soil is cropped. Then also, among other things, uptake of herbicides and water by the plant should be included.

CONCLUDING REMARKS

The development of simulation models appears to be one of the routine methods used when problems of pollution and leaching are encountered. This practice has led to a plethora of models, which often at first sight, and indeed also after detailed inspection, are quite similar. One suspects that in many cases the real incentive for developing yet another model is not so much the application of computer modeling to an unexplored area, but is what Van Keulen et al. (1981) have called: the attitude that implies "anything you can do, I can do better", if not a basic coolness

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to, or mistrust of, the complex models of others. On the other hand, there is some justification for a decision to develop a new model despite the large number and diversity of existing models, because the way in which underlying concepts are programmed in models is quite often difficult to understand for users other than the original developer. Furthermore, technical problems are often encountered when model implementation is attempted on different computer systems. Moreover, there is usually much understanding to be gained from developing one's own model, instead of copying someone else's.

In order to use models like those listed in table 1 for practical purposes, it is necessary to be able to estimate required parameter values from independent, standard measurements. An accurate and easily-available method to estimate parameter values would allow models to be applied to sites where detailed information on the temporal pattern of relevant processes is lacking. If parameter values can be accurately estimated, models that are more research-oriented may also be useful for analysis of practical questions concerning agricultural practices. If it is inevitable to use parameters that are site-specific and can only be obtained by complicated and time-consuming methods (e.g., determination of mineralization and denitrification rates), it is sometimes possible to correlate such parameters to easily-obtainable and/or time-independent system properties. Examples are the correlation between mineralization and soil texture (Van Veen et al. 1985, Richter et al. 1988), and between F_m and $(F_e + Al)_{ox}$ (Van der Zee and Van Riemsdijk, 1986; see case study 2).

As discussed earlier a prerequisite for a model to be attractive for users outside the designers' group (or indeed outside the scientific community) is the existence of appropriate documentation, in the form of a user's manual. Such a manual should discuss the relevant theory, explain how it is incorporated into the model, which language is used, what input is required, and of course the objectives for which the model was developed and is applicable. Also needed is a discussion of the model limitations, of the simplifications used, and it should be indicated when the model cannot be used. Moreover, it should contain information as to the determination or estimation of the parameters required; possibly it should suggest default parameter values which apply to an "average" situation. In Europe the existence of such user-friendly documentation for leaching models is the exception rather than the rule. Also for the models presented as case studies documentation, other than scientific papers, is lacking, though at least the protocol mentioned in the context of case study 2 offers the possibility of application of the model to practical situations.

Even well-tested and user-friendly models should be used with caution if employed by external users. Especially when used by non-modelers (e.g. planners and politicians), the danger exists of misinterpretation of results and of too much trust in model predictions. When a model is made available for practical use, the modeler should still be consulted for interpretation of the results because many far-fetched assumptions are used even in the best of models.

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List of addresses of authors of models mentioned in table 1 for which no publication is available as yet.

Ackerer, P.
Institut de Méchanique des fluides
2 Rue Boussingault
f- 67083 Strasbourg Cédex
France

Chen, Wenlin
Institute for Agricultural Resources, Environment and Remote Sensing
Beijing Agricultural University
Beijing
P.R. China

Lafolie, F.
INRA Station de Sciences du sol et d'Agronomie
Domaine St.Paul
Flontfavet
France

Maciejewski, S.
Hydroengineering Institute of the Polish Academy of Sciences
ul. Cysterow 11
80-953 Gdansk
Poland

Vogel, T.
Dept. of Irrigation and Drainage
Thakurova 7
16629 Prague 6
CSSRnd