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MODELING AGRICULTURAL-ENVIRONMENTAL PROCESSES IN CROP PRODUCTION

Proceedings of a 2 — 4 June 1980 Task Force Meeting

G. Golubev and I. Shvytov, Editors

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PREFACE

The International Institute for Applied Systems Analysis began its work on modeling the environmental impacts of crop production in 1978. The objective was to clarify what was known about applying mathematical models to the assessment of the environmental impacts of crop production, and the focus was on the environmental impacts of dry farming. The most important field-scale environmental effects of dry farming--which can potentially lead to such large-scale environmental impacts as eutrophication, water pollution, and cropland losses--were identified as soil erosion, nitrogen leaching, and phosphorus and pesticide losses.

The work in this field was begun by considering the hydrological and major natural biogeochemical processes, which, through a chain of events, cause these environmental effects. It became apparent that there are many mathematical models describing single processes such as water percolation, runoff, nitrogen mineralization, nitrification, denitrification, phosphorus precipitation and adsorption, evapotranspiration, nutrient uptake, pesticide degradation, etc. Moreover, a few complex models (CREAMS, ARM, ACTMO, etc.) have been developed. One of these complex models, CREAMS, was transferred to IIASA and used in a number of the Institute's National Member Organization countries.

Our experience in collecting and using various mathematical models convinced us not only of the necessity of refining collaborative efforts in this field, but also of the need to discuss some methodological questions. We pursued these matters at two meetings: a planning workshop in June 1978 and an April 1979 conference on environmental management of agricultural watersheds. A third meeting on modeling agricultural-environmental processes in crop production--which is reported in these proceedings--focused on:

- discussions of the state of the art of developing mathematical models for environmental processes in crop production;
- improving the guidelines for completing the IIASA research on mathematical modeling of the environmental effects of agriculture; and
- refining the Institute's collaborative work with other organizations.

This volume presents the papers presented at this third meeting in the form in which they were received from their authors. The paper on CREAMS is missing, as it will be treated in detail elsewhere.

The volume closes with a short review of the main points brought out at the meeting.

The editors would like to express their thanks to all those who contributed to this Task Force Meeting, whether by formal presentations, or through participation in the discussions. The editors are grateful to the chairmen and rapporteurs of the sessions (see Appendix), whose reports were used to prepare the final paper. We would also like to express our appreciation to Pamela Hottenstein and Caroline Goodchild for their technical and organizational help.

GENADY N. GOLUBEV
IGOR A. SHVYTOV
Editors

CONTENTS

THE MODELLING OF ENVIRONMENTAL IMPACTS OF CROP PRODUCTION

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INTRODUCTION

Agricultural management policies based on intensive use of land, water and chemicals have greatly increased the efficiency of crop production in the twentieth century. The policies have also produced distributions of chemical residuals in the environment which may be hazardous to human health and natural ecosystems. The environmental pollution problems associated with agricultural production are extremely difficult to resolve. The effects of agricultural practices on chemical losses from cropland and the ultimate fate of chemicals once they leave cropland are poorly understood. Even if this were not the case, the efficiency of food and fiber production is so critical to the world's economy that policy makers are reluctant to impose pollution control practices which may lower production levels. The environmental impacts of crop production can be managed rationally only if two critical information needs are met. First we must be able to quantitatively assess the environmental damages associated with crop production practices. Second, the likely effects of pollution control practices on crop production levels and farm income must be determined and practices identified which will have minimal negative impact on food production. Perhaps the most critical challenge facing agricultural and environmental scientists in the remainder of this century is to provide the information needed to develop agricultural management policies which feed the hungry without poisoning the poor (and the affluent).

Mathematical models have become necessary tools for the study of agricultural pollution, mainly because past empirical experience has provided little of the quantitative information needed. A variety of modelling approaches have evolved in the last ten years, and this paper is a brief attempt to categorize models related to water quality and to give some examples of models which have been developed at Cornell University over the past several years.

CATEGORIES OF MODELS FOR ANALYZING AGRICULTURAL NONPOINT SOURCE POLLUTION

Water quality problems caused by crop production are typically associated with nonpoint source pollution, which is the contamination of water bodies by chemicals and sediment contained in diffuse runoff and percolation water flows from land surfaces. Provision of the information discussed in the previous section requires estimates of pollutant losses or loadings from cropland to water bodies, assessment of water quality impacts of pollutant loadings, and determination of economic effects of control practices. The author is familiar with only one model which attempts to provide all of this information (Wineman, _et_ _al_., 1979). More typically models are designed for only one of the three types of analyses and can be classified as

1. Chemical and Sediment Loading Models
2. Water Quality Impact Models
3. Planning and Management Models

Water quality models are not unique to nonpoint sources since they are in general designed to predict the response of a water body to both point and nonpoint sources. The literature contains hundreds of examples of such models and they are omitted from this discussion. Sediment loading models are also omitted, partly in the interest of brevity, but also as a reflection of the fact that sediment *per se* is seldom a critical or manageable water quality problem. Rather, sediment is important mainly as a carrier of chemicals, and sediment loading models are integral components of many chemical loading models.

Chemical Loading Models

Chemical loading models have been constructed to predict the following losses from croplands: dissolved and solid-phase nutrients, salts, and pesticides in runoff, and dissolved nutrients, salts and pesticides in percolation or watershed base flows. The models are developed for either field or watershed scale and fall into three distinct groups.

Continuous simulation models are the most analytical models and are based on systems of differential equations for solute movement. Essentially all of the models apply to groundwater problems, and most focus on nitrate or phosphate movement. Examples are given by Davidson *et al*. (1978), Czyzewski *et al*. (1980), van Veen (1977) and Shah *et al*. (1975). Continuous simulation models require calibration and have seen limited field testing.

Discrete simulation models solve chemical transport problems by repetitive mass balance calculations for discrete time steps and are generally more operational than the continuous models. Discrete simulation models are often based on previously developed hydrologic and sediment transport models. Examples include models for nitrogen in percolation by Addiscott (1977) and Saxton et al. (1977), watershed models for nutrients by Williams and Hann (1978) and Tseng (1979), and field-scale models for nutrients and pesticides developed by Donigian et al. (1977) and Knisel et al. (1979).

A final group of models are functional models which do not attempt to simulate the fundamental processes which affect chemical losses. Rather they are simple predictive equations, often empirical, which can provide rough estimates of the quantities of chemical losses. Functional models are designed to provide information rapidly with relatively little data input. Examples are the nitrate leaching model of Burns (1974, 1975) and the general "loading functions" proposed by McElroy et al. (1976).

Planning and Management Models

Planning and management models are in principle the most useful models for policy making since they determine economic impacts of potential pollution control practices. In theory, the models can provide estimates of trade-offs between agricultural production and environmental quality objectives. However, the economic components of the models are much better developed than components for prediction of pollution, which are commonly limited to sediment losses estimated by the Universal Soil Loss Equation. All planning and management models are based on budgetting approaches and are usually solved by linear programming.

Three different scales of models are apparent. Regional impact models are used for macro-scale studies of farm and consumer income (Heady and Vocke, 1979; Taylor and Frohberg, 1977). Watershed planning models such as those of Onishi and Swanson (1974), Casler and Jacobs (1975) and Scherer (1977) are applied to specific water quality problems and evaluate impacts of management practices, subsidies and taxes on pollution and farm income. Farm management models estimate the effects of pollution control on the activities of individual farmers. Examples are given by Smith *et al*. (1979), Coote *et al*. (1976) and Miller and Gill (1976).

EXAMPLES

The remainder of this paper is a description of four operational models which have been developed at Cornell University for the analysis of agricultural nonpoint source pollution. Using the terminology of the previous section, three of the models are chemical loading models, including two discrete simulation models and one functional model. The fourth model is a farm management model. The purpose of the examples is to illustrate some general characteristics of models used to evaluate environmental impacts of crop production and also to provide a progress report on a modelling research program which the author has been involved in for several years. The discussion is limited to the general structures of the models and some results of their applications. Mathematical details are provided in the cited references.

Watershed Loading Functions

The estimation of pollutant export in streamflow from large agricultural watersheds is difficult. The basic modelling problem is how to recognize the great spatial variability of a watershed's land surface without resorting to a model which is so complex that data and computer requirements render it impractical. The approach used in the present case was the application of a functional model to each of a watershed's spatial units and then aggregating results from all units in the watershed. The model is described in Haith and Tubbs (1980). Earlier versions are in Haith and Tubbs (1979) and Haith and Dougherty (1976).

The structure of the loading functions is shown in Figure 1. Unit source areas or fields which are homogeneous with respect to soils and crops are identified using a random sampling procedure. Separate estimates are made for dissolved and solid-phase losses of the chemical of interest. Dissolved chemicals are carried in runoff as predicted by the U.S. Soil Conservation Service's Curve Number Equation (CNE). Snowmelt runoff is based on a degree-day melt equation and the CNE. Solid-phase chemicals move with sediment losses as predicted by the Universal Soil Loss Equation (USLE). Both the CNE and USLE are applied on an event basis and hence predictions can be made for any time period of interest. Solid-phase chemical concentrations are based on concentrations in the soil and dissolved concentrations are extrapolated from field experimental studies. Concentrations are multiplied by runoff or soil loss to produce edge-of-field chemical loadings. These loadings are converted to watershed export by multiplication by transport and attenuation factors. The factors are assumed to be equal to one for dissolved loadings. Solid-phase attenuation factors are given by the watershed's sediment delivery ratio.

The loading functions were used to estimate nitrogen (N) and phosphorus (P) losses from the 391 km^2 Pequea Creek watershed in Pennsylvania. Water quality sampling data provided measurements of dissolved and

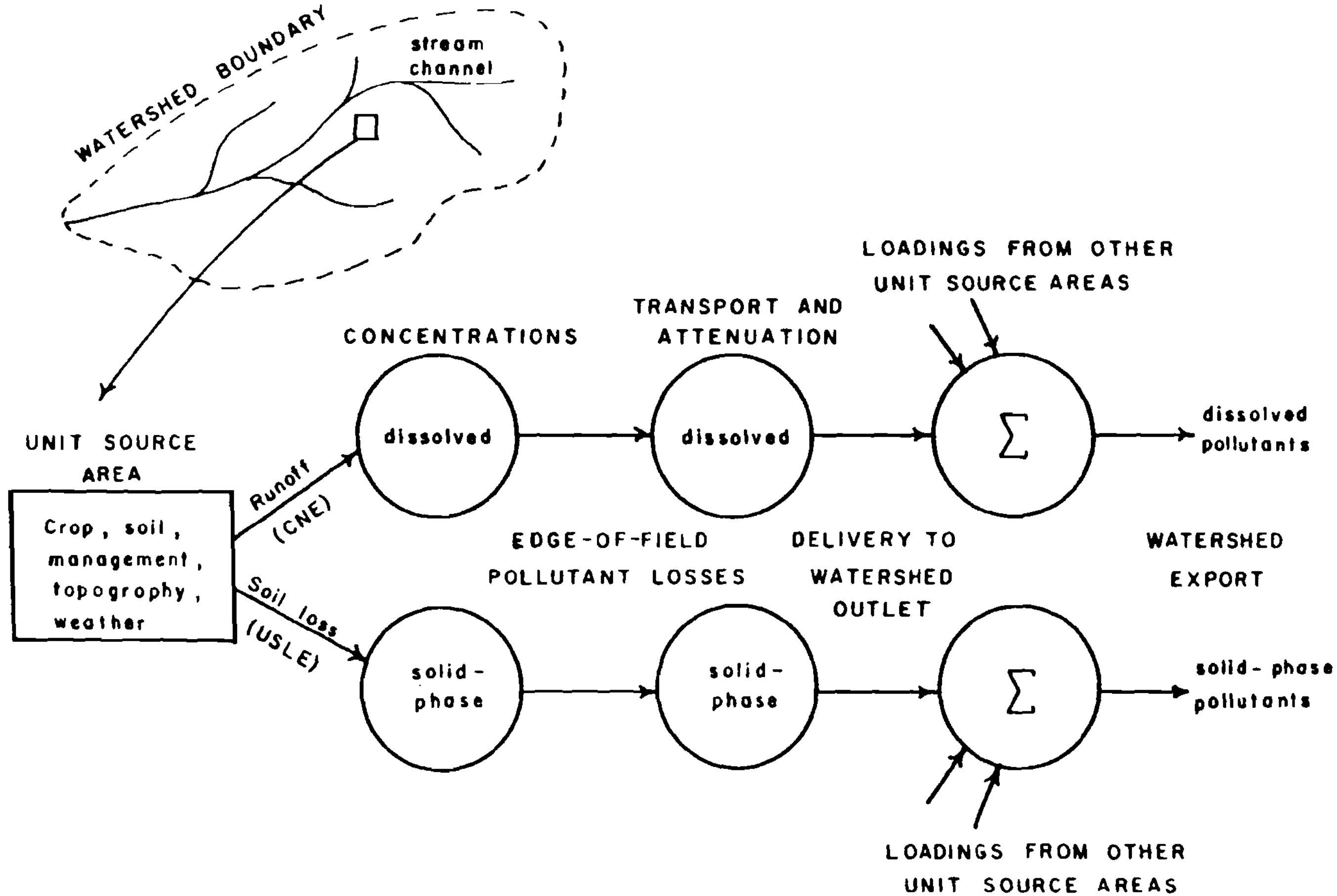

Figure 1. General Methodology for Watershed Loading Functions

solid-phase N and total P in runoff from the watershed for a 16-mo period in 1977 and 1978. Predictions are compared with observations in Table 1. Nitrogen predictions were relatively accurate, but total P predictions (dissolved & solid-phase) were less so. Since data was not available to test the model's predictive ability for the dissolved and solid-phase P fractions, further testing will be necessary.

Pesticide Runoff Model

This model simulates the behavior of pesticides in the soil and estimates dissolved and solid-phase losses in runoff. The model is described in Haith and Tubbs (1980) and Haith (1980).

The general components of the model are shown in Figure 2. Runoff losses are based on the total pesticide in the surface centimeter of soil. This quantity is assumed to decay exponentially with time and when a precipitation event occurs, is partitioned into adsorbed and dissolved constituents based on a single parameter linear adsorption isotherm. Runoff losses are predicted by the CNE and soil losses are determined by an event-based version of the USLE. The model was tested using data for atrazine losses from two small catchments (P2 and P4) in Watkinsville, Geoergia. Predictions are compared with observations for 17 major precipitation events in 1973-1975 in Table 2. The model's accuracy clearly varies among storms but the magnitudes of measured and predicted total losses for the three-year period compare favorably. Correlation coefficients between measured and predicted atrazine losses for the 17 events are 0.95, 0.92 and 0.94 for solid-phase, dissolved and total runoff losses.

	Dissolved Nitrogen	Solid-Phase Nitrogen	Total Phosphorus
		(10^3 kg)	
Predicted by Loading Functions	128.7	725.0	330.7
Measured in Direct Runoff	129.8	797.4	234.5

Table 1. Comparison of Predicted and Observed Nutrient Export from Pequea Creek, Feb., 1977 - May, 1978.

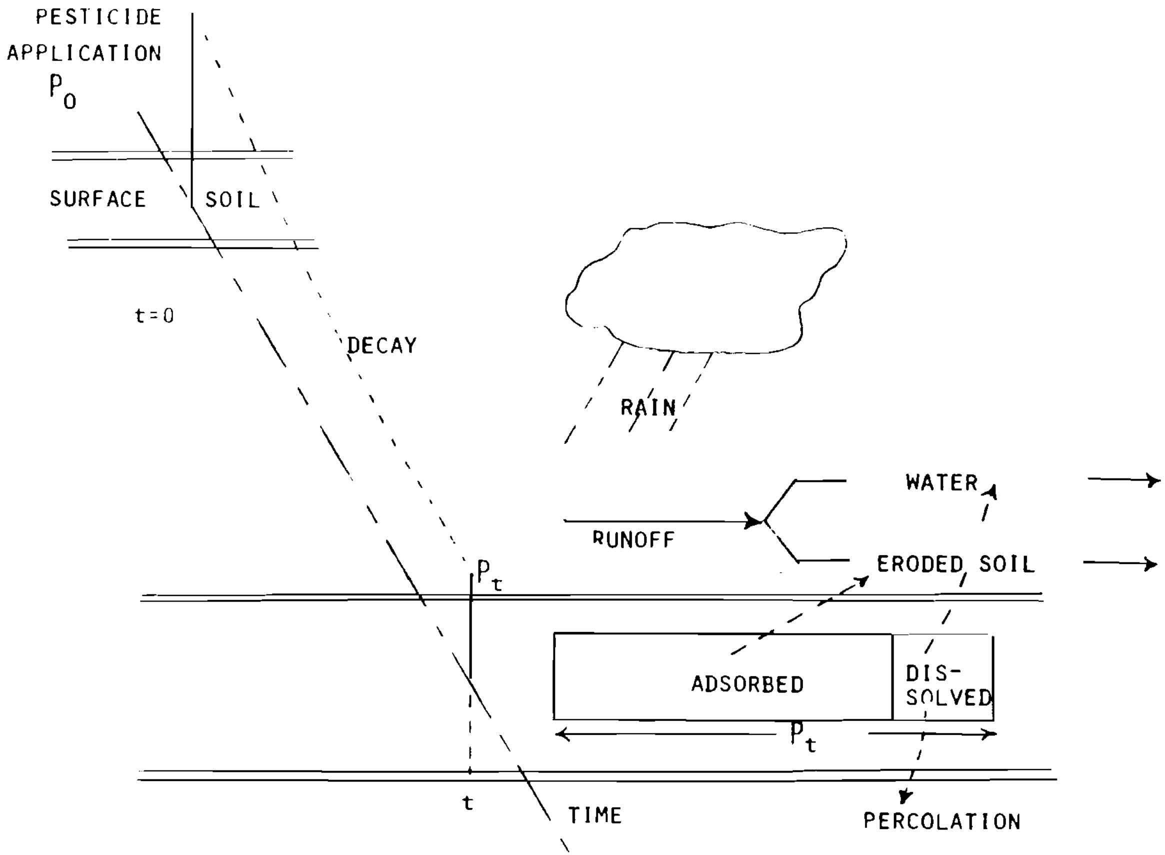

FIGURE 2. COMPONENTS OF PESTICIDE RUNOFF MODEL

Event	Solid-Phase Pesticide in Runoff Measured	Solid-Phase Pesticide in Runoff Predicted	Dissolved Pesticide in Runoff Measured	Dissolved Pesticide in Runoff Predicted	Total Pesticide in Runoff Measured	Total Pesticide in Runoff Predicted
	(g/ha)					
Catchment P2						
1	0.6	0	10.3	0	10.9	0
2	7.0	15.2	40.7	41.7	47.7	59.6
3	1.0	0	3.0	0	4.0	0
4	0	0	3.0	0	3.0	0
5	0.2	0.4	1.7	2.1	1.9	2.5
6	0.5	0.1	1.2	0.2	1.7	0.3
7	0.2	0	0.5	0	0.7	0
8	0.3	0.2	4.1	2.4	4.4	2.6
9	1.5	1.4	4.6	7.2	6.1	8.6
Total	11.3	17.3	69.1	53.6	80.4	70.9
Catchment P4						
10	1.2	6.4	22.7	40.3	23.9	46.7
11	0.2	0	2.2	0	2.4	0
12	0.1	0	0.6	0.5	0.7	0.5
13	0	0.1	6.2	1.1	6.2	1.2
14	0.1	0	1.3	0.2	1.4	0.2
15	0	0.2	0	4.2	0	4.4
16	0.1	0.1	1.1	1.0	1.2	1.1
17	0.1	0	2.5	0.1	2.6	0.1
Total	1.8	6.8	36.6	47.4	38.4	54.2

Table 2. Comparison of Predicted and Observed Atrazine Losses in Runoff from Two Small Georgia Catchments, 1973-1975.

Cornell Nutrient Simulation (CNS) Model

The CNS model is the most complicated of the three chemical loading models since it includes soil moisture budgets in two soil layers and detailed descriptions of soil chemical behavior. The model predicts runoff, sediment and percolation losses, solid-phase and dissolved N and P in runoff and dissolved N in percolation. Model details are in Haith and Tubbs (1980), and earlier versions are described by Tubbs and Haith (1977) and Haith (1979).

The CNS model consists of a daily soil moisture model (Figure 3) and monthly models for soil N (Figure 4) and P (Figure 5). The monthly runoff, percolation and sediment loss values required for nutrient mass balances are obtained by summing the daily values predicted by the soil moisture model. The monthly time step for nutrient calculations produces a model which is computationally very efficient, and simulation runs of 25 years or more can be obtained for less than $10 of computer time.

Runoff in the CNS model is based on the CNE, but curve numbers are adjusted continuously based on soil moisture in the surface (top 10-cm) zone. Evaporation and transporation, as well as cover factors for the USLE are based on a crop canopy model. Crop nutrient uptake is determined from a sigmoid growth function. Dissolved nutrient losses in runoff are functions of dissolved N and P in the top centimeter of the surface zone.

The CNS model has been tested using data from field studies at Aurora, N.Y. and Watkinsville, Ga. Table 3 shows testing results for the same two Georgia catchments which were used in pesticide model testing. Predictions in general compare favorably with observations. The major discrepancy is in the prediction of dissolved P losses in runoff from

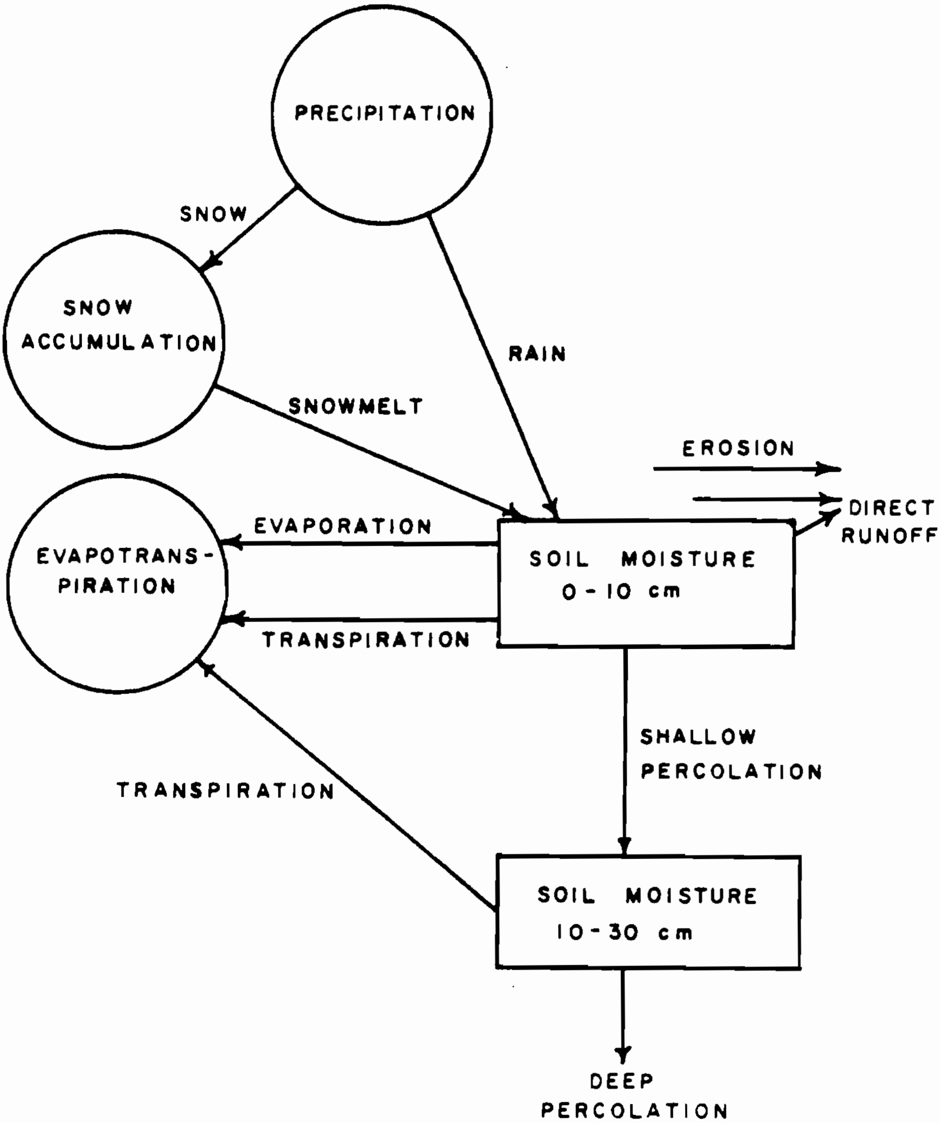

Figure 3. CNS Soil Moisture Model

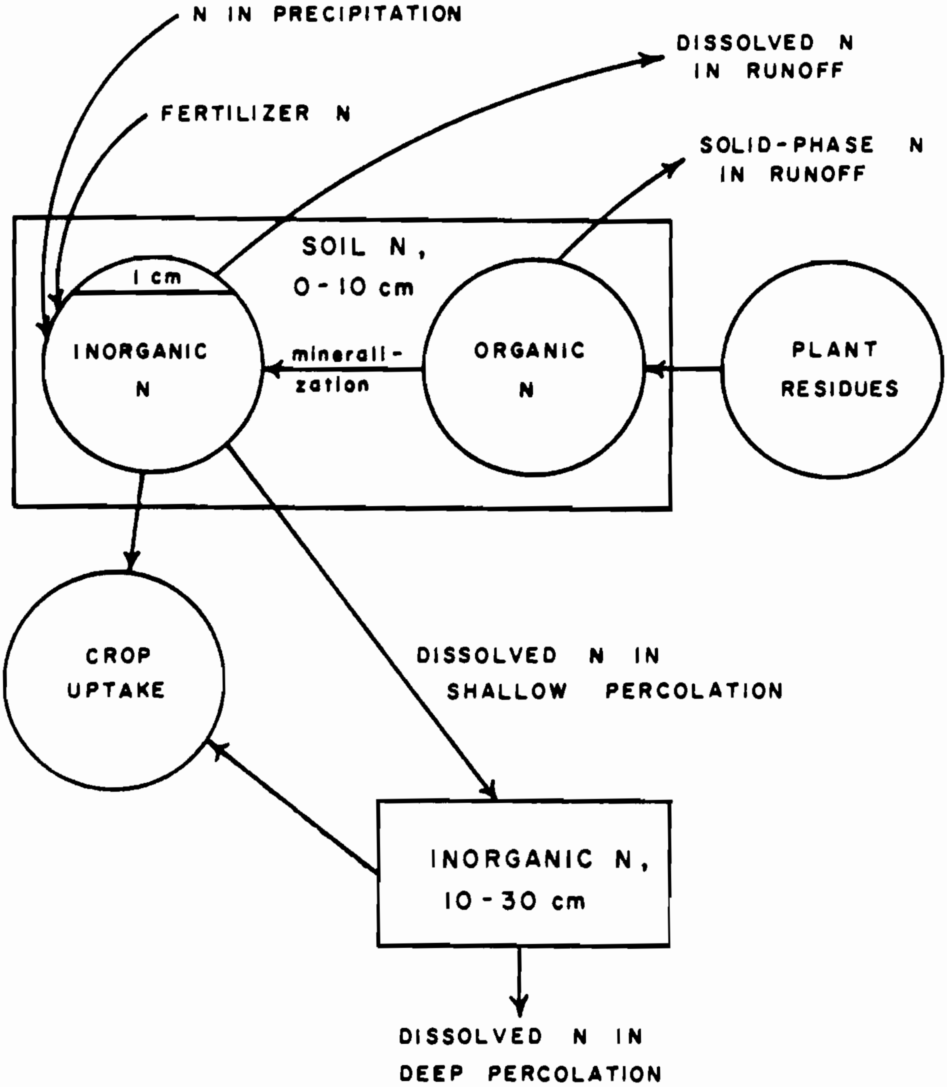

Figure 4. CNS Nitrogen Model

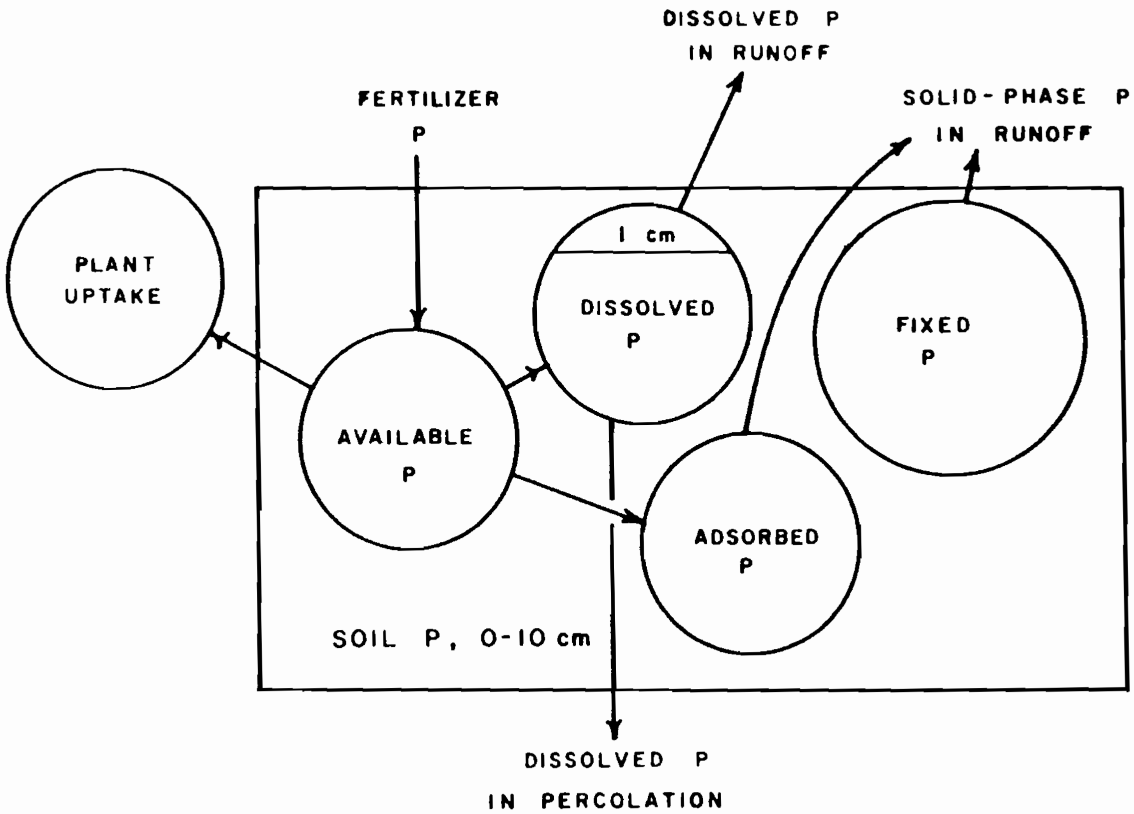

Figure 5. CNS Phosphorus Model

	Catchment P2		Catchment P4	
	Measured	Predicted	Measured	Predicted
Runoff (cm)	28.0	40.2	19.7	23.3
Sediment (T/ha)	7.3	9.5	1.9	1.6
Dissolved N in Runoff (kg/ha)	3.6	5.6	2.0	2.4
Solid-Phase N in Runoff (kg/ha)	9.4	8.2	3.5	2.1
Dissolved P in Runoff (kg/ha)	0.31	0.46	0.34	0.19
Solid-Phase P in Runoff (kg/ha)	5.8	4.5	1.6	0.6

Table 3. Comparison of CNS Model Predictions with Observed Runoff, Sediment and Nutrient Losses for Two Georgia Catchments (P2, P4), May 1974 - Sept., 1975

catchment P4. The observed losses appear to be partly due to leaching of P from crop residues, a phenomenon which is not included in the CNS model.

A Farm Management Model (HDF1)

The HDF1 model (Haith and Atkinson, 1977) is a relatively simple linear programming model designed to evaluate issues related to nutrient management on dairy farms. As indicated in Figure 6, the model captures the major nutrient cycles on a dairy farm and can be used to explore the relationships between nutrient and sediment losses, farming practices and income. The major activities are herd size, crop-soil combinations, and fertilizer and manure applications. Constraints can be placed on total N losses, dissolved and solid-phase losses of N and P in runoff and cropland erosion. Total N loss is estimated as all cropland N not used by crops. Runoff losses of N and P are determined by loading functions similar to those used in the watershed model (Figure 1).

Table 4 shows the results of an application of the model to a 124-ha dairy farm in Jefferson County, New York. Three types of plans are presented. The first is an income maximizing plan produced with no restrictions on pollutant losses. The remaining two sets of plans show effects of constraints on total N and erosion.

SUMMARY

Mathematical models are important tools for resolving issues related to the environmental impact of crop production. Chemical loading models provide estimates of chemical inputs to water bodies and planning and management models can be used to evaluate trade-offs between environmental

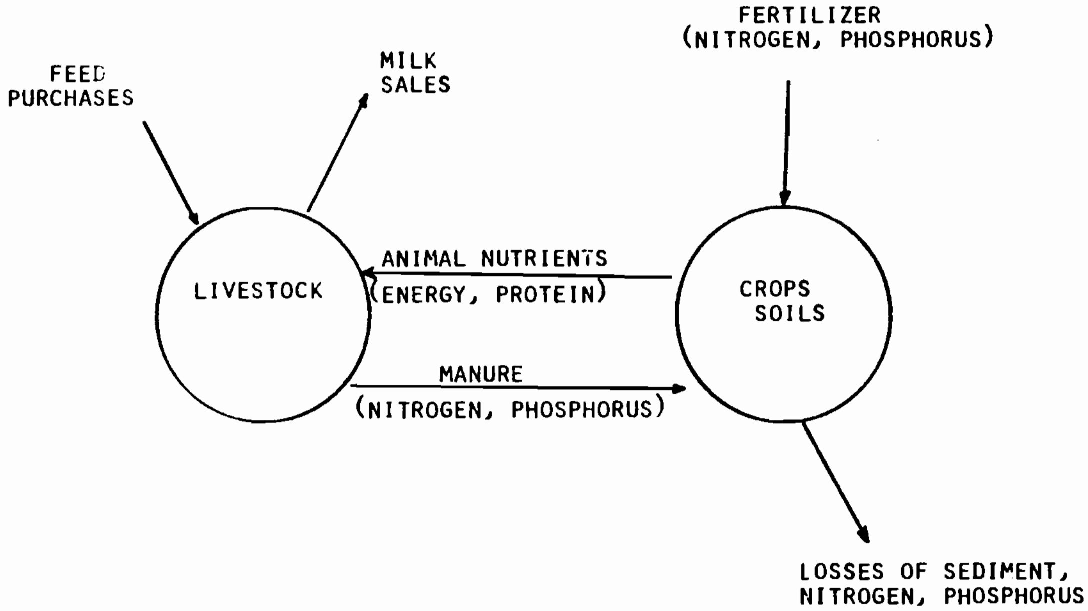

FIGURE 6. DAIRY FARM NUTRIENT CYCLES IN HDF1 MODEL

	Income-Maximizing Plan	Plans with Total Nitrogen Loss Constrained to			Plans with Total Erosion Constrained to		
		60	40	20 kg/ha	3	2	1 T/ha
Net Income ($/yr)	36,610	29,155	19,437	9,718	27,073	18,084	9,095
Herd Size (# of cows)	150	118	79	39	111	74	38
Land in Corn-Oats-Alfalfa-Alfalfa Rotation (ha)	80	63	42	21	61	41	22
Pasture Land (ha)	31	24	16	8	23	16	8

Table 4. Effects of Nitrogen Loss and Erosion Constraints on a 124-ha Dairy Farm in Jefferson Co., N.Y.

and food production objectives. Four examples of models were discussed in this paper. Testing of the three transport models indicated that they provide reasonable estimates of nutrient, pesticide and sediment losses from croplands. The farm management model which was presented provides a simple means of determining income effects of pollution control practices.

It can be anticipated that models such as these will be used with increasing frequency in the future. To the extent that agriculture is perceived to have significant environmental impacts, there will be future needs for quantitative information to aid rational policy making. In the absence of reliable experience and field data, mathematical models will remain one of the few viable means of providing the necessary information.

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A Field-Scale Model for Nonpoint Source Pollution Evaluation[1/]

W. G. Knisel[2/]

Mathematical models to assess nonpoint source pollution and evaluate the effects of management practices are needed to adequately respond to the Water Quality Legislation of the past 10 years. Action agencies must assess nonpoint source pollution from agricultural areas, identify problem areas, and develop conservation practices to reduce or minimize sediment and chemical losses from fields where potential problems exist. Monitoring every field or farm to measure pollutant movement is impossible, but landowners need to know the benefits before they apply conservation practices. Only through the use of models can pollutant movement be assessed and conservation practices planned.

Models developed for these purposes include the Pesticide Runoff Transport (PRT) model to estimate runoff, erosion, and pesticide losses from field areas (Crawford and Donigian, 1973); the Agricultural Runoff Model (ARM) to estimate runoff, erosion, and pesticide and plant nutrient losses from field areas (Donigian and Crawford, 1976); and the Agricultural Chemical Transport Model (ACTMO) to estimate losses from field or basin size areas (Frere, Onstad and Holtan, 1975). Bruce, et al. (1975) developed an event model to estimate pesticide losses from fields during single runoff-producing storms. These models are expensive when several years of data are simulated, and all require calibration. Beasley, et al. (1977) developed the ANSWERS model to estimate runoff and erosion and sedimentation from basin sized areas. This model has been used to identify sources of erosion and to consider conservation practices for erosion control, but it does not estimate nutrient or pesticide movement.

In 1978, the U.S. Department of Agriculture, Science and Education Administration, Agricultural Research (USDA-SEA-AR), began a national project to develop relatively simple and inexpensive mathematical models for evaluating nonpoint source pollution. A model that does not require calibration was planned, since very little calibration data are available. The initial efforts were concentrated on field scale, since that is where conservation management systems are applied. A field was defined as an area with relatively homogeneous soils under a single management practice that was small enough that rainfall variability was minimal. Requirements for the model were that it be simple and yet represent a complex system, be physically based and not require calibration, be a continuous simulation model, and have the potential to estimate runoff, erosion, and adsorbed and dissolved chemical transport. A field-scale model has been developed and is operational.

The purpose of this paper is to present the concepts and describe application of the field scale model. Details of the model cannot be given because space

[1/] Contribution from the U.S. Department of Agriculture, Science and Education Administration, Agricultural Research.

[2/] The author is a hydraulic engineer, USDA-SEA-AR, Southwest Rangeland Watershed Research Center, Tucson, Arizona. This paper represents contributions from seven lead scientists and 40 contributing scientists in SEA-AR.

is limited, but each component is described. A manuscript in the process of publication will describe the model in detail and give instructions for its use.[3/]

CREAMS MODEL STRUCTURE

The model reported in this paper consists of three major components: hydrology, erosion/sedimentation, and chemistry. The hydrology component estimates runoff volume and peak rates, evapotranspiration, soil water content, and percolation, all on a daily basis. The erosion component estimates erosion and sediment yield including particle size distribution at the edge of the field. The chemistry component includes a plant nutrient element and a pesticide element. Stormloads and average concentrations of adsorbed and dissolved chemicals are estimated in the runoff, sediment, and percolation fractions.

The Hydrology Component

This component consists of two options, depending upon availability of rainfall data. If the user is limited to daily rainfall data, Option 1 provides a means of estimating storm runoff. If hourly or breakpoint (time-intensity) rainfall data are available, Option 2 offers the user an infiltration-based method of estimating storm runoff.

Option 1: Williams and La Seur (1976) adapted the Soil Conservation Service (1972) curve number method for simulation of daily runoff. The method relates direct runoff to daily rainfall as a function of curve number (Fig. 1). Curve

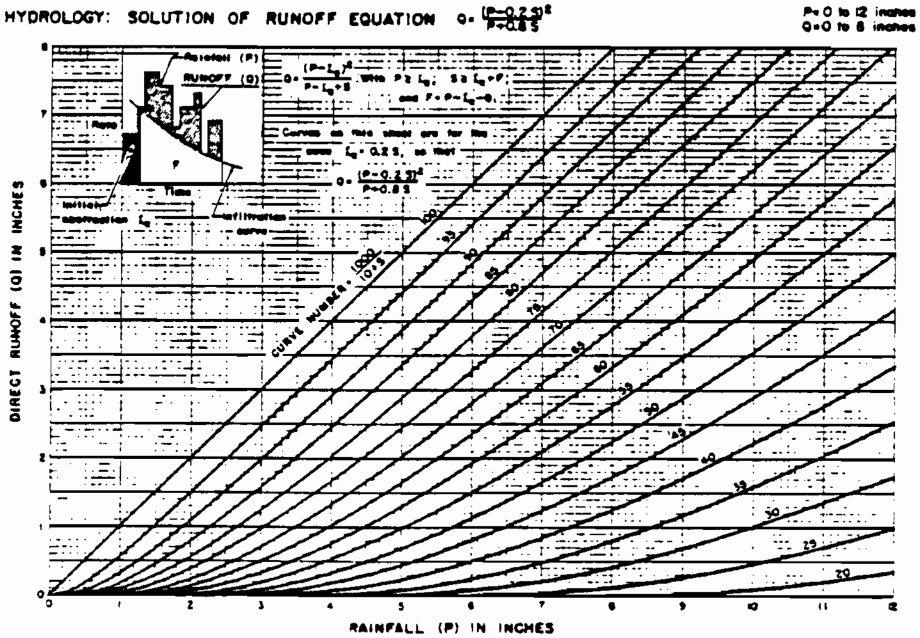

Figure 1. Soil Conservation Service Curve number method of storm runoff estimation (USDA, Soil Conservation Service, 1972).

[3/] U.S. Dept. of Agri., Science and Education Administration. CREAMS: a field scale model for estimating Chemicals, Runoff, and Erosion from Agricultural Management Systems. To be published as a USDA-SEA Conservation Research Report.

number is a function of soil type, cover, management practice, and antecedent rainfall. The relationship of runoff, Q, to rainfall, P, is

$$Q = \frac{(P\ 0.2S)^2}{P + 0.8S} \tag{1}$$

where S is a retention parameter related to soil moisture. A water balance is calculated by

$$SM_t = SM + P - Q - ET - O \tag{2}$$

where SM is initial soil moisture, SM_t is soil moisture at day t, P is precipitation, Q is runoff, ET is evapotranspiration, and O is percolation below the root zone. Eq.(2) estimates the soil water for determining the retention parameter, S, in Eq. (1).

The percolation component uses a storage routing technique to estimate flow through the root zone. The root zone is divided into 7 layers -- the first layer is 1/36 of the total root zone depth, the second layer 5/36 of the total, and the remaining layers, all equal in thickness, are 1/6 of the root zone depth. The top layer is approximately equivalent to the chemically active surface layer and the layer where interrill erosion is active. The soil water capacity for each layer is defined as the field capacity, and percolation cannot occur until the field capacity is exceeded. Percolation through each layer is based on the saturated hydraulic conductivity for the layer.

The peak rate of runoff, q_p, (required in the erosion model) is estimated by the empirical relationship (Williams and LaSeur, 1976)

$$q_p = 200D^{\left(0.7 + 0.23e^{-4.7D}\right)}\, C^{0.159}\, Q^{\left(0.917D^{0.0166}\right)}\, L^{-0.187} \tag{3}$$

where D is drainage area, C is mainstem channel slope, Q is daily runoff volume, L is the watershed length-width ratio, and e is the base of natural logarithms. Although Eq. (3) was developed and tested for basin-sized areas, it has been found applicable to field-sized areas as well.

<u>Option 2</u>: The infiltration model is based on the Green and Ampt (1911) equation (Smith and Parlange, 1978). A defining diagram of the infiltration model is given in Fig. 2. The concept assumes that the soil contains some

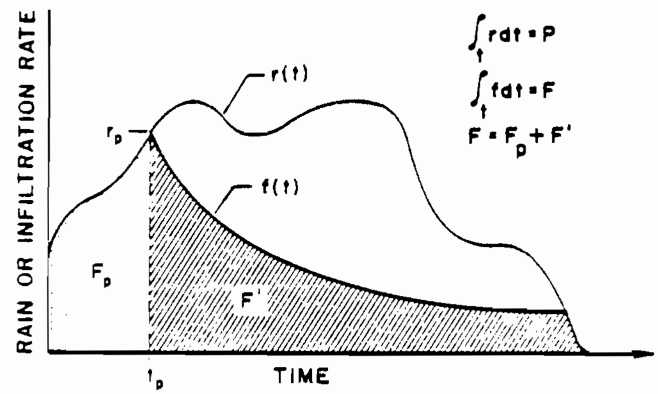

Figure 2. Schematic representation of runoff model using infiltration approach (Smith and Parlange, 1978).

water initially in a surface infiltration-control layer at the time rainfall occurs. When rainfall begins, the soil water content in the control layer approaches saturation and surface ponding occurs at some time, t_p (Fig. 2). The amount of rain that has already infiltrated at time of ponding, designated F_p in Fig. 2, is analogous to the initial abstraction in the SCS curve number model (Option 1), but it is a function of rainfall rate in this option. After the time of ponding, the Green and Ampt (1911) equation assumes that water moves as a sharply defined wetting front with a characteristic capillary suction, H_c, as the principle driving force. At any time, the potential gradient is

$$g = \frac{H_c + L}{L} \tag{4}$$

where L is the depth of wetting. The flow, f, is the product of effective saturated conductivity, K_s, and the gradient, or

$$f = K_s\left(\frac{H_c + L}{L}\right). \tag{5}$$

The infiltrated depth, F, (Fig. 2) is

$$F = L(\Theta_s - \Theta_i) \tag{6}$$

where Θ_s is the water content at saturation and Θ_i is the initial water content. The infiltration capacity, f_c, becomes

$$f_c = K_s \frac{H_c\phi(\Theta_s - \Theta_i) + F}{F} \tag{7}$$

where Θ_s approaches the soil porosity, ϕ, and, letting $G = \phi H_c$ the infiltrated depth at t_p is

$$F_p = \frac{G(\Theta_s - \Theta_i)\, K_s}{r - K_s} \tag{8}$$

where r is rainfall rate. If $D = (\Theta_s - \Theta_i)$, and approximating the infiltration curve of Fig. 2 by a series expression for the natural logarithm, the infiltrated depth in a time interval, ΔF, is

$$\Delta F = \sqrt{4A(GD + F) + (F - A)^2} + A - F, \tag{9}$$

where $A = \frac{K_{si}\Delta t}{2}$. The average infiltration rate for any interval i, $\bar{f}_i$, is

$$\bar{f}_i = \frac{\Delta F_i}{\Delta t_i} \tag{10}$$

and runoff during the interval, q_i, is rainfall rate for the interval minus the infiltration rate, $r_i - \bar{f}_i$. Total runoff is the sum of all q_i for the storm. Thus, the infiltration-based model has three parameters: G, D, and K_s.

The percolation estimated is similar to that used in Option 1, except that a single layer below the infiltration control layer represents the root zone. Percolation is calculated using average profile soil water content above field capacity and the saturated hydraulic conductivity, K_s.

Peak rate of runoff is estimated in Option 2 by attenuating the rainfall excess using the kinematic wave model for flow over a simple plane (Wu, 1978). The plane is approximated by the field slope and flow length.

Evapotranspiration: The evapotranspsiration (ET) element of the hydrology component is the same for both options. The ET model, developed by Ritchie (1972), calculates soil evaporation and plant evaporation separately. Evaporation is based on heat flux and is a function of daily net solar radiation and mean daily temperature. Daily radiation and temperature are interpolated by fitting a Fourier series to mean monthly radiation and temperature (Kothandaraman and Evans, 1972). Evaporation is calculated in two stages: the first is potential soil evaporation to modify the moisture flux based upon plant canopy or leaf area index, and the second stage is a function of time and an evaporation constant. Plant evaporation is computed as a function of soil evaporative flux and leaf area index. If soil water is limiting, plant evaporation is reduced by a fraction of the available soil water. Evapotranspiration is the sum of plant and soil evaporation but cannot exceed potential soil evaporation.

Erosion

The erosion component of the CREAMS model considers the basic processes of soil detachment, transport, and deposition. The concepts of the model are that sediment load is controlled by either transport capacity or the amount of sediment available for transport, whichever is less. If sediment load is less than transport capacity, detachment may occur; deposition occurs if sediment load is greater than transport capacity. The model represents a field comprehensively by considering complex slopes for overland flow, concentrated channel flow, and impoundments or ponds. The model can estimate particle size transport for the primary particles -- sand, silt, and clay -- and large and small aggregates. Detachment and deposition do not occur simultaneously. In deposition, the model calculates sediment sorting. Temporary ponding can result in transport of only the finer particles.

The detachment process is described by a modification of the Universal Soil Loss Equation (USLE) (Wischmeier and Smith, 1978) for a single storm event. This interrill detachment, D_{IR}, in the overland flow element is expressed as

$$D_{IR} = 4.57EI\ (S_{of} + 0.014)\ KCP/(q_p/Q), \tag{11}$$

where EI is storm rainfall energy, S_{of} is the slope of the overland flow, q_p is runoff peak rate, Q is runoff volume, K is the soil erodibility factor, C is the cover factor, and P is the management practice factor. The rill detachment process, D_R is expressed as

$$D_R = (6.84 \times 10^6)\ n_x Q q_p^{1/3} (x/22.1)^{n_x - 1}\ S_{of}^{\ 2} KCP(q_p/Q) \tag{12}$$

where x is the distance down slope, n_x is slope-length exponent, and Q, q_p, K, C, and P are defined as above. As shown in Eq. (11), interrill erosion is a function of rainfall detachment and transport, and from Eq. (12) rill erosion is a function of transport capacity denoted by the runoff volume and peak rate. Both equations contain the K, C, and P factors of the USLE (Wischmeier and Smith, 1978). Sediment transport for the overland flow element is estimated by the Yalin transport equation (Yalin, 1963) modified for mixtures of sediment having varying sizes and densities.

The concentrated flow or channel element of the erosion model assumes that the peak rate of runoff is the characteristic discharge for the channel, and detachment or deposition is based on that discharge. Detachment can occur when the shear stress developed by the characteristic discharge is greater than the critical shear stress for the channel. Bare channels, grassed waterways, and combinations of bare and grass channels can be considered by the model for as many as 10 channel segments. Discharge is assumed to be steady state, but spatially varied, increasing downstream with lateral inflow. Friction slope and shear stress are estimated from solution of the spatially varied flow equations. The solutions consider drawdown or backwater effects in the channel as a result of channel outlet control.

Water is often impounded in field situations, either as normal ponding, where a channel flows through a restriction at a fence line or a road culvert, or as outflow from an impoundment-type terrace. Any such restriction reduces the flow velocity and coarse-grained sediments and aggregates can settle out of the flow. Deposition in impoundments is a function of the fall velocity of the particles and particle travel time through the impoundment. The fraction of particles passing through the impoundment, FP, of a given size, i, is given by the exponential relation

$$FP_i = A_i e^{B_i d_i} \tag{13}$$

where d_i is the equivalent sand-grain diameter and A and B are coefficients dependent upon impoundment surface area and depth, and settling velocity of the particles.

In addition to calculating the sediment transport fraction for each of the five particle size classes, the model computes the sediment enrichment ratio, which is based on the specific surface area of the sediment and organic matter and the specific surface area for the residual soil. As sediment is deposited in transport, the organic matter, clay, and silt are the principle particles transported, and this results in high enrichment ratios. The enrichment ratios are important in adsorbed chemical transport.

Chemical Component

Plant Nutrients: The basic concepts of the nutrient component are that nitrogen and phosphorus are adsorbed to soil particles and are lost as sediment is transported, that soluble nitrogen and phosphorus are lost with surface runoff, and that soil nitrate can be leached by percolation, denitrified, or taken up by plants.

Nitrogen and phosphorus are mixed with the soil, and the amounts lost with sediment are a function of sediment yield and enrichment ratio. A logarithmic function is used to relate nitrogen and phosphorus losses to enrichment ratios.

The chemical model component assumes that an arbitrary surface layer 1 cm deep is effective in chemical transfer to sediment and runoff. Soluble nitrogen and phosphorus are assumed to be thoroughly mixed with the water in the top centimeter. This includes soluble forms from the soil, surface-applied fertilizers, and plant residues. These soluble nutrients are imperfectly extracted by overland flow. The extraction from this active layer is expressed by an empirical extraction coefficient. All broadcast fertilizer is added to the surface active layer, whereas only a fraction would be added by fertilizer incorporated with the soil.

When infiltrated rainfall saturates the surface active layer, soluble nitrogen moves into the root zone below the layer from which chemicals are extractable. Nitrate in the rainfall contributes to the total in both this layer and the root zone.

Fertilizer addition and mineralization of organic matter both increase soil nitrate. Mineralization is calculated by a first-order rate equation from the amount of potential mineralizable nitrogen and is modified by soil water content and temperature. Optimum mineralization rates occur at soil temperatures of 35°C. Soil temperature is approximated by air temperature, as calculated in the hydrology component of the model.

The model assumes that plant uptake of nitrogen under ideal conditions is described by a normal probability distribution curve. The potential uptake is reduced to the actual by a ratio of actual plant evaporation to potential plant evaporation. A second option for estimating nitrogen uptake is based on plant growth and the plant's nitrogen content.

Soil nitrate is available to plants for uptake. It can also be leached out of the root zone, or denitrification can reduce it. The description of nitrate leaching in the model assumes uniform mixing of the draining water and the nitrate remaining in the soil water. The amount of nitrate leached is a function of the amount of water percolated out of the root zone, as estimated by the hydrology component of the model.

Denitrification of soil nitrate in the root zone occurs when the soil water content exceeds field capacity, i.e., when percolation occurs. The amount of denitrification is based upon soil temperature and the organic carbon content of the soil. The model estimates organic carbon from the organic matter content in the root zone. The rate constant for denitrification at 35°C is calculated from the amount of organic carbon and is adjusted for temperature assuming a twofold reduction for each 10-degree decrease in temperature.

Thus, the plant nutrient component of the chemical model estimates nitrogen and phosphorus losses in sediment, soluble nitrogen and phosphorus in the runoff, mineralization, uptake by the crop, nitrate leached by percolate through the root zone, and denitrification in the root zone. The model computes loads of each component, accumulates over the year, and calculates average concentrations of nitrogen and phosphorus in runoff.

Pesticides: The pesticide model was developed to estimate concentrations of pesticides in runoff (water and sediment) and total mass for each storm during the period of interest. The model can accomodate up to 10 pesticides simultaneously in a single run. It is structured to consider foliar application of pesticides separately from soil-applied pesticides, because dissipation from foliage is more rapid than that from soil. The model can also consider multiple applications of the same chemical, as is done with insecticides.

As in the plant nutrient component, a surface active layer that is 1 cm deep is assumed. Movement of pesticides from the surface is a function of infiltrating water and pesticide mobility parameters. Pesticide in runoff is partitioned between the solution, or water, phase and the sediment phase by the following relationships:

$$(C_w\, Q) + (C_s\, M) = a\, C_p \tag{14}$$

and

$$C_s = K_d\, C_w \tag{15}$$

where C_w is pesticide concentration in water, Q is volume of water per unit volume of stirred runoff interface or surface active layer, C_s is pesticide concentration in sediment, M is the mass of soil per unit volume of interface, a is an extraction ratio of the amount of soil extracted per unit volume in the stirred runoff interface, C_p is the concentration of pesticide residue in the soil, and K_d is the coefficient for partitioning the pesticide between sediment and water phases. The concentration C_w is assumed to be the average concentration in solution that reaches the field edge but is determined by extraction of the pesticide into the runoff from the soil interface in the field. The term C_s is the pesticide concentration in the soil material at the runoff-soil interface after extraction. Only a small part of this mass extraction actually reaches the edge of the field and is calculated as a product of concentration, sediment mass, and the enrichment ratio. The sediment mass and enrichment ratios are calculated by the erosion component of the model.

Pesticide washed off of foliage by rain changes the concentration in the soil. The amount calculated as available for washoff is updated between storms by a foliar degradation process. Pesticide residue in the runoff interface layer is adjusted for downward movement and washoff from foliage.

SUMMARY

A physically based daily simulation model has been developed by SEA-AR scientists to evaluate nonpoint source pollution from agricultural fields. The model simulates processes in hydrology, erosion, and plant nutrient and pesticide losses as affected by management practices. It does not require calibration, and the computer program is computationally efficient -- it costs only a few dollars per year of computations. The hydrology component has been tested in 30 watersheds in 13 land resource areas of the U.S.; the erosion component has been tested in five land resource areas; the chemistry component has been tested in three land resource areas. A comprehensive publication of CREAMS is in progress which includes model concepts and a user manual that aids in parameter and coefficient estimation.

ACKNOWLEDGEMENTS

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REVIEW OF SIMULATION MODELS FOR NITROGEN BEHAVIOUR IN SOIL IN RELATION TO PLANT UPTAKE AND EMISSION.

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INTRODUCTION

Nitrogen is one of the major nutrient elements for plants. Already in ancient times many agricultural measures were directed to an optimalization of the nitrogen supply to crops. In some cases insufficient nitrogen supply caused soil depletion often with drastic effects for crop production and environment (soil erosion by lack of vegetation). Manures and fertilizers have proven to be excellent remedies against soil depletion and ensure good crop yields provided other conditions are fulfilled. It is remarkable that there exists a certain uneasiness about the abundant use of nitrogen fertilizers because instead of being a remedy against soil depletion, it might cause a further depletion of the soil organic matter and so induce serious agronomic and environmental harms in the future.

Direct harmful effects of the use of nitrogen fertilizers on the environment are leaching of nitrates to soil water reservoirs and emission of nitrogen oxides and ammonia into the atmosphere.

For the study of these complex effects mathematical models have been developed. Depending on the ultimate goal the models differ widely in concept. Moreover, models were developed by scientists specialized in different fields which hindered communications, so that even models with the same goal may differ significantly in concept.
In the next section the most important differences between existing models will be discussed. It was not possible to review all of the many models on nitrogen behaviour in soil, which are developed in the last decade, because of lack of space. Therefore only a number of selected models will be dealt with in this review.

CRITERIA FOR MODELS

For reviewing mathematical models or simulation models, as they are usually called, different aspects should be considered. In this review the dynamical aspects, aims, time horizont, differences in concept and geometry will be discussed.

Dynamical aspects

Models can be divided into budgeting models and dynamic models. Budgeting models often consider a complete growing season, i.e. they contain data for annual fertilizer gifts, manure, biological N_2-fixation as input, and leaching of N, volatilization of NH_3, denitrification losses and N in the harvested crops and in animal products as output. Despite their simplicity it is often difficult to obtain this type of data. Especially, data on denitrification losses are seldom based on measurements but are mostly determined by balancing the budget. For fertilizer efficiency studies these types of balances can be very useful.

Dynamic models are based on a description of the system by differential equations. The processes considered are similar to those of budgeting models, but usually described in much more detail. For instance mineralization may be described by numerous microbiological reactions, and leaching by multilayer transport equations. The differential equations are often numerically integrated. A subdivision can still be made for mathematical solutions using explicit methods only and for those ones using also implicit models. The explicit method has the advantage that the construction of the programme is much clearer, and that modifications can easily be introduced. A disadvantage of the explicit method is that the computation time is considerably longer than for implicit methods. For models which are mainly oriented to scientific understanding long computation times are no serious drawback, but for forcasting and management models it is a drawback.

Within this manuscript budgeting models are not further reviewed, the other criteria apply to dynamic models only.

Aims

Shytov and Vasiliev (1980) distinguished between models which are mainly developed for better scientific understanding, for forecasting and for management purposes. Such a division is rather arbitrary because well developed models designed for "better understanding" are able to provide data for forecasting or management purposes. as well. The amount of input data required is, however, often so large that this gets inpractical. The role of models which are designed primarily for better understanding is very important, they are superb tools to promote in-depth discussions on complex systems, and allow organization of information, which enables the identification of gaps in our knowledge. The role of forecasting and management models is of course not less important; in fact they apply the knowledge gained from the first type of models. The models designed for better understanding are often characterized by careful biological, chemical or physical description of the mechanisms of the processes included, while forecasting and management models may apply rather simple regression equations. Although for such regression equations adaptation to local circumstances is always required, the models in which they are applied, are convenient because the number of input data is comparatively low and often relatively easy to obtain.

Time horizont

The time horizonts of soil nitrogen models differ enormeously. Models used to follow rainfall or irrigation required usually time steps of hours or days; many leaching models use therefore identical time steps. The simulated period is limited to a few weeks. Also denitrification models, in which the water phase is an important variable, require small timesteps. Models describing mineralization, immobilization and other microbiological processes (denitrification excluded) consider longer timesteps. The simulated period ranges from a growing season to a few years. Models for the prediction of soil organic matter losses may consider even timesteps of a whole year, while the simulated period may extend many decades.

Differences in concept

Soil nitrogen models can roughly be divided into three groups:

- Models which concentrate on transport processes such as leaching of nitrogen and volatilization of NH_3.
- Models which concentrate on the availability of mineral N for plants and therefore on the formation and depletion of soil organic matter.

- Models which concentrate on aerial dry matter production and therefore on limitations of the production caused by insufficient availability of mineral N.

Part of the models considering leaching actually consist of a description of the flow of water in a soil. The flow in three directions is carefully considered; but all biological transformations are only represented by one simple source term. Other leaching models consider only the vertical flow of water but include phases for mobile and stagnant water with an exchange of nitrogen compounds between both phases. The models oriented on the fate of mineral N mostly include descriptions of microbiological processes. Often, both the carbon and nitrogen cycle are included and interrelated. In some of them the microbiological biomass is the key variable. On the contrary transport equations are often very simple. The models oriented to aerial dry matter production concentrate usually on photosynthetic production, on respiration and on a careful calculation of the evapotranspiration and its relationships to the uptake of soil-N. Soil water and soil nitrogen are rather simple growth limiting factors in such models.

Geometry

Most models are multilayer models i.e. calculations are made for a soil columm with infinite horizontal dimension while the vertical distance is divided into a number of layers, what is considered to be representative for the total system under study. Only a few models consider three dimensional aspects, in particular those ones, which are used to simulate waterflow and oxygen diffusion. A very limited number of models does not consider geometric aspects, these ones are not suitable to calculate vertical transport processes.

REVIEW OF MODELS

The division of total system-models into the three mentioned categories, i.e. a) models, which concentrate on transport processes such as water and NO_3^- movement, b) models, which concentrate on the availability of mineral N for plants and microorganisms, as the result of microbial activity and c) models, which are developed primarily to simulate the effect of nitrogen on crop growth and vice versa, is rough and open for discussion. It offers, however, the reviewers a possibility to organize the very large number of models, which have been developed so far.

The models of category a) can be characterized by their use of waterflux description to calculate N-transport. The calculation of water transport is very time consuming (Beek and Frissel, 1973), what brought some modelers to simplify this description to a transport equation, where waterflux is not calculated but is included as input (Van Veen and Frissel, 1980; Bosatta, 1980).

The main equation to calculate waterflux (Gupta *et al.*, 1978) is

$$C' \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} [K(h) \frac{\partial H}{\partial z}] - S \qquad (1)$$

where C' = soil water capacity, $\frac{d\theta}{dh}$, $cm^3\ cm^{-3} \cdot cm^{-1}$

θ = volumetric water content, $cm^3\ cm^{-3}$

h = pressure head, cm

K = hydraulic conductivity, cm day^{-1}

H = total head, $h + z$, cm

S = sink term for root extraction, $cm^3\ cm^{-3}\ day^{-1}$

t = time, day

z = soil depth, cm.

The relation between the hydraulic conductivity and water content is described in various ways. A typical example is the relation by Simmons *et al.* (1980) used by Tanji *et al.* (1980).

$$K = \alpha^2 K_m \exp[\beta(\theta - \theta_0)] \qquad (2)$$

where α = scale factor

K_m = scale mean hydraulic conductivity, cm

θ_0 = saturated water content, $cm^3\ cm^{-3}$

β = location-dependent parameter.

Another key equation is the one for the water sink term due to water extraction by the roots. Tanji *et al.* (1980) used (Nimah and Hanks, 1973).

$$S = K(h)[h_r - h)/R(z)] - \frac{RDF(z)}{\Delta z \Delta x} \qquad (3)$$

where h_r = root water pressure at the root-soil interface, cm

R = radius of waterflow to roots, cm

RDF = root distribution function defined as the proportion of roots in Δz

Δx = radial distance between roots, cm.

Transport of mineral N, mainly NO_3^-, is calculated by multiplying the N-concentration in soil water and the waterflux. Most models of this category include ion exchange and describe biological nitrogen transformations, such as mineralization, nitrification, hydrolysis, uptake by plants, etc. by first order rate kinetics. A typical model of this category is the forementioned model of Tanji *et al.* (1980) which is developed primarily to simulate the effect of different irrigation practices on the fate of N in soil. The model of Wagenet (1980) is rather similar to the one of Tanji *et al.*, in description and objective. The main difference is the presence in the Wagenet model of options to simulate heat-flux. Another model of this category is the model of Rao *et al.* (1980) which is mainly developed to calculate leaching of N and the uptake of N by plants after application of fertilizer N, animal manure or plant residues (Fig. 1). To calculate mineralization of N from organic matter use is made of the C/N-ratio of the organic matter which implies the simulation of C transformations.

Although the model of Selim and Iskander (1980) which is designed to study the effects of the application of N-containing waste water by infiltration, emphasizes water and NO_3^- movement, it differs from the aforementioned models in its treatment of moisture content and hydrolic conductivity both which are input parameters and so, are not calculated. Michaels-Menten kinetics are used to simulate N-uptake by plants. Also the models of Duffy *et al.* (1975)

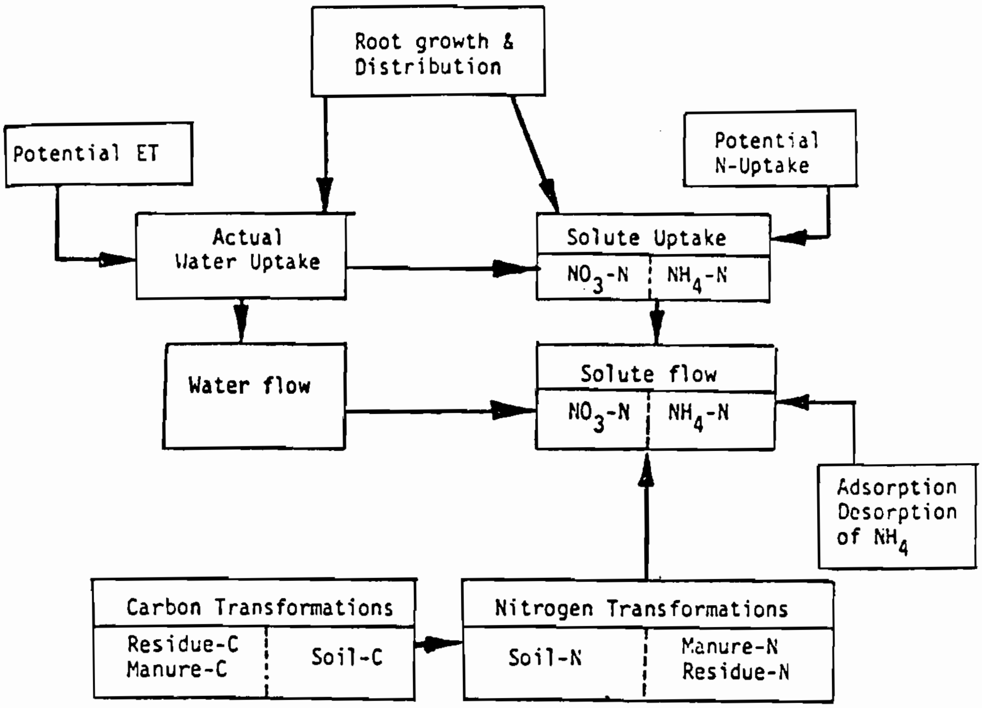

Fig. 1 Flow diagram showing the relationship in the model of Rao *et al.* (1980). ET = Evapotranspiration.

and Watts and Hanks (1978) stress the effect of transport processes of water and N on the uptake of N by plants. The former model has been developed to predict N-concentrations in the tile effluent as a function of farm management practices and climatic conditions and the latter aims to describe net changes of N in the root zone of irrigated corn.

To calculate nitrogen requirements under various soil and climatic conditions Kruh and Segall (1980) developed a model in which emphasis is on N and water movement. It includes rainfall, irrigation and transpiration, and also contains a more detailed description of biological N-transformations and interactions of the N and C cycles than the aforementioned models. Their description of water and heat-flux is based on the work of De Wit and Van Keulen (1972). Also the original model of Beek and Frissel (1973) included detailed descriptions of nitrification, immobilization, mineralization besides detailed descriptions of water, NO_3^- and heat movement through soil. Nitrification was described with first order rate kinetics with the rate constant being dependent on the number of nitrifying cells. Their model of mineralization and immobilization was one of the first descriptions, where organic matter is divided into different components with different decomposition rates. In this way it was possible to account for differences in availability as substrate for microorganisms of different components of plant residues and soil organic matter such as sugars, celluloses, lignins and proteins.

Cameron and Kowalenko (1976) developed a model to simulate nitrogen flow pathways in an unsaturated soil. The exchange phenomena of NH_4^+ were treated explicitly using a non linear Freundlich equilibrium model and a Langemuir kinetics model to describe adsorption and desorption of NH_4^+. Nitrification and ammonification followed first order kinetics.

The model of Beek and Frissel can be regarded to be the base of the model of Van Veen and Frissel (1980). This model can be considered to be representative for the models of category b). Besides descriptions of physical-chemical processes such as volatization of ammonia, leaching, fixation of ammonium on clay minerals, oxygen and NO_3^- diffusion, it includes detailed descriptions of microbially mediated processes, nitrification denitrification, mineralization and immobilization. The mathematical formulations of the rates of the microbial processes explicitly include growth and death of the microbes involved. Growth and activity of the heterotrophic biomass, which is involved in mineralization and immobilization, in oxygen consumption and thus, in denitrification, is considered to be dependent on the availability of C- and N-compounds as substrate. Similar to the Beek and Frissel (1973) model it accounts for differences in availability as substrate of organic matter components by splitting crop residues and native soil organic matter into six fractions (Fig. 2). A unique feature of this model is that each of those fractions are utilized for biosynthesis and energy supply by a fraction of the biomass. The size of each of those fractions is proportional to the ratio of the size of the C-pool decomposed by this fraction of the biomass to the total C-content. Decomposition and related growth are described using Monod kinetics. Death of the biomass is described with first order rate kinetics.

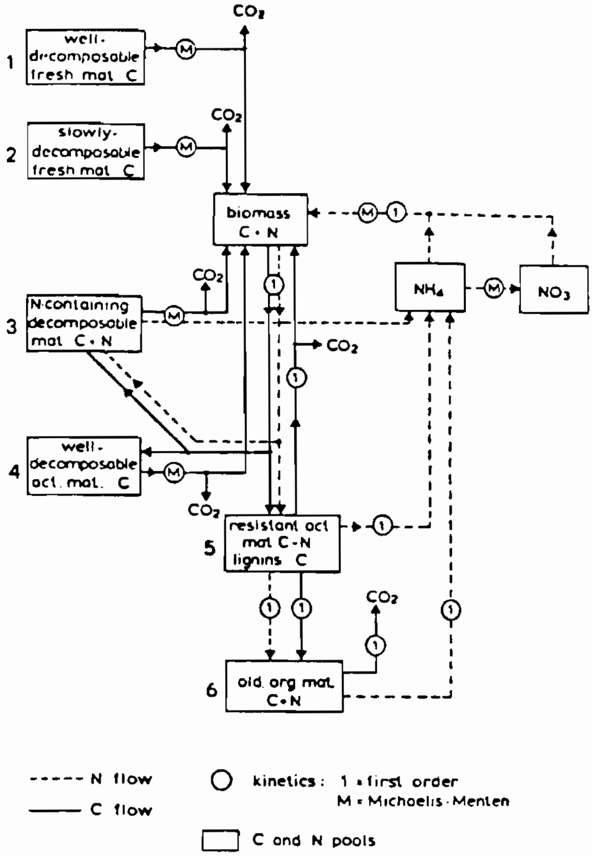

Fig. 2 Flow diagram showing the relationships in the mineralization - immobilization part of the model by van Veen and Frissel (1980).

The two steps of nitrification, i.e. ammonium and subsequently nitrite oxydation, are described explicitly with the use of Monod kinetics. The description on microbial activity in relation to C and N-supply is used in the submodel of denitrification for the calculation of the oxygen consumption in both waterlogged and unsaturated soils. Oxygen supply is thought to occur via air-filled pores into the surrounding soil or in case of waterlogged soils from the atmosphere above the soil. The critical point in this submodel is the calculation of the occurrence of anaerobiosis, when oxygen supply does no longer meet oxygen consumption. Then denitrification is calculated.

Although this model has been developed to simulate the fate of N in the intensive agricultural soils of North Western Europe, it shows many similarities with the model of McGill *et al.* (1980)(Fig. 3) which is used to describe N in the virgin grassland of North America. The major identical concepts of the description of mineralization and immobilization which in both models is the core of the model, were (Van Veen *et al.* 1980).

- C is the main control on biomass
  and biomass in turn controls N-uptake and release;
- several organic fractions are included to deal with
  differences in quality and availability of substrates
- biomass turnover or death is treated explicitly.
  This concept acknowledges microbial productivity as
  essential to the dynamics of the terrestrial N cycle;
- mineralization and immobilization are treated separately
  and explicitly.

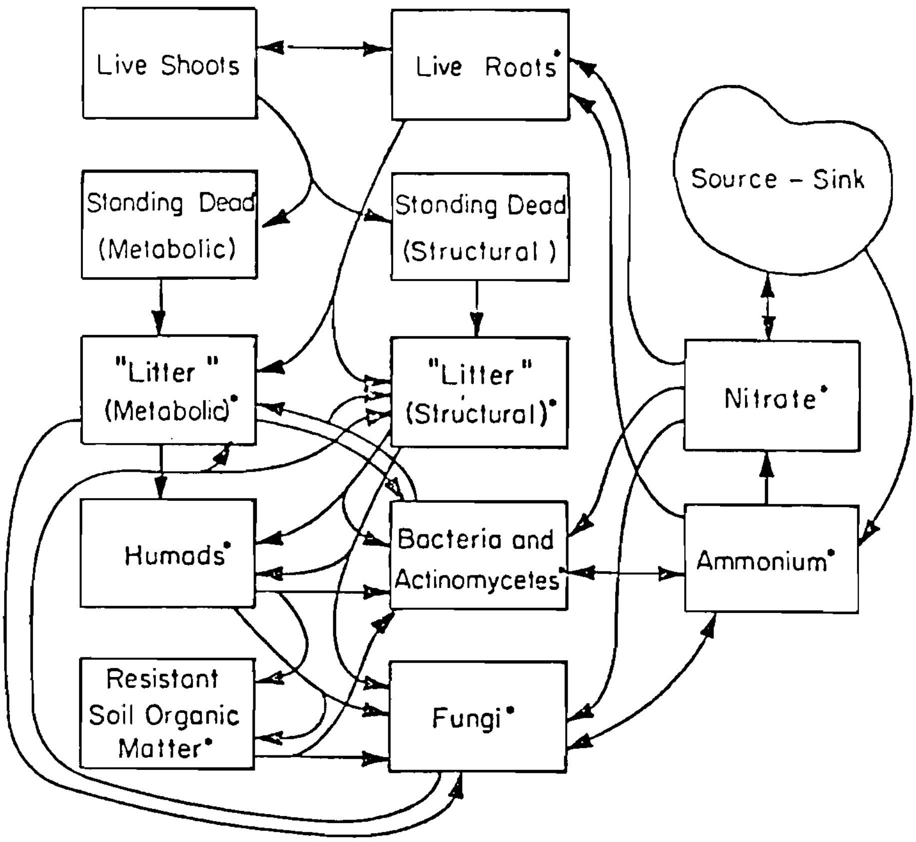

Fig. 3 Flow diagram showing part of the relationships of the model by McGill *et al.* (1980).

Major differences between the two models with respect to the description of microbial activity are related to the C/N-ratio of the biomass, which is variable in the McGill *et al.* model and fixed in the Van Veen-Frissel model, to microbial death which in the McGill *et al.* model is dependent on freezing and thawing as well as density-dependent and the McGill *et al.* model explicitly includes fungi- and bacteria as separate groups. The McGill *et al.* model also includes nitrification, but does not differentiate between ammonium and nitrite oxidizers, denitrification, leaching and plant growth.

Based on the Van Veen and Frissel model, Juma and Paul (1980) developed a very detailed description of microbial activity in relation to mineralization and immobilization of N. It contains features to simulate the fate of tracers such as ^{14}N, ^{15}N, ^{12}C and ^{14}C independently. The model of Bosatta (1980) also emphasizes the role of microorganisms in the soil N- cycle. The description of microbial growth is based on the model of Parnas (1975). The model is mainly intended to describe mineralization and leaching from the mor layer of a forest site. Organic matter is divided into only two pools, one containing the C compounds, the other one the C-N compounds. Although it is simpler than the Van Veen-Frissel model, also in other aspects, many of the characteristics are similar.

Smith's (1979) model describes the fate of C, N, P, K together in one complex model which also emphasizes the dynamics of microorganisms in soil organic matter decomposition processes. Organic matter is divided into live and dead plant components and live and dead microbial components. Similar to the Van Veen and Frissel and McGill *et al.*

models this model also includes explicitly the effect of adsorption of organic matter on its decomposition. Decomposition rates follow Michaeles-Menten kinetics. The description of the dynamics of the microbial population explicitly includes growth, maintenance, waste metabolism and death. The nitrogen submodel also describes nitrification as a two step reaction, leaching, input of N by rain and fertilizers application, exchange of NH_4^+ and it contains a simple calculation of N-losses due to denitrification.

The third category includes models which are mainly developed to simulate the effect of N on crop production. It concerns models which emphasize N-uptake and the fate of N in the plant. A good example of this group is PAPRAN, a model developed by Seligman and Van Keulen (1980). It is designed to study the biological and economical efficiencies of different crop and pasture management systems of semi-arid regions. The model represents dry matter production, as related to water use of the plant and N availability, allocation of dry matter, death of vegetative tissue, N-uptake, which is calculated from the difference between actual N content of the plant and an optimum concentration, and allocation and translocation of N. Furthermore the model contains a rather detailed description of mineralization and immobilization of soil N, considering two soil organic matter fractions; volatilization of ammonia, and leaching are also included. The model of Greenwood *et al.* (1974) is less extensive, than PAPRAN but also gives a detailed description of NO_3^- -N-uptake by plants and N-dependent plant growth and of NO_3^- -N and water movement through soil. The model was derived to predict crops responses to nitrogen fertilizer under different soil and wheather conditions. Jones *et al.* (1974) developed a N-model, which could be inserted into SIMCOT II, a model designed to simulate cotton growth and yield. The nitrogen submodel is a rather empirical description emphasizing N-uptake by plants and N in the plants. Daily uptake is determined by N supply from the soil, demand of N for new growth and maximum daily plant absorption for the existing conditions. The supply of N from the soil is calculated from an empirical formulation of N-mineralization from soil organic matter and from fertilizer input.

A root zone N-simulation model to evaluate the long term effects on soil root zone-N of various sewage sludge application rates was developed by O'Brien and Mitsch (1980). It includes mineralization, nitrification, denitrification, plant uptake, ammonia volatilization and leaching of nitrate. Plant uptake of N is decribed by Michaels-Menten kinetics, other transformation rates follow first order rate kinetics. Soil organic matter is divided in a stable and unstable fraction. The time horizont is considerably longer than for most of the aforementioned models, up to 50 years.

The model of Bhat *et al.* (1980) is designed to predict the various transformations of N in soil after application of farm wastes Although it includes several descriptions of plant-related processes, such as N-uptake, crop growth, distribution of dry matter and N between shoots and roots and C and N additions through dead plant material, it also describes microbially mediated soil N transformations, such as ammonification, immobilization and dentrification and water and N movement processes.

Besides models, which describe the total N cycle in soil or at least a number of processes of the soil-N cycle, descriptions have also been published of separate processes. Because of space limitations, we will only mentioned a few examples of those models.

Nitrification can be considered to be the most frequently described process of the soil-N cycle. Many descriptions are based on the work of McLaren and his group (e.g. McLaren, 1969; 1971). Other examples of models on nitrification in soil systems are from Paul and Domsch (1972), Saunders and Bazin (1973) and Laudelout *et al.* (1977).

Models on denitrification can be devided in two groups. The first group consists of models which deal with the kinetics of the process of NO_3^--reduction only. Denitrification has been decribed with first order rate kinetics with respect to the NO_3^- concentration (Stanford *et al.* 1975), zero order kinetics (Focht, 1974) and Michaels-Menten type kinetics (Cho and Mills, 1979). The second group of denitrification models consists of models which are developed to describe not only NO_3^--reduction but also the occurrence of anaerobiosis in soil including a description of oxygen behaviour in soil (Van Veen and Frissel, 1979; Leffelaar, 1979; Smith, 1980).

A model on ammonia volatilization after ureum hydrolysis was developed by Parton *et al.* (1980). Burns (1976) developed a model to predict leaching of NO_3^- uniformly incorporated to a limited depth or destributed throughout a soil profile. A detailed model on leaching has also been developed by Addiscott (1980). The description is based on the concept that water and solutes in the soil can be partitioned between a mobile and a retained phase.

This review is based on the proceedings of a workshop on N-models held at Wageningen, in January 1980 (Frissel and Van Veen, eds 1980). Because of lack of space we have not dealt intensively with details of kinetics of the processes or with their justification based on experimental data and the present state of our knowledge of the N-cycle in soil. Those subjects are discussed in the forementioned proceedings.

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A CRITICAL EVALUATION OF A HYDROLOGICAL LAYER MODEL FOR FORECASTING THE REDISTRIBUTION OF UNADSORBED ANIONS IN CULTIVATED SOILS

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SUMMARY

Tests of the accuracy of a simple hydrological layer model for predicting the redistribution of soluble unadsorbed anions in cultivated soils are summarized and discussed in the light of the mechanisms of leaching thought to be involved. The results show that the predictions of the model were in broad agreement with the experimental data, but that holdback effects (even within the relatively small aggregates of a seedbed) could influence the accuracy of the model, especially when leaching occurred shortly after the application of salt. Nevertheless, the model provides a simple method of estimating leaching which has been successfully applied to data from a wide range of cultivated soils and has been used as a basis of a method for adjusting N fertilizer practice for differences in nitrate leaching.

INTRODUCTION

Losses of nitrate by leaching are generally greatest when uptake of water and N by crops are small. In northern latitudes this is most likely to occur in winter and spring, when growth is slow or the soil is fallow. There are substantial residues of inorganic N left in the soil at harvest, but the proportion which remains in the following spring depends largely on the amount of winter rainfall (van der Paauw 1962 and 1963; Lidgate 1978). Losses of both residual and freshly-applied N can also occur in the spring, especially when heavy rain occurs before a crop becomes fully established (van der Paauw 1972). The N lost from the rooting zone will eventually find its way into underground water supplies or more directly into surface waters via natural or artificial drainage channels, where it can become a pollution hazard (Cooke 1976). It is important, therefore, from both agricultural and environmental standpoints to devise practical methods for predicting the extent of nitrate leaching in a wide range of situations.

Mechanistically leaching is the net result of a number of complex interacting processes which combine to disperse a band of nitrate as it is displaced through the soil during mass flow (Kirkham and Powers 1972; Greenwood and Burns 1979). The relative importance of these various processes depends largely on the pore structure of the soil and the rate and direction of water movement through it. In weakly-structured soils containing a large proportion of single-grained particles, dispersion is more likely to be controlled by microscopic 'mixing' processes within each pore (diffusion and hydrodynamic dispersion) and by turbulent effects created by the irregular shapes of the pores. In soils with a more well-defined crumb structure, where there is a wide pore size distribution, dispersion will depend more on the different rates of water movement through pores of different length and diameter. In some circumstances, water flow can be almost completely inhibited in narrow and dead-end micropores within aggregates, and when the soil is wet, nitrate can only enter and leave these by diffusion. The extent of dispersion is then governed by the relative proportions of nitrate inside and outside the aggregates when rainfall occurs.

Although leaching is concerned primarily with the displacement of ions from the soil during periods of heavy rainfall, upward movement of water and nitrate can also occur during evaporation (especially when it is near the surface) and this can also affect the way in which nitrate is dispersed within the profile. Because upward movement occurs at relatively low water contents, the soil solution flows mainly through the micropores. However, despite these superficial differences, the processes which control dispersion during the upward displacement are identical to those for drainage, although their relative importance may be different.

Inevitably these mechanisms are far too complex for any quantitative theory to have been derived from detailed consideration of the individual processes involved. Attempts have therefore been made to identify the processes, or features of these processes, that are considered to be of greatest importance and to incorporate these into models of leaching. Two different modelling approaches have been used, one based on classical flow theory (Gardner 1965; Kirkham and Powers 1972) and the other based on hydrological layer principles similar to those of the plate-layer theory of chromatography (Glueckhauf 1955). Recently Greenwood and Burns (1979) have critically examined both approaches. Their main conclusions may be summarized as follows :

(1) Many different models are capable of giving quite accurate predictions of the extent of leaching in field soils, although it is unlikely that any single model will hold for all situations on all soils.

(2) Contrary to many tacitly held beliefs, models developed from the flow theory approach are not based on any more fundamental principles than those based on hydrological layer principles.

(3) Flow theory models require detailed input data that is unlikely to be widely available, whereas most hydrological layer models make use of information which is routinely collected by meteorologists and soil surveyors.

(4) Models based on the hydrological layer approach are generally less expensive to run than flow theory models as they require less computing time.

On the basis of these criteria it was proposed that the best practical approach to estimating the leaching of nitrate from field soils was likely to be that offered by the hydrological layer type of model (e.g. Bresler 1967; Terkeltoub and Babcock 1971; Burns 1974; Addiscott 1977).

Unfortunately tests of most of these models have largely been restricted to one or two comparisons with experimental data under a somewhat limited range of environmental conditions. Information about their range of application is therefore fragmentary. The primary object of this paper is to discuss the results of both new and published experiments aimed at testing the validity of one particular hydrological layer model (that of Burns 1974). The second object is to discuss the suitability of the model for more widespread predictive purposes.

THE MODEL

Details of the model have been given by Burns (1974). It was designed for use on weakly-structured cultivated soils that do not form severe cracks or fissures. The model assumes that the soil is divided into a series of layers each characterised by its water content at field capacity. Each increment of rainfall increases the water content of the top layer, diluting the nitrate in the soil solution. After equilibration, the excess solution over that needed for field capacity is transferred to the next layer where it is thoroughly mixed with the soil solution already present, before the excess is once again lost to the layer below. The process continues until percolation ceases or until the required depth is reached. During dry periods, the model assumes that evaporation removes water from the surface layer until the soil water content falls to a fixed minimum (the evaporation limit); water is then extracted from the next layer and moves upwards to the surface before vaporizing. This induces movement of nitrate which is treated in the same way as downward movement. The water extraction is repeated for successive layers down the profile until the evaporative demand is satisfied. The amount of evaporation is calculated from E_o (open water surface evaporation) by the procedure of Stanhill (1958) which allows for the reduction in water loss that occurs as the soil dries out.

RESULTS AND DISCUSSION

Computer Simulation

The accuracy of the model was tested using the results of a series of leaching experiments carried out at Wellesbourne between 1970 and 1973 (Burns 1974 and 1981). The main experiments were designed to measure the influence of rainfall and evaporation on the redistribution of chloride (or, in one experiment, nitrate) applied to the surface of cultivated sandy loam and clay loam soils under fallow conditions over a period of several months. Other shorter-term experiments to measure the changes in distribution of chloride in the sandy loam soil after the application of controlled amounts of irrigation in various treatments were also included.

The weather patterns varied considerably between experiments in the different years, and provided an excellent test of the flexibility of the model. In 1970 there was a prolonged dry spell after the initial sampling (during which there was significant upward movement of nitrate and chloride to the surface) before substantial leaching occurred. In 1971, on the other hand, an extremely intense rainstorm about 1 week after chloride application caused rapid downward displacement, with further redistribution only occurring relatively slowly thereafter. The weather pattern in 1972 was less extreme than in the previous two years, with a more even distribution of rainfall and evaporation, so that there was a morė gradual movement of chloride through the profile during the experiment. The model was used to predict the changes in distribution of the anion from measurements of its initial distribution within the profile for all of the experiments using daily values of rainfall, irrigation and evaporation.

A summary of a statistical analysis of the fit of the model to the experimental data following the variations in weather conditions is given in Table 1. This shows that the predictions of the model were highly correlated with the data in all cases. As the intercepts of the

Table 1 Statistical analysis of the fit of the model to the field data

Year	Anion	Soil type	Number of data	Correlation coefficient	Slope and standard error of regression line
1970	chloride	sandy loam	84	0.869***	1.12 ± 0.061
1970	nitrate	sandy loam	84	0.830***	1.37 ± 0.088
1971	chloride	sandy loam	168	0.871***	1.40 ± 0.033
1972	chloride	sandy loam	56	0.962***	0.93 ± 0.029
1972-73	chloride	clay loam	46	0.979***	1.06 ± 0.030

***Highly significant ($P < 0.001$)

regression equations were never significantly different from zero, the regression data are presented as the slopes of the lines which pass through the origin. All but one of these are slightly greater than one, indicating a general tendency of the model to overestimate the chloride contents of the layers slightly. These deviations were greatest for the nitrate treatment in the 1970 experiment (where microbial reactions influenced the results) and in the 1971 experiment (where the displacement of chloride was consistently underestimated). Nevertheless, the results of this analysis show that in all other cases, the models gave very satisfactory predictions of the amounts of leaching which occurred, particularly in view of the narrowness of the soil layers used in these measurements.

Although these results show that the overall fit of the model to the experimental data was generally quite satisfactory, there was evidence of small but systematic deviations which were particularly noticeable during the early stages of all the experiments (Burns 1981). The patterns of these deviations appeared to be related to how quickly the first substantial rainfall occurred after salt application. This delay must have affected the proportion of salt which was able to penetrate the aggregates before leaching occurred, and it is extremely likely that the resulting displacement was influenced by the extent to which the anions were held back within the aggregates during displacement. The model assumes complete and instantaneous equilibration of all anions within each layer during leaching and some deviation from the experimental data was therefore inevitable. Thus in the 1972 experiment in the sandy loam soil, where the movement of chloride into the soil crumbs was enhanced by frequent showers which were just sufficient to moisten the surface, more chloride was held back within the surface regions of the soil when leaching occurred than was predicted by the model (see Fig 1). Although the effect is small, similar trends of the

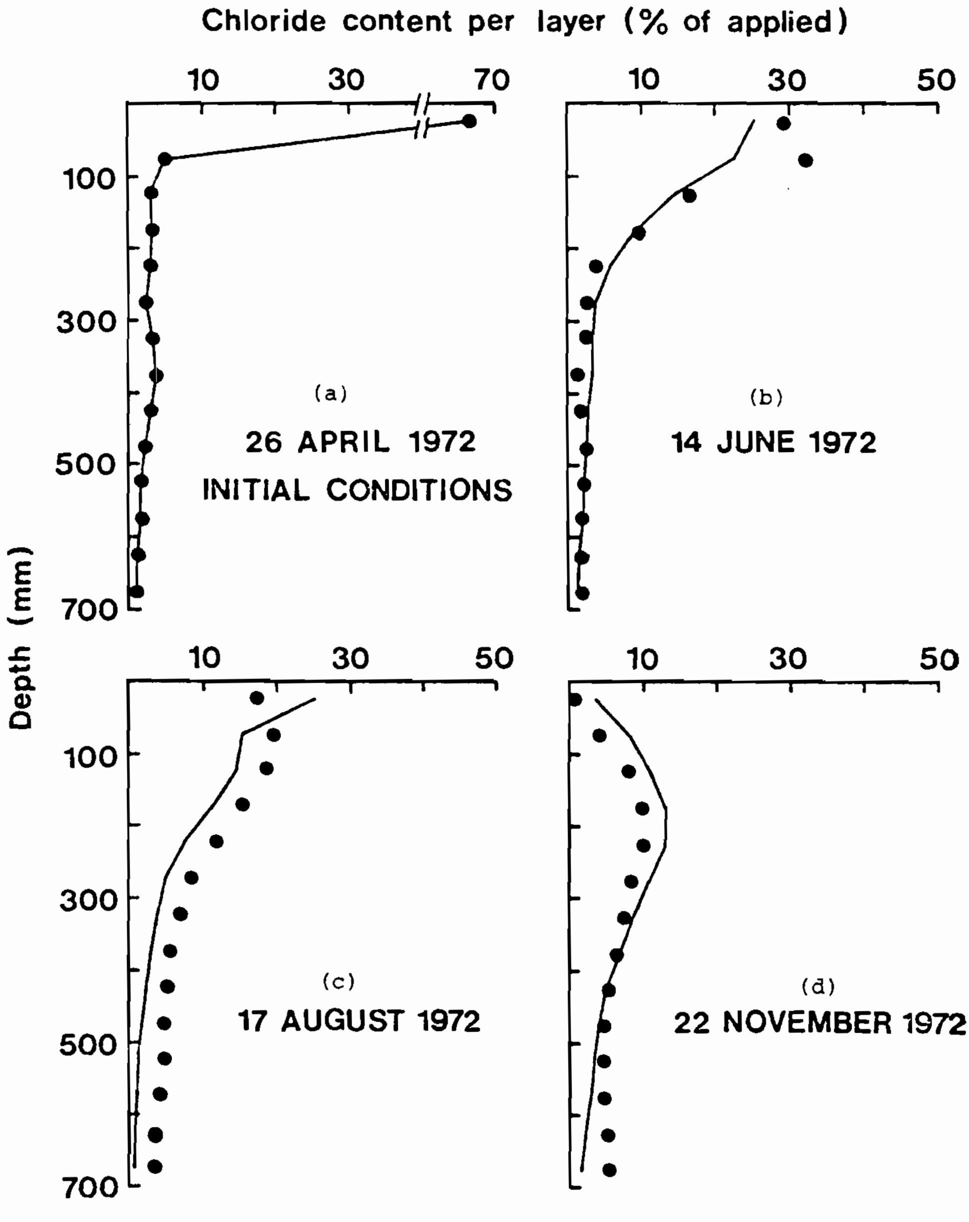

Figure 1. The redistribution of chloride in a sandy loam soil in 1972. The initial distribution is given in (a); the lines in (b) to (d) are the predictions of the model. The points represent the experimental data.

same magnitude were also consistently observed when leaching resulted from the application of controlled levels of irrigation (Burns 1981). In the 1971 experiment, on the other hand, most of the chloride still remained in the macropores around the aggregates when the first heavy rainfall occurred, within a few days of salt application. Thus much of this chloride was carried along by the rapidly moving drainage water which passed through these macropores, allowing little time for equilibration with the solution in the bulk of soil, with the result that the model substantially underestimated the extent of leaching (see Fig 2).

The importance of these holdback effects will clearly depend on the size of the aggregates and on the rate of water movement through the soil. In the above experiments, the soils had all been cultivated to produce a seedbed and the aggregate size was generally small. Under these conditions, the model was able to give a good overall representation of the changing shape of the salt distribution as it was leached downwards, provided that the leaching was delayed long enough to ensure some equilibration of the applied salt within the soil solution in the surface layer. However, holdback effects are likely to be of much greater importance in uncultivated or in cracking soils, where the structural units can be much larger, especially under conditions where high rainfall intensities are the norm (e.g. in the tropics). To predict leaching in these circumstances it may be necessary to incorporate the concept of mobile and immobile soil solution phases into the model (much as has been suggested by Addiscott 1977), together with a procedure for defining the redistribution of salts between these phases during the period immediately after their application.

Simple versions of the model

There are a number of advantages of using the model for predicting the leaching of unadsorbed anions from the surface regions of cultivated soils. Apart from its relatively small requirement in the use of

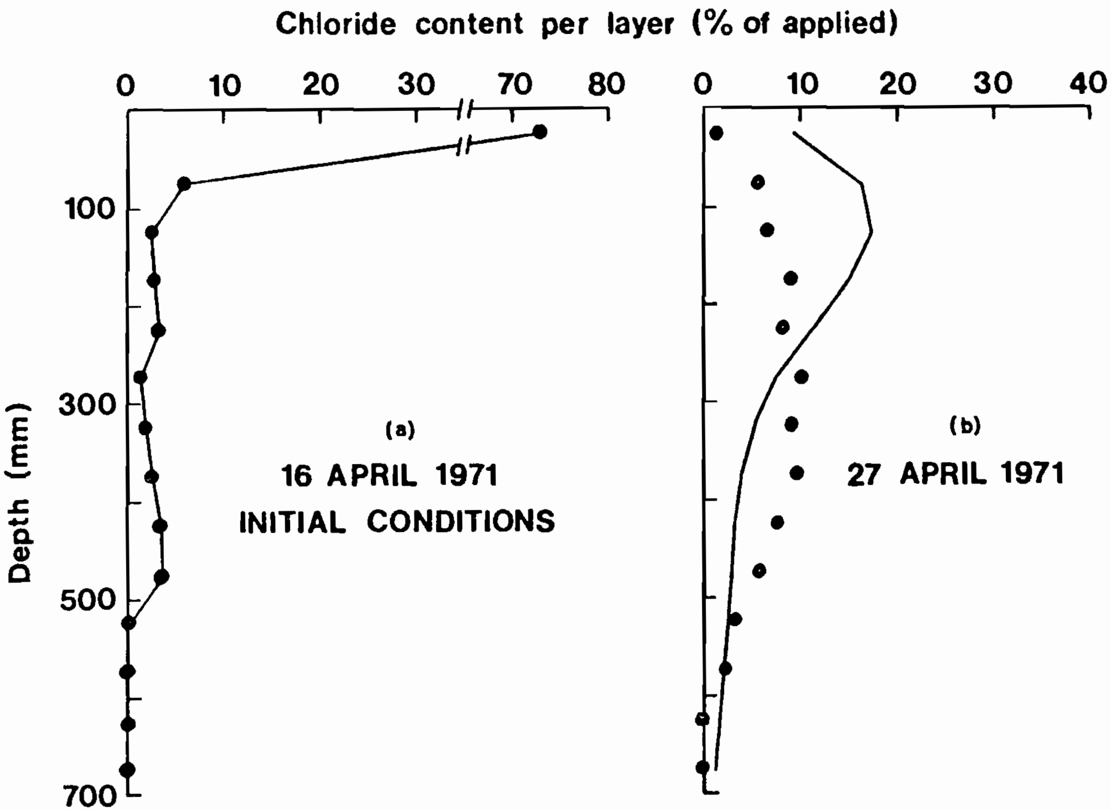

Figure 2. The redistribution of chloride during the early stages of leaching in a sandy loam soil in 1971. The initial distribution is given in (a); the line in (b) is the prediction of the model. The points represent the experimental data.

computing time, which may enable it to be reprogrammed on the modern generation of microcomputers, the model can also be further simplified to give forms which allow rapid estimates of leaching to be made. For example, where detailed information on the changes in shape of the leaching distribution are not required, estimates of total losses of nitrate or chloride from a given depth in the profile during a predominantly wet period may be calculated using a single equation. For surface-applied salts, this takes the form (Burns 1975) :

$$f = \left(\frac{P}{P+100_m} \right)^{h/10}$$

where f is the fraction of nitrate or chloride displaced below a depth h (mm) in the soil, θ_m is the volumetric field capacity and P is the total amount of water draining through the soil (mm). Because of the small amount of information required for these simplified models, they are particularly suitable for comparing with independent data from published experiments. Preliminary tests of the performance of this equation showed that it gave accurate estimates of displacement in cultivated soils which were not susceptible to swelling or cracking (Burns 1975). In the following exercise, further tests have been carried out using nitrate leaching data of Wild and Babiker (1976) for four different arable soils with θ_m values ranging from 0.17 to 0.33.

Values of the mean depth of rain penetration (P/θ_m) were taken from their data and used in the above equation to estimate the mean displacement of nitrate (at f = 0.5) in each of their treatments. These are compared with the corresponding observed displacement of the nitrate peak after leaching in Fig 3. The graph shows that the predictions of the simplified model were highly correlated with the experimental data. The regression line was also not significantly different from the line of perfect agreement, and any minor bias that may have been introduced from the use of the model can be explained by asymmetry in the shapes of the nitrate distributions after leaching, which would have caused the

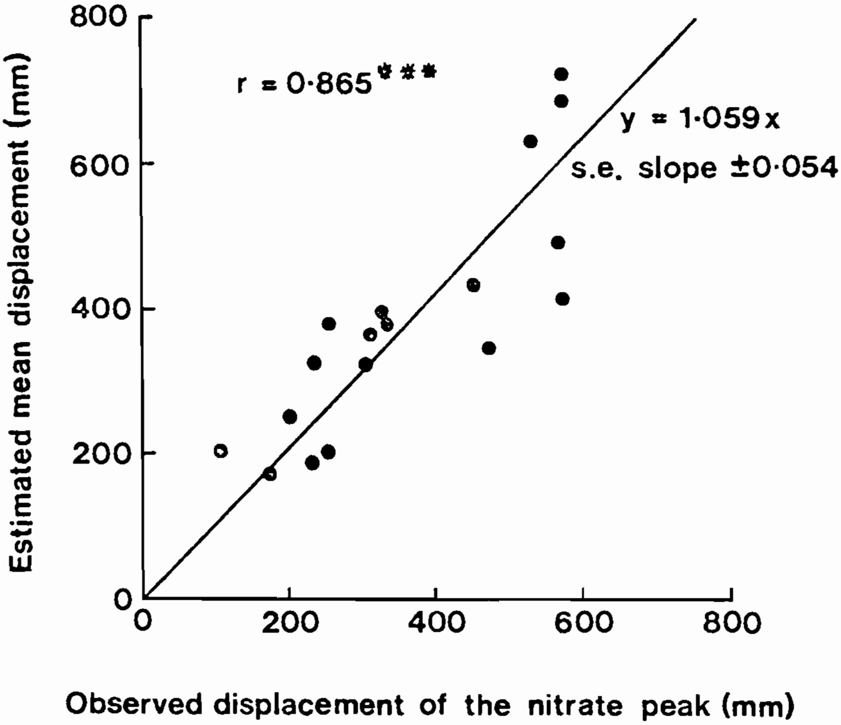

Figure 3. Regression of the estimated mean displacement of nitrate on the observed displacement of the nitrate peak in independent experiments of Wild and Babiker (1976) on 4 different soils.

mean depth of displacement to exceed the depth of the nitrate peak.

The above equation has been used to develop a practical method for estimating the influence of the leaching of fertilizer nitrate during the growing season on the yield of crops (Burns 1980). The method is based on the fact that the rate at which plant roots absorb nitrate is unaffected by its concentration at the root surfaces, provided this is above a very low concentration. In consequence, it is the proportion of the root system that is exposed to nitrate rather than the mean concentration in the soil that determines its availability to the crop. Thus in the method it was assumed that every crop on every soil had a characteristic critical rooting depth. Any nitrate leached below this depth was considered to be unavailable to the crop, whereas any nitrate above it was equally available no matter how it was distributed. Tests of the method showed it was able to explain some of the variations in yield response of different crops to N fertilizer in different experiments at one site over a number of years, (see Fig 4). Thus it would appear that the model is not only able to make predictions of the losses of nitrate from cultivated soils in carefully monitored leaching experiments, but that the predictions may also be helpful for forecasting how to adjust N fertilizer practice for differences in nitrate leaching.

CONCLUSIONS

The displacement of nitrate during leaching is governed by the pore structure of the soil and the rate of water movement through it. Nitrate remaining in the macropores is likely to be displaced more rapidly than that held in the micropores, and models which assume complete and instantaneous equilibration of all parts of the soil solution during leaching can therefore have only limited accuracy. Nevertheless the results show that one such model can give quite adequate representations of the losses of nitrate from cultivated soils

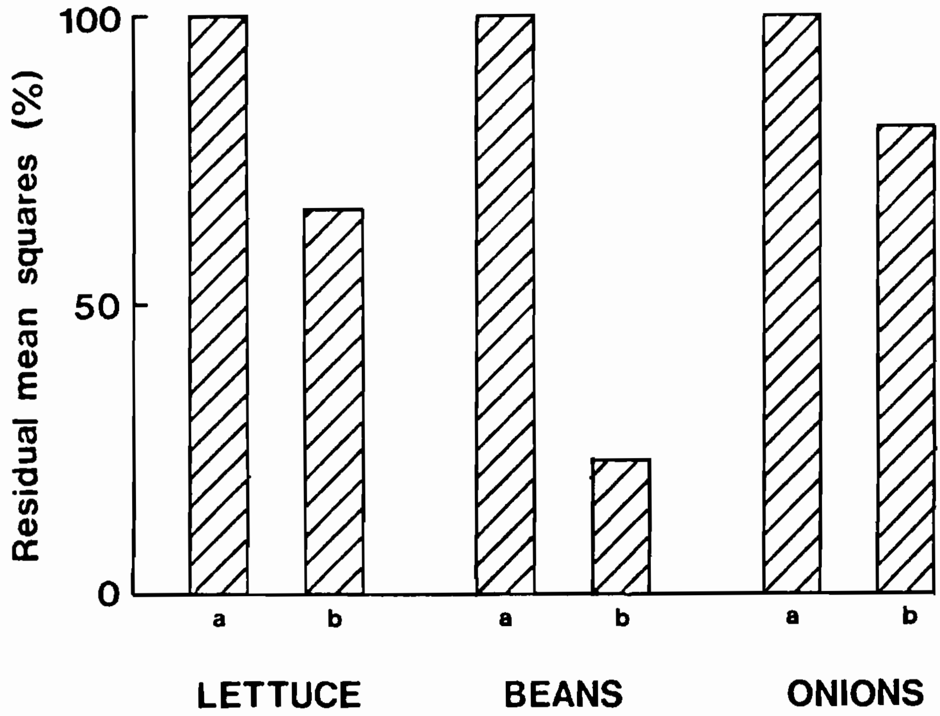

Figure 4. Residual mean squares after fitting a polynomial equation to data for the yield response of 3 crops to N fertilizer: (a) using the amounts of fertilizer applied and (b) using the amounts applied after adjusting for the differences in the estimated losses of nitrate by leaching between the various experiments.

where the aggregate size is small, provided that leaching does not occur too soon after fertilizer application. This model is also useful for obtaining approximate estimates of the losses of nitrate from the rooting zones of different crops, especially when only limited information about the soil and weather conditions is available.

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MODELLING NITRATE MOVEMENT IN PROFILES THAT CONTAIN SOIL, HEAVY CLAY AND CHALK

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ABSTRACT

A simple computer model based on the sizes and porosities of the structural units of soil, clay subsoil and chalk was used to simulate the nitrate concentration profiles that have developed by leaching beneath an area of old grassland first ploughed up in 1959 and left fallow since. Three profiles taken fairly close to each other differed considerably in the depth at which chalk was found, and in one the clay recurred below the first layer of chalk. However, the model simulated nitrate concentrations reasonably well in all three profiles but tended to over-estimate concentrations in the chalk immediately beneath the subsoil clay. The results suggested that nearly all the nitrate originated from the ploughing-up of the old grassland and the resulting breakdown of soil organic nitrogen, and that this nitrate readily penetrated the subsoil clay, up to 10 m thick that lies above the chalk.

INTRODUCTION

Interest in modelling the movement of nitrate in the soil has been stimulated by the concern of the agricultural community about the loss of an increasingly expensive resource and the concern of environmental authorities about nitrate as a pollutant of water supplies. In the United Kingdon, as much as one-third of the £200 m spent annually on nitrogen fertilisers may be wasted by leaching, and over 100 public supply boreholes now produce groundwater with nitrate concentrations intermittently or continuously above 11.3 mg N l^{-1}, the WHO recommended limit, (Young *et al.*, 1979). Nitrate in water supplies is seen as a health risk because of the possibility of methaemoglobinaemia in very young children (Comley, 1945) and the possible association with gastric cancer (Tannenbaum *et al.*, 1977), but it should be noted that only one death in the United Kingdom was attributed to nitrate in water between 1950 and 1975 and that followed the use of well water polluted with coliforms (Tayler, quoted by Wild, 1977).

The movement of nitrate and other ions in the soil has been modelled by a variety of approaches, including miscible displacement theory (Nielsen and Biggar, 1962), chromatography theory (Frissel *et al.*, 1970; Kolenbrander, 1970), other forms of layer model (Bresler, 1967; Burns, 1974; Addiscott, 1977) and that of Scotter (1978) which centres on the effect of wormholes and fissures. Considerable progress has also been made in modelling the movement of nitrate through chalk (Young *et al.*, 1976, 1979), but principally on outcrops of aquifers where soil and other superficial deposits were thin. Less work of this nature seems to have been done where superficial deposits are thick enough to influence nitrate movement appreciably.

MODELLING APPROACH

This paper is concerned with the problem of sites where the surface soil is separated from the chalk by an appreciable thickness of heavy clay, as at Rothamsted. This situation requires a model that can be applied with continuity through soil, clay and chalk, and which is based on characteristics that can be defined reasonably well in all three media. This makes it difficult to use models based on the flow equations, because of the great spatial variability of hydraulic conductivity in clay and chalk and even in some surface soils.

An earlier paper (Addiscott, 1977) described a model for aggregated soils based on the division of the soil solution into mobile and non-mobile (retained) phases, of which only the mobile phase is displaced during water movement. Solute equilibration between the phases was assumed to occur when movement ceased. The phases were defined with reference to the soil moisture characteristics. This model proved reasonably successful in simulating changes in nitrate concentration in soil layers after autumn application of calcium nitrate (Addiscott, 1977). It also simulated changes in chloride concentration in drainage from the Rothamsted Drain Gauges (lysimeters) following autumn application of calcium chloride (Addiscott *et al*., 1978). However, to obtain a simulation for the deeper (40-inch) gauge, it was necessary to transfer most of the water defined as mobile to the retained phase in the layers below 0.5 m, which contained heavy subsoil clay. The need for this modification suggests that the model is unsuitable for simulations through soil, clay and chalk in this form.

An alternative form of the model assumes that the retained phase is held within the aggregates whilst the mobile phase moves in a film on the outside of the aggregates. The phases can then be defined in terms of the sizes and porosity of the aggregates and the thickness of the mobile film. Also, if the aggregates are assigned a specific geometry, solute movement between the phases can be simulated as occurring by diffusion rather than simple equilibration. In this form of the model, the aggregates are assumed to be cubic. Size and porosity are characteristics that can be measured or estimated for the structural units of the soil, clay and chalk, and this model was therefore used to attempt the simulation of movement through the three media. Further information on this model will be presented at the meeting and will also be found in a forthcoming publication (Addiscott, [illegible]).

MATERIALS AND METHODS

Borings were made in November 1977 as part of a co-operative project between Rothamsted Experimental Station (R.E.S.) and the Water Research Centre, Medmenham (W.R.C.) at Rothamsted on a permanent fallow site. The soil was a flinty clay loam of the Batcombe series (Avery, 1964) overlying Clay-with-Flints which in turn rests upon the chalk. Chalk was reached at very variable depths, ranging over a small area between four and eleven metres. The area was in permanent grass for more than 200 years before it was ploughed up in December, 1959 and has remained as bare fallow subsequently, cultivated only for weed control and receiving no nitrogen fertiliser. The site is of interest because of the conclusion by Young *et al*. (1979) that the mineralisation of soil organic nitrogen following the ploughing-up of established grassland or long-term grass leys results in very large nitrate leaching losses into aquifers.

Cores were taken in 1 m lengths with a percussion drill down to the depths shown in the figures and subsampled. Water was extracted by the high-speed centrifugation method of Edmunds and Bath (1976) and analysed using standard AutoAnalyser techniques (W.R.C. procedure). Samples from boreholes 2 and 3 were also examined by R.E.S. procedures. Soil samples were extracted with 2*M* KCl 0.1*N* in HCl and chalk samples by centrifugation, ammonium and nitrate being determined by the methods of Varley (1966) and Litchfield (1967) respectively on the AutoAnalyser. In the figures, W.R.C. analyses are shown for borhole 1 and R.E.S. analyses for boreholes 2 and 3. All the chalk data is from the unsaturated zone.

COMPUTER SIMULATIONS

Inputs to the model

The model needs (a) rainfall/evaporation data, (b) nitrate input data, (c) parameters defining the sizes and porosities of the structural units, and (d) diffusion parameters. These were supplied as follows.

(a) Rainfall/evaporation data were presented as the drainage through the 20-inch Drain Gauge, which gives a measure of the excess of rainfall over evaporation and any previous deficit for a given period.

(b) Mineralisation of soil organic N was found to be proportional to the square root of time in laboratory experiments (Stanford and Smith, 1972). Soil samples taken from the 0-23 cm layer of the permanent fallow site in 1959, 1963, 1970 and 1978 and analysed for total N showed similarly that the decrease in total N (N_0-N_t) was related to the square root of time (t), by the regression

$$N_0-N_t = 922\ t^{\frac{1}{2}} + 19\ ;\ r^2 = 0.9997\ (p<0.001)$$

where N_0-N_t was in kg ha^{-1} and t in years. This relationship provided a convenient means of presenting mineral N input. Eleven percent of the mineral N found in profiles 2 and 3 was ammonium-N, nearly all of it in the soil and clay, but this does not necessarily imply that eleven percent of the total N input remained as ammonium.

(c) Sizes of structural units are presented to the model as normal or log-normal distributions defined by a mean and standard deviation. The distribution is likely to be log-normal for soil aggregates (Gardner, 1956), such a distribution being characteristic of the breakage of solids (Epstein, 1948). Size distributions were assumed to be normal in the clay and chalk unless breakage was thought to have influenced size (e.g. at clay/chalk interfaces). The means and standard deviations used at various depths are shown in Table 1. Values for the top two layers were based on measurements. Not much is known about size distributions in the Clay-with-Flints at depth, but it is thought that there are widely spaced fissures through which nearly all vertical water movement occurs. This was simulated by using the model in a mode that assumes the cubes to be stacked upon each other so that water flows only over the four vertical faces, giving in effect a grid of fissures. The size of the cubes (i.e. the spacing of the fissures) was assumed to increase with depth initially but to decrease again near the chalk surface. The structural units of the chalk were taken to be around 200 mm in size and not to vary with depth. Simulations were made assuming the water to flow around four or six faces of the chalk cubes. The clay and chalk were assumed to have porosities (p) of 0.35 and 0.5 respectively (Williams, 1978, and personal communication). If the values of volumetric moisture content (θ) and air fraction (f) indicated that the water-filled porosity (p_w) was less than p, p_w was used in place of p for diffusion calculations in the cubes. In the soil and clay, 8.8 percent of p or p_w was taken to exclude nitrate, this figure being based on earlier experiments. The thickness of the mobile film was calculated from θ, f, p and the cube size unless p_w was less than p, when it was given a predetermined general value (usually 0.2 mm).

(d) The diffusion parameters needed include the cube size and p or p_w (above). Nitrate must be present predominantly as calcium nitrate, for which the diffusion coefficient in free solution was assumed to be similar to that for calcium chloride taken from tables (1.17×10^{-5} cm^2 s^{-1}). The tortuosity factor in the structural units was taken to be numerically similar to p or p_w.

Climatic inputs and time-dependant operations were in units of one month, except the calculations for diffusion in the structural units which were made five times more frequently.

Simulations of nitrate concentrations in the profile

The three profiles to be discussed differed greatly from each other although they all came from within a small area (Figures 1-3). Profile 1, the simplest, showed surface soil and then subsoil clay to 3 m, some chalk marl between 3 and 4 m, and chalk below 4 m. Profile 2 was more disturbed. There was subsoil clay to 10 m but the chalk found there continued only to 14 m, where chalk marl recurred and was followed by further clay from 15 to 20 m. This profile may have been in a chalk pipe. In profile 3, the clay was found down to 11 m but the chalk was then continuous.

There were marked fluctuations in both nitrate concentration and water content down all three profiles (Figures 1-3 and Table 1). To check that the fluctuations in nitrate concentration were not simply dilution effects associated with fluctuations in water content, correlations between nitrate concentration and water content were calculated. In profile 2 there was a strong negative correlation ($r = -0.763$; $p<0.001$), suggestive of a dilution effect, but in profile 3 where the fluctuations were also large the correlation was negligible ($r = 0.04$; NS), and in profile 1 the correlation was positive (but non-significant, $r = 0.26$).

Nitrate concentrations in profile 1 (Figure 1, solid line) were fairly constant in the chalk to 11 m and then declined rapidly to a minimum of 3 mg l^{-1}. There were discontinuities at the clay-chalk interface and at 14 m. The model simulated the concentrations in the soil and clay reasonably well but did not initially simulate the concentrations in the chalk because it predicts only the amount of nitrate movement and not the time scale over which it occurs.

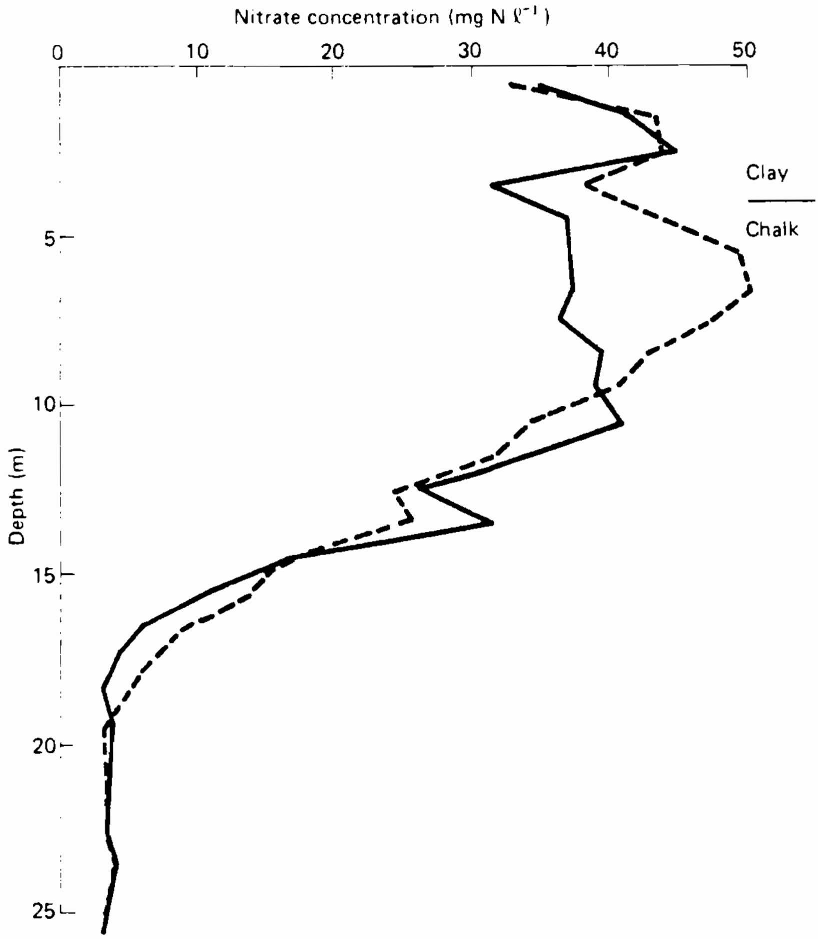

Figure 1. Nitrate concentrations in interstitial water. Profile 1.
——— measured; ----- simulated

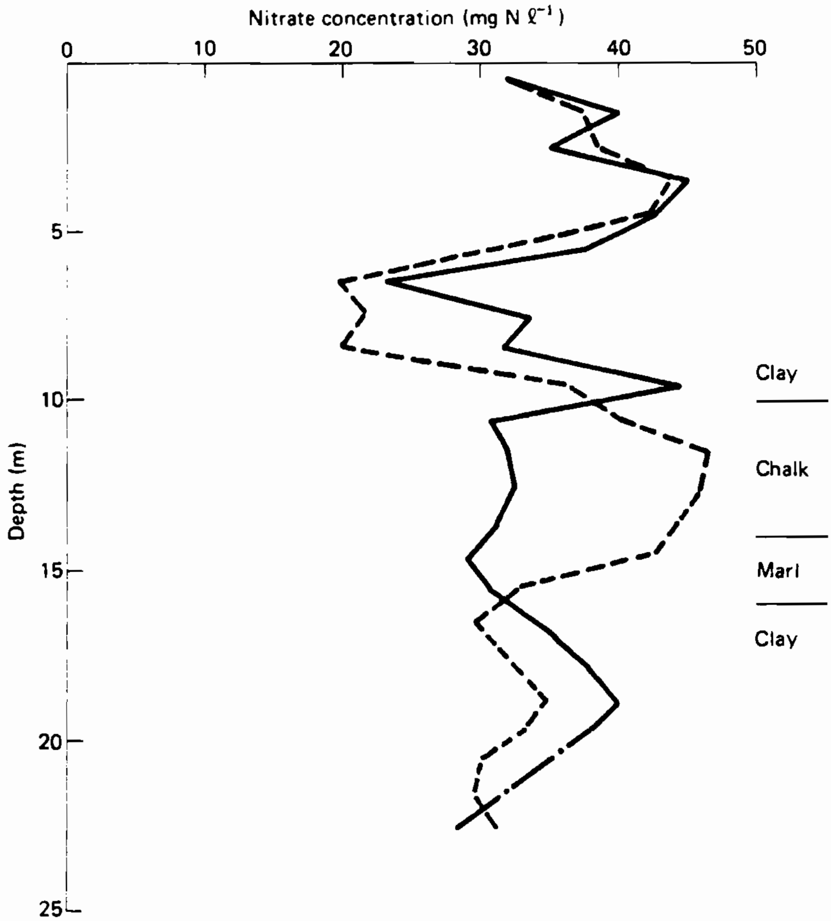

Figure 2. Nitrate concentrations in interstitial waters. Profile 2.
——— measured; ------ simulated.

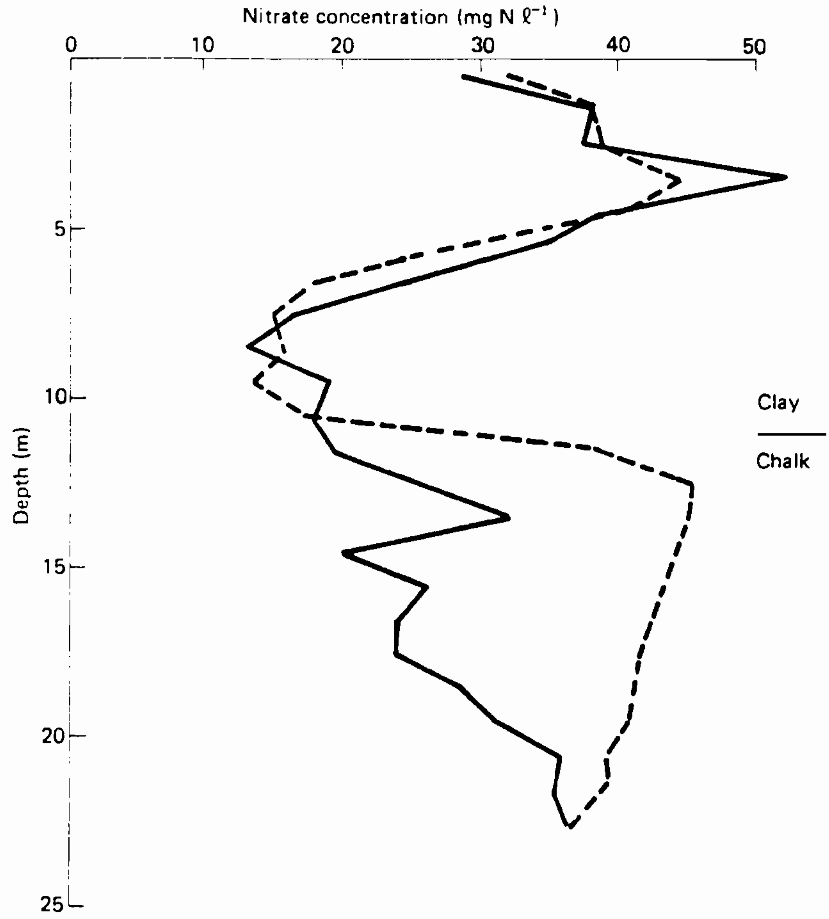

Figure 3. Nitrate concentrations in interstitial water. Profile 3.
——— measured; ------ simulated

Young *et al* (1979) concluded that bands of nitrate move downwards at about 1 m $year^{-1}$. This was simulated by making the model print for the layer *x* m below the clay the concentration that would have been found *x* years earlier had instantaneous flow occurred in the chalk. This resulted in the simulation shown in Figure 1 which showed correctly where the concentration decreased and partially reproduced the discontinuities but showed unduly large nitrate concentrations in the section of the profile immediately below the clay.

Profile 2 (clay-chalk-clay) was treated as if it were all soil and clay in that no time-scale correction was applied. The model simulated the nitrate concentrations in soil and clay quite satisfactorily but again predicted over-large concentrations in the chalk beneath the first section of clay (Figure 2).

The model alao simulated satisfactorily the nitrate concentrations in the soil and clay of profile 3, but once again showed over-large concentrations in the chalk immediately beneath the clay whether or not the time-scale correction was applied in the chalk (Figure 3).

DISCUSSION

The model used is basically simple and has not been widely tested. Considering this, the depth of the profiles (23-26 m) and the lengthy period covered by the simulations (just under 18 years), the results are probably as good as can reasonably be expected. The problem of the over-large nitrate concentrations simulated in the chalk immediately beneath the clay clearly needs further investigation, and the model as a whole is still undergoing development. It must also be remembered that although some of the layer inputs (Table 1) were based on measurement, some were "guesstimates". The simulation results should therefore be interpreted with caution, but allow some provisional conclusions to be drawn.

When the measured nitrate profiles were first examined, there was considerable discussion as to whether the nitrate found in the chalk had leached from the surface soil or whether it was "fossil nitrate" that had been in the chalk for a long time before the ploughing in 1959. The fact that the profiles could be simulated reasonably well on the assumption that the nitrate had leached from the surface strongly suggests that this is what happened, although it does not, of course, prove it. In the same way, these results also support the conclusion of Young et al. (1979) that large losses of nitrate by leaching occur when old grassland is ploughed up and soil organic nitrogen is mineralised, since the simulations were made with N input solely from mineralisation. Inputs of N in rain and by dry deposition are likely to have been small in comparison (possibly 5 percent of that supplied by mineralisation). The results from profile 1 also accord with the value of ca 1 m $year^{-1}$ calculated by Young et al. (1979) for the rate of downward movement of bands of nitrate in chalk.

The model did not include any allowance for denitrification, since there seemed to be no reliable way of predicting its occurrence. Not all the nitrate in the simulated profile was found in the measured profile, but this is as likely to reflect the inadequacies of the model as the occurrence of denitrification. Clearly denitrification cannot have occurred on any very large scale.

Table 1 Inputs for each metre layer: Mean size of structural unit (side of cube) (mm), number of sides on which flow occurs, volumetric moisture content (θ_v).

	Profile 1			Profile 2			Profile 3		
Layer	Mean size	Flow sides	θ_v	Mean size	Flow sides	θ_v	Mean size	Flow sides	θ_v
1	16.7 l	6	0.315	16.7 l	6	0.273	16.7 l	6	0.271
2	90 n	4	0.555	90 n	4	0.246	90 n	4	0.265
3	90 n	4	0.533	90 n	4	0.253	90 n	4	0.260
4	10 l	6	0.360	300 n	4	0.218	300 n	4	0.190
5	10 l C	6	0.400	500 n	4	0.170	500 n	4	0.222
6	C		0.424	1000 n	4	0.194	1000 n	4	0.234
7	C		0.445	1000 n	4	0.386	2000 n	4	0.220
8	C		0.447	1000 n	4	0.337	3000 n	4	0.188
9	C		0.465	1000 n	4	0.371	3000 n	4	0.177
10	C		0.418	10 l	6	0.269	3000 n	4	0.220
11	C		0.428	10 l C	6	0.383	2000 n	4	0.228
12	C		0.416	C		0.327	10 l C	6	0.321
13	C		0.466	C		0.306	C		0.367
14	C		0.331	C		0.335	C		0.330
15	C		0.397	C		0.363	C		0.321
16	C		0.314	300 n	4	0.322	C		0.318
17	C		0.400	300 n	4	0.391	C		0.319
18	C		0.385	300 n	4	0.330	C		0.327
19	C		0.426	300 n	4	0.242	C		0.329
20	C		0.364	300 n	4	0.251	C		0.302
21	C		0.389	300 n	4	0.323	C		0.322
22	C		0.406	300 n	4	0.323	C		0.300
23	C		0.405	300 n	4	0.323	C		0.333
24	C		0.409						
25	C		0.391						
26	C		0.380						

Notes.
1) Standard deviation of size distribution taken as 0.4 x mean. n denotes normal, l log-normal.
2) Size inputs for first two layers based on measurement. Remainder are values considered possible but are not amenable to verification.
3) Layer 1, soil and clay; subsequent layers are clay unless marked C. Layers marked C are chalk, with assumed mean size 200 mm and 6 flow sides unless otherwise stated.
4) Values of θ_v derived from measured gravimetric moisture contents.

The simulations, if correctly based, imply that fissures on a grid with 1-3 m spacing and carrying thin films of mobile water (ca 0.2 mm thick) on vertical faces are sufficient for agricultural leachates to penetrate the clay in such a way as to produce nitrate concentrations up to 30-40 mg N l^{-1} in the unsaturated chalk below, i.e. concentrations exceeding the WHO maximum limit for potable water. There must therefore be doubt as to whether even a fairly thick superficial deposit of clay can protect an aquifer from nitrate pollution unless it is unfissured.

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RETENTION, TRANSFORMATIONS, AND TRANSPORT OF PESTICIDES IN SOIL-WATER SYSTEMS: MODEL DEVELOPMENT AND EVALUATION[1]

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ABSTRACT

Mathematical models currently available for describing the fate of pesticides in soil-water systems were reviewed. Processes influencing the fate of pesticides considered in this review were: retention (adsorption-desorption), transformations (chemical and/or biological degradation), and transport with water. A number of simulation models, with varying degrees of complexity and scope, are presently available. However, verification and extensive use of these models has generally been difficult owing to inadequate methods for measuring and/or estimating the necessary model input parameters. The ability to devise and numerically solve complex simulation models presently exceeds the available experimental base data to verify these models. Given the uncertainities of the model parameters and the field-scale spatial heterogeneity, deviations of a factor of 2 or more between simulated and measured conditions may be acceptable. Therefore, for general use, simple models with a minimum number of inputs may provide sufficient information about the fate of pesticides in agricultural ecosystems. Only limited amounts of field-data are available to verify even the simple pesticide models.

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INTRODUCTION

Various processes and factors govern the fate of soil-applied pesticides. An understanding of these processes and factors can lead to better management practices and reduce the potential for contamination of surface and groundwater resources. Major process that determine pesticide behavior in agricultural ecosystems are: 1) retention by soil (adsorption-desorption), 2) transformations (chemical and/or microbiological degradation), 3) leaching (transport with water through the soil profile), and 4) plant uptake (weed and crop species). Only the first three processes were considered in this paper. In view of the number of excellent reviews (e.g., Haque and Freed, 1974; Leistra, 1973; van Genuchten and Cleary, 1978; Anderson, 1980) dealing with modeling the behavior of pesticides in the environment, the scope of this paper is limited to an examination of the success and/or failure of various models to simulate pesticide behavior in soils under laboratory and field conditions. In this regard, various simulation models proposed to date are briefly reviewed, and the difficulties encountered in their verification and use are discussed.

REVIEW OF MATHEMATICAL MODELS

Using principles of conservation of mass and the continuity equation, the partial differential equations for water and solute transport in soils can be derived. The equation for one-dimensional transient soil-water flow with simultaneous soil-water extraction by plant roots is given by,

$$\frac{\partial \Theta}{\partial t} = -\frac{\partial}{\partial z}\left[K(\Theta)\left(\frac{\partial h}{\partial z} - 1\right)\right] - U(z,t) \qquad [1]$$

The symbols used in Eq. [1] and elsewhere in this paper are defined in the Appendix. The equation describing convective-dispersive pesticide transport is,

$$\frac{\partial}{\partial t}(\Theta C+\rho S) = -\frac{\partial}{\partial z}\left[-\Theta D\frac{\partial C}{\partial z} + qC\right] - \sum_{i=1}^{n} Q_i \qquad [2]$$

The term in the brackets on the r.h.s. of Eq. [2] is the convective-dispersive pesticide flux, and Q_i are various sink terms accounting for pesticide loss (degradation). For steady water flow conditions (i.e., $\partial\theta/\partial t = 0$), Eq. [2] reduces to,

$$\frac{\partial C}{\partial t} + \frac{\rho}{\theta}\frac{\partial S}{\partial t} = D\frac{\partial^2 C}{\partial z^2} - v\frac{\partial C}{\partial z} - \frac{1}{\theta}\sum_{i=1}^{n} Q_i \qquad [3]$$

where, $v=(q/\theta)$ is the average pore-water velocity. Eqs. [1] and [2] are solved sequentially in order to describe the simultaneous transient flow of water and pesticides. Functional relationships between adsorbed (S) and solution (C) concentrations of pesticides as well as the rate laws governing pesticide degradation must be specified to solve Eqs. [2] or [3].

When the adsorption-desorption reactions are instantaneous, equilibrium exists between the solution and adsorbed-phase pesticide concentrations (C and S, respectively). The equilibrium relationship between C and S is specified by the adsorption-desorption isotherm. In Table 1, various equilibrium isotherm models are summarized. Among these, the linear and Freundlich isotherms have been the most common models used for pesticide adsorption-desorption on soils and sediments. Over the range of solution concentrations associated with agricultural applications of pesticides, linear isotherms may be adequate (Rao and Davidson, 1980).

Various rate laws have been proposed for the cases where adsorption-desorption reactions are not instantaneous (Table 2). Note that most of the equilibrium models listed in Table 1 can be derived from those shown in Table 2 by assuming the steady-state conditions ($\partial S/\partial t = 0$). Also the models in-

Table 1. Summary of models used for describing equilibrium adsorption of pesticides during flow (Adapted from van Genuchten and Cleary, 1978).*

MODEL	EQUATION	REFERENCE
1.1 (linear)	$S=k_1C+k_2; \quad k_2 \geq 0$	Lapidus and Amundson (1952) Lindstrom et al (1967)
1.2 (Langmuir)	$S=\dfrac{k_1C}{1+k_2C}$	Tanji (1970) Ballaux and Peaslee (1975)
1.3 (Freundlich)	$S = k_1C^{k_2}$	Lindstrom and Boersma (1970) Swanson and Dutt (1973)
1.4	$S = k_1Ce^{=2k_2S}$	Lindstrom et al (1971) van Genuchten et al (1974)
1.5 (Modified Kjelland)	$S=\dfrac{CS_m}{C+k_1(C_m-C)\exp[k_2(C_m-2C)]}$	Lai and Jurinak (1971)
1.6 (Fraction near equilibrium)	$S=(FREQ)\ k_1\ C^{k2}$	van Genuchten et al (1974) Wood and Davidson (1975)

* See Appendix for definition of symbols

Table 2. Summary of models used for describing nonequilibrium adsorption of pesticides during flow (Adapted from van Genuchten and Cleary, 1978).*

MODEL	EQUATION	REFERENCE
2.1 (linear)	$\frac{\partial S}{\partial t} = k_r\ (k_1C+k_2\ -S)$	Lapidus and Amundson (1952) Oddson et al (1970)
2.2 (Langmuir)	$\frac{\partial S}{\partial t} = k_r\ (\frac{k_1C}{1 + K_2C}\ -S)$	Hendricks (1972)
2.3 (Freundlich)	$\frac{\partial S}{\partial t} = k_r\ (k_1C^{k_2}\ -S)$	Hornsby and Davidson (1973) van Genuchten et al (1974)
2.4	$\frac{\partial S}{\partial t} = k_r\ e^{k_2S}(k_1Ce^{-2k_2S}\ -S)$	Lindstrom et al (1971)
2.5	$\frac{\partial S}{\partial t} = k_r\ (S_m-S)\ \sinh k_2(\frac{S_m - S}{S_m\ -S_i})$	Fava and Eyring (1956) Leenheer and Ahlrichs (1971)
2.6 (Two-site)	$\frac{\partial S}{\partial t} = \frac{\partial S_1}{\partial t} + \frac{\partial S_2}{\partial t}$, where $\frac{\partial S_1}{\partial t} = k_1 C^{k_2} \frac{\partial C}{\partial t}$ $\frac{\partial S_2}{\partial t} = k_r\ (k_1C^{k_2} - S_2)$	Selim et al (1976) Cameron and Klute (1977)

* See Appendix for definition of symbols

cluded in Tables 1 and 2 assume the adsorption-desorption processes to be reversible. When the adsorption-desorption are reversible, but nonsingular, different values are assigned to the rate coefficients for adsorption and desorption (e.g., van Genuchten et al., 1974).

Two basic types of rate laws have been used to describe the kinetics of pesticide degradation in soils: the "power rate" model and the "hyperbolic rate" model. In Table 3, Models 3.1 and 3.2 are examples of the first type, while Model 3.3 is an example of the latter type of degradation model. Although the hyperbolic rate law, based on Michaelis-Menten enzymatic kinetics, may be more appropriate for pesticides, the first-order kinetic equation (Model 3.1) has been successful in describing pesticide degradation in soils. Two aspects of these models must be recognized: (1) The rate of degradation (Q) can be set proportional to either the total pesticide concentration ($\Theta C+\rho S$), or the solution-phase concentration (ΘC); the distinction between these two choices is not always specified by many authors. (2) The value of the degradation rate coefficient is determined by environmental factors, principally temperature and soil-water potential. Walker (1976 a,b) presents an empirical regression equation, based on experimental data, for describing this dependence. The reader is referred to an excellent review by Goring et al (1974) for a discussion of pesticide degradation in soil.

From the foregoing discussion, it is apparent that various mathematical submodels have been proposed for describing retention and degradation of pesticides and other solutes. Analytical or numerical solutions to Eq. [3] are available for various initial and boundary conditions as well as the type of retention or degradation submodel. Therefore, the problem in modeling pesticide behavior in soils is not one of lack of models or numerical methods for solving these models, but that of selecting a simulation model that has been verified.

Table 3. Summary of models used for describing the kinetics of pesticide degradation in soils.*

MODEL	EQUATION	REFERENCE
3.1	$Q = -k_{d1}(\theta C + \rho S)$	Liestra (1973)
3.2	$Q = -k_{d_1} C^{k_{d_2}}$	Hamaker (1966)
3.3	$Q = \dfrac{-k_{d_1}}{k_{d_2}+C}$	Hamaker (1966)

* See Appendix for definition of symbols.

VERIFICATION OF SIMULATION MODELS

Ideally, a conceptual model should include all processes that determine the fate of pesticides in soils. Furthermore, procedures for independently measuring the necessary input parameters associated with each process in the model must be available. The validity of a mathematical model can then be judged by comparing model predictions with experimental results obtained under well-defined initial and boundary conditions. Unfortunately, for complex and heterogeneous systems such as field soils, an idealized approach to model verification is not feasible. Neither all the processes that determine the pesticide behavior in soils are known nor is a quantitative description of these processes always possible. Also, methods for measuring model input parameters are generally unavailable. Many of the model parameters are therefore estimated based on "best-fit" to experimental data. However, conceptual models may be forced to describe measured data, precluding process identification and model verification (Davidson et al., 1980). In the following paragraphs, we will discuss selected examples of attempts to verify conceptual-process models for describing pesticide adsorption-desorption and transport in soils.

Adsorption-Desorption and Transport

Davidson and Chang (1972) reported that the equilibrium linear isotherm (Model 1.1, Table 1) model failed to describe picloram herbicide movement in Norge loam soil column. van Genuchten et al (1974) evaluated Models 1.3, 1.6, 2.3 and 2.4 for describing picloram herbicide movement at several pore-water velocities (14 to 142 cm/day) a column in Norge loam soil. They also considered the adsorption-desorption isotherms to be nonsingular. They concluded that the assumption of instantaneous adsorption was valid only at low velocities (14 cm/day) and that Model 1.3 could describe measured data. Model 1.6 predicted the data from the higher velocity experiments only if the parameter FREQ was introduced and allowed to decrease with increasing velocity. Note that FREQ represents the fraction of total adsorption "sites" in equilibrium during flow and a decreasing value of FREQ indicates increasing nonequilibrium conditions for adsorption-desorption. van Genuchten et al (1974) also reported that Models 2.3 and 2.4 could describe measured data only when the rate coefficients were varied with pore-water velocity. Wood and Davidson (1975) investigated fluometuron herbicide movement during transient water flow in Cobb fine sandy loam soil columns. They reported that Model 1.6 predicted the fluometuron data when the value of FREQ varied between 0.5 and 0.75, where as Model 1.3 (which is Model 1.6 with FREQ=1.0) underpredicted the leaching of fluometuron. Rao et al (1979) evaluated the ability of Model 2.6 to describe the movement of 2,4-D and atrazine herbicides in three soils during steady water flow. They also found that model parameter values required to describe the measured data were significantly different for each set of experimental conditions (pore-water velocities and/or concentrations).

The mathematical models listed in Tables 1 and 2 appear to be inadequate for describing pesticide adsorption-desorption during pesticide transport in soils. Nonequilibrium adsorption-desorption models generally tend to describe measured data somewhat better than equilibrium models. It should be recognized, however, that the nonequilibrium models contain a larger number of parameters (and therefore greater degrees of freedom for parameter optimization schemes) which need to be measured. Most laboratory batch adsorption experiments suggest that the adsorption-desorption processes are quite rapid; 60–80% of the reaction is completed within a few minutes and equilibrium is achieved within a few hours. Rate coefficients calculated from such experiments are large enough that equilibrium conditions should prevail during water flow in the range of pore-water velocities employed by most researchers. Based on such findings, we may conclude that the apparent nonequilibrium pesticide adsorption-desorption observed during flow is not due to the kinetics of the reaction at the soil-solution interface. The degree of nonequilibrium appears to be determined by the rate at which pesticide molecules are transported to the soil surfaces or adsorption "sites". van Genuchten and Wierenga (1976) proposed a model where the soil-water was divided into "mobile" and "immobile" regions, and the convective-dispersive solute transport was limited to the "mobile" soil-water region. The rate of pesticide adsorption-desorption on the "sites" residing within the immobile soil-water region was controlled by diffusive mass transfer across the mobile-immobile soil-water interface. A similar model was described by Leistra (1977). Although such a model appears to be conceptually pleasing, the model parameters need to be determined for each set of experimental conditons (van Genuchten et al., 1977; Rao et al., 1979, 1980 a,b) for the same soil column.

Transformations

Considerable research effort has been directed towards an investigation of transformations, metabolic pathways, and persistance of pesticides in soils. Several excellent reviews of this research are available (e.g., Crosby, 1973; Kaufman, 1976; Laveglia and Dahm, 1977). However, very few publications provide sufficient data suitable for a quantitative analysis of pesticide degradation in soils. Experimental investigations of simultaneous transport and transformations of pesticides in soils, under laboratory or field conditions, are not common. Pesticide degradation rates reported in the literature generally are measured under laboratory incubation conditions.

Based upon an exhaustive literature search, Ou et al (1980) calculated the first-order rate coefficients (k_d) and half-lives ($t½$) for degradation of a broad spectrum of pesticides in soils. Their data is summarized in Table 4. Field data are based on the dissappearance of the parent compound (solvent-extractable), while laboratory data are for mineralization (rate of $^{14}CO_2$ evolution from ^{14}C-labeled compounds) or for parent compound disappearance under aerobic or anaerobic incubation. In most cases, half-lives under field conditions are smaller than those under laboratory conditions (Table 4). Laboratory studies are generally designed to characterize a single degradation process, while under field conditions, several processes can lead to parent compound disappearance (e.g. volatilization, microbial degradation, leaching).

It is important to note that the coefficients of variation (% CV) in Table 4 are about 60-80%. Considering the fact that the degradation rates included in Table 4 cover a range of soil types and environmental conditions, the % CV values are surprisingly small. The data in Table 4 suggest that for a majority of pesticides, the degradation rate coefficient can be estimated within a factor of 2 or 3, using the database presently available.

FIELD-SCALE SIMULATION MODELS

Several models with varying degrees of complexity and conceptualization of the system processes can be developed. However, numerical solutions of such complex models require large amounts of computer time. Methods to independently measure the model input parameters are also inadequate.

Table 4. First-order rate coefficients (k_d) and half-lives ($t_{1/2}$) for degradation of pesticides under laboratory and field conditions. (From Rao and Davidson, 1980).

Pesticide		Rate Coeff. (day^{-1})		Half-Life (days)	
		Mean	%CV	Mean	%CV
A. HERBICIDES					
2,4-D	Lab.*	0.066	74.2	16	56.25
	Lab.	0.051	23.5	15	33.3
	Field	3.6	83.3	5	100.0
2,4,5-T	Lab.	0.029	51.7	33	66.7
	Lab.*	0.035	82.9	16	68.8
ATRAZINE	Lab.*	0.019	47.4	48	68.8
	Lab.	0.0001	70.4	6900	71.5
	Field	0.042	33.3	20	50.0
TRIFLURALIN	Lab.*	0.008	65.5	132	82.6
	Lab*(anaerobic)	0.025	-	28	-
	Lab.(chain)	0.0013	-	544	-
	Field	0.02	65.0	46	41.3
BROMACIL	Lab.*	0.0077	49.4	106	42.5
	Lab.	0.0024	116.2	901	116.2
	Field	0.0038	100.0	349	76.8
TERBACIL	Lab.*	0.015	33.3	50	26.0
	Lab.	0.0045	124.0	679	124.5
	Field	0.006	55.0	175	88.6
LINURON	Lab.*	0.0096	19.8	75	18.7
	Field	0.0034	41.2	230	29.3
DIURON	Lab.	-	-	-	-
	Field	0.0031	58.1	328	64.6
DICAMBA	Lab.*	0.022	80.2	14	85.7
	Lab. (ring)	0.0022	-	309	-
	Lab. (chain)	0.0044	-	147	-
	Field	0.093	16.1	8	12.5

(Continued)

Table 4. Continued

Pesticide		Rate Coeff. (day^{-1}) Mean	%CV	Half-Life (days) Mean	%CV
PICLORAM	Lab.*	0.0073	58.9	138	67.4
	Lab.	0.0008	111.3	8600	184.2
	Field	0.033	51.5	31	77.4
DALAPON	Lab.*	0.047	-	15	-
TCA	Lab.*	0.059	103.4	46	119.6
	Field	0.073	-	22	-
GLYPHOSATE	Lab.*	0.1	121.0	38	139.5
	Lab.	0.0086	93.0	903	191.8
PARAQUAT	Lab.*	0.0016	-	487	-
	Field	0.00015	-	4747	-
B. INSECTICIDES					
PARATHION	Lab.*	0.029	48.3	35	82.9
	Field	0.057	101.8	18	44.4
METHYL PARATHION	Lab.*	0.16	-	4	-
	Field	0.046	-	15	-
DIAZINON	Lab.*	0.023	108.7	48	62.5
	Lab.	0.022	-	32	-
FONOFOS	Lab.*	0.012	-	60	-
MALATHION	Lab.*	1.4	71.4	0.8	87.5
PHORATE	Lab.*	0.0084	-	82	-
	Field	0.01	30.0	7.5	24.0
CARBOFURAN	Lab.*	0.047	87.2	37	94.6
	Lab.	0.0013	-	535	-
	Lab.*(anaerobic)	0.026	50.0	44	95.4
	Field	0.016	87.5	68	61.8

(Continued)

Table 4. Continued

Pesticide		Rate Coeff. (day^{-1}) Mean	%CV	Half-Life (days) Mean	%CV
CARBARYL	Lab.*	0.037	56.8	22	40.9
	Lab.(chain)	0.0063	101.6	309	91.9
	Field	0.10	79.2	12	91.7
DDT	Lab.*	0.00013	130.8	1657	98.3
	Lab.*(anaerobic)	0.0035	82.9	692	123.4
ALDRIN and DIELDRIN	Lab.*	0.013	-	53	-
	Field	0.0023	100.0	1237	198.4
ENDRIN	Lab.* (anaerobic)	0.03	53.3	31	61.3
	Field(aerobic)	0.0015	-	460	-
	Field (anaerobic)	0.0053	-	130	-
CHLORDANE	Field	0.0024	104.2	1214	202.1
HEPTACHLOR	Lab.*	0.011	-	63	-
	Field	0.0046	119.6	426	82.6
LINDANE	Lab.*	0.0026	-	266	-
	Lab.(anaerobic)	0.0046	-	151	-
C. FUNGICIDES					
PCP	Lab.*	0.02	60.0	48	60.4
	Lab. (anaerobic)	0.07	44.3	15	100.0
	Field	0.05	-	14	-
CAPTAN	Field	0.231	-	3	-

*These rates are based on the disappearance of solvent-extractable parent compound under aerobic incubation conditions, unless stated otherwise.

Use of such comprehensive simulation models at a field-scale is confounded by two major problems. First, the soil physical, chemical, and biological characteristics vary spatially as well as temporally even within a single field. For example, soil-hydraulic conductivity, solute dispersion coefficient, average pore-water velocity, and similar flow "intensity" parameters are log-normally distributed (Nielsen et al., 1973; Biggar and Nielsen, 1976). Therefore, estimates of these parameters are prone to considerable errors unless a large number of samples are taken (cf. Warrick et at., 1978). Most simulation models consider the model parameters to be deterministic and do not accomodate their stochastic nature. Second, the field-measured values of model output parameters (e.g., pesticide concentration distribution in the soil profile) also vary considerably owing to soil heterogeneity. Such variability is expected to be larger when an entire watershed is sampled as compared to when a small field is sampled. Thus, in using simulation models at a field-scale, we must recognize the limitations imposed by uncertainities in the measured data used for model verification as well as the uncertainity in model input parameters and the associated confidence limits that should be placed on the model data output.

Under field conditions, the pesticide behavior is determined by a multitude of dynamic processes which occur simultaneously. A comprehensive field-scale simulation model should, ideally, couple in an appropriate manner, the inter-relationships between these processes. However, time-varying boundary conditions (e.g., rainfall, pesticide applications) can not be precisely specified under field conditions. The very complexity of the field problem and the soil heterogeneity suggest that we must look for much less accuracy in simulations of field experiments compared to laboratory experiments. Based upon experiences with development and testing simulation models for describing nitrogen dynamics in the crop root zone (Rao et al., 1980c), it appears that fairly simple models may be able to provide sufficiently accurate predictions of the fate of pesticides for field-scale applications.

A simple model for pesticide dynamics in soils should, at the minimum, include the following processes: (I) water and solute transport, (II) adsorption-desorption and, (III) degradation. Fairly simple approaches, based on the "piston displacement" concepts, could be successfully used to describe water and pesticide transport (e.g. Rao et al., 1980c). Approximate analytical solutions are also available to compute pesticide concentration distribution profiles during water infiltration and redistribution (DeSmedt and Wierenga, 1978). Techniques for approximating transient soil-water and solute transport by a steady-state flow model are discussed by Wierenga (1977). The simplest adsorption-desorption model is the equilibrium linear isotherm (Model 1.1, Table 1). Flow-velocities encountered under field conditions are usually much smaller than those used in laboratory soil column experiments. Thus, with increased contact times between pesticide molecules and the soil surfaces (adsorption sites), the assumption of equilibrium conditions may be more acceptable. An alternate approach would be to use Model 1.6 (Table 1) and define the FREQ parameter as a function of the average pore-water velocity. The degradation of pesticides can be described fairly well by simple first-order kinetics, where the rate coefficient combines the rates of different processes responsible for pesticide dissipation. A constant value for this "global" rate coefficient for degradation appears to be satisfactory (Table 4). However, rate coefficient values can be made a function of soil temperature and soil-water potential following the approach proposed by

Walker (1976 a,b). An important process not included in the above discussion is the plant uptake of pesticides by weed and crop species. We are not aware at this time of any efforts to model this process.

From the large number of field studies conducted on pesticide persistance, only a limited amount data could be used for model verification. Therefore, it is difficult to assess whether or not simplified models are acceptable. The movement, retention, and degradation of propyzamide herbicide during a 100-day period in field plots was described by Leistra et al (1974) using a simple steady-state flow model, Eq. [3], with linear equilibrium adsorption (Model 1.1) and first-order degradation rate (Model 3.1). Similar experiments should be carried out to provide additional data for testing similar simple models. The very accuracy with which laboratory measurements can be made and our mathematical ability to devise complex simulation models seems to be diverting our attention from the development and testing of simple models for field-scale application. Such models are not only easy to design, but necessary input data can be provided from existing data bases. The importance of continued basic laboratory research on processes determining pesticide dynamics in soil-water systems, however, cannot be over-emphasized.

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APPENDIX

C	Solution-phase concentration (ML^{-3})
C_m	Maximum solution concentration (ML^{-3})
D	Pesticide dispersion coefficient (L^2T^{-1})
FREQ	Fraction of adsorption sites in equilibrium
h	Soil-water potential (L)
$K(\theta)$	Soil hydraulic conductivity (LT^{-1})
k_1, k_2, k_3	Empirical adsorption isotherm constants
k_{d1}, k_{d2}	Degradation rate constants (T^{-1})
k_r	Adsorption-desorption rate constant (T^{-1})
q	Darcy soil-water flux (LT^{-1})
Q	Sink term for pesticide degradation ($ML^{-2}T^{-1}$)
S	Adsorbed-phase concentration (MM^{-1})
S_1	Adsorbed concentration on "fast" sites (MM^{-1})
S_2	Adsorbed concentration on "slow" sites (MM^{-1})
S_i	Initial adsorbed concentration (MM^{-1})
S_m	Maximum adsorbed concentration (MM^{-1})
t	time (T)
$t_{1/2}$	Half-life for pesticides in soil (T)
U	Sink term for soil-water uptake by roots (T^{-1})
v	Average pore-water velocity (LT^{-1})
z	Distance (L)
θ	Volumetric soil-water content (LL^{-3})
ρ	Soil bulk density (ML^{-3})

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STATE OF ART OF MODELING OF THE WATER BALANCE PROCESSES IN THE AGRICULTURAL FIELD AND WATERSHED.

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INTRODUCTION.

A topic discussed in this paper is concerned with mathematical models; physical models have become obsolete as practical tools in modern agricultural hydrology.

Regarding present situation in the field of mathematical modeling, it is obviously impossible to enlist and analyse all existing models which might be used for the simulation of hydrological processes in an agricultural area.In general,it can be said that a reliable hydrologic model should be capable to simulate any phase of the hydrologic cycle in such a way that an output from it can serve as an input into specialised agricultural model.However,as it will be seen from the paper of Dr Shvytov,even the models which have been considered as advanced in many ways,have certain limitations for a direct application in the field of agriculture.Attempts to test best models in the world on equal data resulted in the differences up to 400 per cent.

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WHAT CAN BE EXPECTED FROM A WATER BALANCE MODEL IN AN AGRICULTURAL APPLICATION ?

Before answering this question let us provide an example from an experimental agricultural station at Michalovce in eastern part of Czechoslovakia,in the vicinity of which two hundred thousands hectars of land will be intensively used for the production of crops.When there was formulated a request to apply a mathematical model on the data from pilot agricultural scheme,the processes to be simulated were as follows:

a.Groundwater level movement calculation and real time forecast of it for the management of alternative irrigation/drainage system.

b.Real time forecast of spring soil moisture in the zone of areation,for the determination of the period during which the spring works should be performed.

c.Simulation of the consumption of water by various types of plants and its seasonal development and water content in soil after harvesting.

These and other problems require to simulate simultaneously some other processes which may not be adirect matter of interest of agriculturalists.By instance,the simulation of surface runoff volume and its distribution is necessary for the estimation of the amount of water which will remain available after the rain to crops.Soil freezing and thawing process at the end of winter significantly determines the paths for water falling as a spring rain or from snowmelt and should become a part of the model as well.

Beside that the simulation of the hydrological cycle should be rather based on wider aspects of the hydroecological conditions of the region than on more or less specific conditions of a single field.This means that a behaviour of biotic materials,abiotic materials and gradient conditions in a regional scale should be involved into the model.

It can be concluded that before an application of any model agriculturalists should be able to set up certain criteria in accordance with solved problem and carefully test among many available models to which extent they are able to meet them.

C O N S T R A I N T S I N T H E W A T E R B A L A N C E S I M U L A T I O N .

For the purpose of this meeting it could be found perhaps more practical to discuss rather the limitations of present water balance modeling than the positive factors of it.As a main reason for it is a fact, that often,due to the problems unexpected at the beginning,a practical application of any model can easily fail or be temporary delayed during the latter phase of the model application,when it would be much more difficult to switch from one model to another.

Few examples of possible limitations are given in this part.

1.Simulation of year-round conditions.

Physical and chemical processes which drive natural system toward various partial equilibria,are not limited to a certain period of a year,actually,they are far from being constant during a year.However, many water balance models are developed for the simulation under summer conditions i.e.situations when soil is unfrozen,uncovered by snow and air temperature rises above $0^{o}C$.Another models are specialised in winter regime or in the simulation of snow cover and its water content variability.Only few models are concerned with transient conditions of early winter or late autumn regimes.and/or late winter and early spring regimes when a significant part of agricultural works may start or be at the end.Thus simulation of transient conditions should be involved in the hydrological simulation.

2.Problem of an effective rainfall.

Many models simulate the distribution of surface runoff assuming that to obtain an effective rainfall is a minor problem.On the other side water balance models frequently pay a little respect to the formation of the hydrograph although the formation of high floods may sigificantly influence agricultural areas in the vicinity of the river.Similarly,models of soil moisture variability pay a little respect to other factors playing equally significant role in the hydrological cycle.

A problem of the occurence of surface runoff through overrecharged shallow groundwater aquifers is simulated very rarely even if such a type of process may signifxcantly influence leaching of the minerals from upper soil layers and accelerate or delay chemical processes in them.

3. Negelected role of the vegetational cover as a natural reservoir interacting between soil and surface.

A typical feature of many water balance models is an analysis of soil infiltration variability as depending on the duration and rate of rainfall. Role of the vegetation and interception as related to the soil moisture is frequently neglected and special models concerned with the interception simulate interactions between rainfall and vegetation only. Frequently is also omitted loss through evapotranspiration and evaporation from the surface of leaves and process of water release from plant surface to the ground. Thus an increased accuracy in the simulation of soil infiltration process becomes less effective when compared with the accuracy of some other factors.

Even less attention is paid to the seasonal fluctuation of the hydrological processes as depending on natural seasonal pattern of the vegetational changes and on harvesting. Actually, to feed a model with parameters characterising the vegetation is useless without rather difficult and complex field experiments. As an example of many approaches in this field can be given experiments of Aston(1979), Greenwood and Beresford(1979) and Balek and Pavlík(1977).

4. Problem of the water balance model output serving as an input into another models.

With few exceptions present hydrological models can not be used without further modifications for a direct use in various types of models simulating crop production, agricultural pollution, flux of nutrients etc. More effort will be necessary on the side of hydrologists to supply as a model output data describing in sufficiently short intervals and in quantitative terms water budget in zones and regions significant for agriculture.It is felt that a realistic water balance model should be able to supply daily and even hourly results of the water volume available as intercepted water,water accumulated in snow,water contributing to the erosional process as a surface runoff,water accumulated in upper moisture zone,in the zone of capillary rise and water which can be taped by the roots. Model should inform also whether a part of the water is frozen or not.Groundwater level should be simulated as well together with the information whether some water is available to produce baseflow. Potential and actual evaporation/evapotranspiration should become available always and evaporation from open water surface,plant leaves, soil surface and transpiration by vegetation should be given in separate values.

5.A discrepancy between the amount of data used for the calibration of the models and data available in agricultural fields.

An application of many models can easily be found as impossible, regarding the amount of data which they require as an input.Model-builders should be always aware that the quality and quantity of data available in field is not comparable with the data from experimental areas,From very few agricultural fields we can expect more data than daily rainfall,daily temperature and perhaps groundwater level.At some pilot schemes perhaps soil moisture measurements with additional meteorologic data of sunshine,air humidity,wind velocity and soil temperature can be obtained.Instead of blaming agriculturalists for having unsufficient data we should trace another possibilities of the simplification of models or adoption of existing models in such way that a wider application with limited data will become available. Such an approach does not mean necessarily a step back.An utilisation of rapidly developing remote sensing methods which can supply areally representative results which is possible to calibrate by using ground observations from a network of low density.

6.Problems of testing and optimalisation of the models.

Dooge(1978) stated that at least a part of the model research should be spent on the model testing than on the development of new models.It is true that the methods permitting to test reliability of models and optimalisation of parameters are not always considered as an equally valuable part of the model work.Some models only use trial and error method as a source of information on the selection of adequate parameters and model testing is limited to the data from experimental basins which in many cases have been already used for the model development. Perhaps some exception can be found in the field of stochastic models; on the other side these models are too theoretical for an agricultural application and require rather long input sequences of information. Often when the model appliedto another catchment,than an experimental field,fails to meet requested results and authors tend to blame rather an inadequacy of data than the model itself.As cited from Dooge:"Practitioner is faced by a cacophony of noise which in many cases can be interpreted as ..my model solves all problems."

On the other side,it should be stated that a limited information from standart network should not last forever and it is a responsibility of the practitioners to extent the observational network as much as possible.

7.Problem of the involvement of man's influence on the hydrological cycle.

There can be found special models concerned with one or several aspects of actual or hypothetical influence of man on the hydrological cycle(Green 1980).What is needed,however,is a standart model in which beside natural processes influence of man can be simulated simultaneously.In agriculture at least influence of irrigation and drainage, pumping and reacharge and changes of crops as they influence infiltration/interception together with the role of urbanisation should be involved into the water balance models.Also a role of changing agricultural techniques should somehow appear in the modeling.It can be said that an ability of the model to simulate man's role in water balance changes of an agricultural field should be one of the decisive factors when a selection among several models is made.

8.Transportation and regionalisation of results from an agricultural field.

This problem has become so significant in present hydrology that a whole part of forthcoming Unesco Symposium on the influence of man on the hydrological regime(1980) will be devoted to it.

Soon or later results obtained for a single field ,which may have an experimental character, are to be extended to vast areas of the region outside of field limits.However,at present hydrologists are unable to define boundaries of the validity of the achieved results.Neither there is an objective method for some more definite conclusion.A similar situation exists in the areal extension of the validity of collected data.A special book published by Unesco (1980) based on case studies may assist in the solution of such a problem.Principles of remote sensing and satellite hydrology(WQB 1980), already applied to some projects,may contribute significantly toward the solution of this problem.

9.System approach application.

In some cases a problem may arise not from the model itself but from the paths leading to its successful application.Working methods of system engineering approach should be applied whenever possible. An example of such an approach based on the conclusions of Buras(1972) consists of following points:

a.Definition of the problem to be solved by the model work,results from a close cooperation between practitioner and modelbuilder.

b.Identification of data available for the model results from the survey in archives,yearbooks,reports and databanks.

c. Identification of the simulated system, field, area, consists of field survey, identification by maps, analysis of existing projects, reports and papers concerned with regional problems, soil, hydrological and hydrogeological survey, ecological analysis and study of the vegetational pattern. Other means of identification should be used when available.

d. Identification of constraints in the model work, results from the appreciation of computer facilities, manpower, budget etc.

e. Selection of the model or alternatively rejection of the model application should not be made before previous problems have not been adequately solved.

f. Proposals for further extensions of the observational network and extension of the identification of the system when the model will be used for managerial purposes.

C O N C L U S I O N S .

We can conclude that before any selection of the model for agricultural purposes, all possible limitations should be considered. Only some of them, based on the personal experience of the author, have been discussed in this paper. Rather the limits of present state of art than the state of art in modeling itself have been discussed here, however, experience with the application of various types of models in the agriculture and other fields have resulted in a point of view which prefers to be more sceptical at the beginning of the model work than at the end of it.

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MODEL OF SURFACE RUNOFF FROM SLOPE

Miloš H o l ý [1)]

A b s t r a c t

The method of deriving the model of surface runoff is based on the mathematical expression of the basic laws of the movement of water. The equation of continuity is derived from the equation expressing the quantitative relations between water flowing down slopes, water falling on the soil surface in form of precipitation and water infiltrating into the soil. The equation of motion is derived considering the effect of the most important forces affecting the erosion process /water gravity, hydrostatic pressure, friction on the slope surface, the impact of rain drops impinging on the soil surface/. Both equations form a system of non-linear partial differential equations with two unknown functions expressing the depth and velocity of the movement of water along the slope in dependence on their location on the slope and on time. The input variable of the model are the intensity and direction of the impinging raindrops, the intensity of infiltration and the physical characteristic of the slope /gradient, lenght and properties of soil surface/.

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The determination of surface runoff is one of the principal stages in the evaluation of non-point pollution. Its dependence on many natural and antropogenic factors makes this very difficult task. A number of solutions to the problem have been offered whose concrete field application has proved difficult and generalizing and whose results do not allow effective measures to be taken in localities which are the principal contributers to such pollution.

In some cases it is therefore purposeful to study not the catchment area as a whole but its individual slopes such as significantly contribute to non-point pollution and whose inclusion in the average conditions of the catchment in some cases, namely in small catchments, makes it very difficult to pinpoint their considerable contribution to the resulting pollution.

One possible solution is the model of surface runoff from the slope whose construction is based on the physical laws of the movement of water.

The following assumptions are used for expressing the basic relations

- the slope surface is a plane forming the angle α with the horizontal plane

- the slope is infinitely wide
- the intensity of precipitation impinging on the slope is even throughout and is merely a function of time
- the intensity of the water infiltrating into the soil is a function of time.

The average velocity of water running of the slope was considered for any point of the slope and at any time.

The laws on the conservation of matter and momentum apply for water running off from the slope. From these relations proceeds the equition of continuity and the equation of movement.

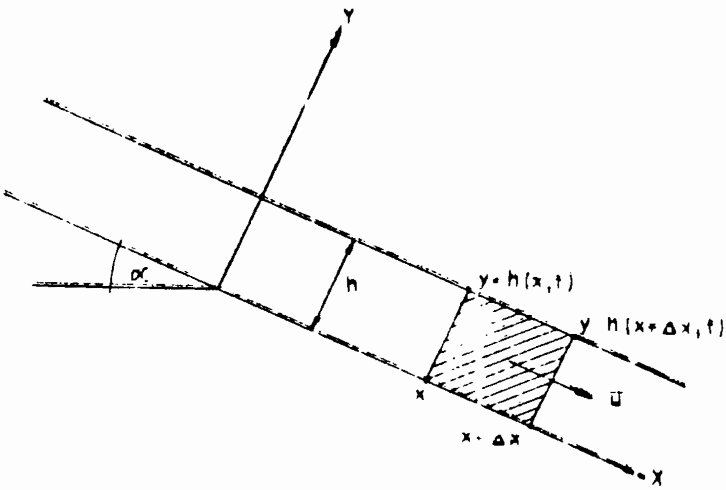

Fig. 1 Scheme for determination of equation of continuity

where X is the coordinate axis in the direction of the surface runoff /cartesian coordinates were used/

Y is the coordinate axis perpendicular to the surface runoff

α is slope gradient

h is height of surface runoff, it is the function of position and time $h/x,t/$

$\bar{u}$ is the average velocity of surface runoff in the direction of the X-axis

$r/t/$ is the intensity of precipitation related to the unit surface of the slope

$i/t/$ is the intensity of infiltration.

Considering elementary runoff on the slope in section $\langle x, x+\Delta x \rangle$ we shall investigate the changes which in this segment occur in the amount of water running off the slope in time interval $\langle t, t+\Delta t \rangle$. The velocity of the movement of water changes with the change of x,y,t.
For the vector of the velocity of the water running off the slope $\vec{w}$ it applies that

$$\vec{w} = [u(x,y,t), v(x,y,t)] , \qquad /1/$$

where u is the component of water velocity in the direction of X

v is the component of water velocity in the direction of Y

Component v is not significant for our problem as we are interested in the flow in the direction of the X-axis.

According to the law on the conservation of matter the difference between water flowing in and running off the slope in section $\langle x, x+\Delta x \rangle$ equals the increment of its volume. The increment is either positive or negative depending on which of the two components, i.e., the inflow or the runoff, is the prevalent factor.

The amount of water which flows into the considered segment in interval $\langle t, t+\Delta t \rangle$ is

$$\int_{t}^{t+\Delta t} \left(\int_{0}^{h(x,\bar{t})} u(x,y,\bar{t})\, dy \right) d\bar{t} \qquad /2/$$

In the same time interval the runoff from the same segment is

$$\int_{t}^{t+\Delta t} \left(\int_{0}^{h(x+\Delta x,\bar{t})} u(x+\Delta x,y,\bar{t})\, dy \right) d\bar{t} \qquad /3/$$

The amount of water in segment $\langle x, x+\Delta x \rangle$ will increase by precipitation by

$$\int_{t}^{t+\Delta t} \Delta x \; r(\bar{t})\, d\bar{t} \qquad /4/$$

and will be reduced by the infiltration of water into the soil

$$\int_{t}^{t+\Delta t} \Delta x \; i(\bar{t}) \, d\bar{t} \qquad /5/$$

The volume of water in the segment $\langle x, x+\Delta x \rangle$ in time t is

$$\int_{x}^{x+\Delta x} h(\bar{x}, t) \, d\bar{x} \qquad /6/$$

The volume of water in the same segment in time $t+\Delta t$ is analogically

$$\int_{x}^{x+\Delta x} h(\bar{x}, t+\Delta t) \, d\bar{x} \qquad /7/$$

According to the law on the conservation of matter it applies that

$$\int_{t}^{t+\Delta t} \left\{ \int_{0}^{h(x,\bar{t})} u(x,y,\bar{t}) \, dy - \int_{0}^{h(x+\Delta x,\bar{t})} u(x+\Delta x, y, \bar{t}) \, dy + \Delta x \left[r(\bar{t}) - i(\bar{t}) \right] \right\} d\bar{t} = \int_{x}^{x+\Delta x} \left[h(\bar{x}, t+\Delta t) - h(\bar{x}, t) \right] d\bar{x} \qquad /8/$$

If we introduce into furhter calculations the mean profile velocity of the surface runoff and assume that h and $\bar{u}$ have continuous derivations of the second order the equation of continuity may be written

$$\frac{\partial(\bar{v}h)}{\partial x}(x,t) + \frac{\partial h}{\partial t}(x,t) = r(t) - i(t) \qquad /9/$$

In order to derive the equation of movement we shall proceed from Newton's second law of motion and shall study the forces which act on water in the considered elementary section of the investigated slope

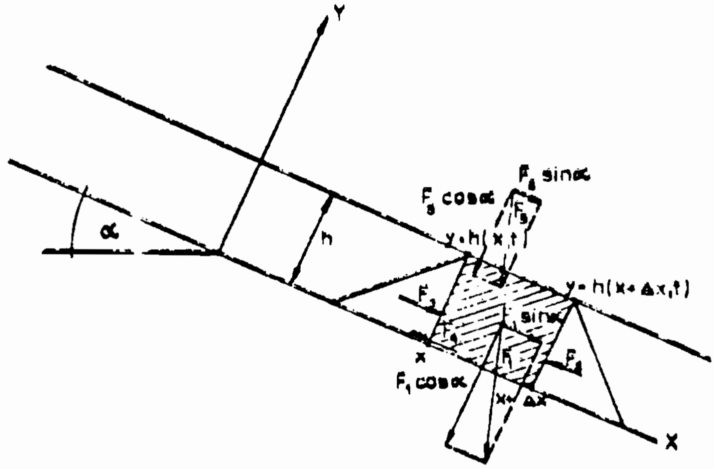

Fig. 2. Scheme for determination of equation of movement.

F_1 is gravity of water in the elementary segment

F_2 is pressure force acting on the water in the elementary segment at distance $x+\Delta x$

F_3 is pressure force acting on the water in the elementary segment at distance x

F_4 is friction force

F_5 is force of water drops impinging on the surface

The magnitude of the individual forces may be expressed as follows

$$F_1 \sin\alpha = \rho g \sin\alpha \int_{x}^{x+\Delta x} h(\bar{x}, t)\, d\bar{x} \qquad /10/$$

where ρ is water density

$$F_2 = \int_{0}^{h(x+\Delta x, t)} p(x+\Delta x, y, t)\, dy \qquad /11/$$

$$F_3 = \int_{0}^{h(x,t)} p(x, y, t)\, dy \qquad /12/$$

$$F_4 = \Delta x\, \tau \qquad /13/$$

$$F_5 = \Delta x\, \rho\, r(t)\, v^* \qquad /14/$$

τ is the function expressing tangential stress

v^* is the velocity of the impingement of raindrops

Newton's law on motion $\frac{d}{dt}(m\, \vec{u}) = \vec{F}$ may for the investigated case be expressed

$$\Delta m \frac{d\bar{u}}{dt} = F_1 \sin\alpha - F_2 + F_3 - F_4 + F_5 \sin\alpha \qquad /15/$$

If suitable expressions for the forces acting on the elementary segment are introduced into Newton's law on motion /15/ we shall obtain an equation for the movement of water running down the slope

$$h(x,t)\frac{\partial \bar{u}}{\partial t}(x,t) + h(x,t)\,\bar{u}(x,t)\frac{\partial \bar{u}}{\partial x}(x,t) =$$
$$= g\sin\alpha\, h(x,t) - g\cos\alpha\, h(x,t)\frac{\partial h}{\partial x}(x,t) -$$
$$- g\cos\alpha\, h^{*}(t)\frac{\partial h}{\partial x}(x,t) - \frac{\tau(h,\bar{u})}{\rho} + r(t)\,v^{*}(t)\sin\alpha \qquad /16/$$

where h is the haight of runoff in the perpendicular direction

v^{*} is the average velocity of impinging waterdrops.

Any consideration of initial conditions must proceed from the fact that the investigated action starts in time $t = 0$. At this point in time precipitation starts acting on the slope surface and the surface runoff is formed. The unknown functions h and $\bar{u}$ have zero value for all x's.

$$h(x,0) = 0 \qquad /17/$$

$$\bar{u}(x,0) = 0 \qquad /18/$$

The determination of boundary conditions depends on the distance between the investigated segment from the water divide of the slope. For the general distance of this segment from the water divide $x_o > x$ it is necessary to determine

$$h \left(x_g , t \right) \qquad /19/$$

$$\bar{u} \left(x_g , t \right) \qquad /20/$$

in accordance with the conditions affecting the formation of the surface runoff.

From the physical point of view it is evident that the system od equations established by the equation of continuity and the equation of movement with the given initial and boundary conditions gives a clearcut solution.

The result of the solution is to obtain the value of the velocity of surface runoff $\bar{u}$ and its height h at any point on the slope. From these values it is then possible to obtain for any profile of the slope the volume of surface runoff, and at the lowest profile of the slope the volume of the total runoff from the slope.

The values which must be substituted to the equation may be obtained by the calculation of known relations, by measurements or by analogy with conditions similar to those which are being investigated. They include: the intensity and duration of the precipitation, the velocity of raindrops impinging on the surface of the slope, the infiltration of the water into the soil, the function expressing tangential stress /determined using laboratory methods/ . Research workers of the Faculty of Civil Engineering of the Czech Technical University in Prague/engrs. Váška, Vrána and Mls/ have made a detail analysis of these variables and instructions for their determination have been issued based on these analyses.

A programme in BASIC language has been constructed for the solution of the system of equations.

Conclusions

The results thus obtained may be used as the basic input data for an arbitrary erosion model possibly for a model of the transport of chemical substances carried by the surface runoff. The problem of the whole catchment is then solved by gradually matching the runoff from the individual slopes.

A HIERARCHICAL APPROACH TO AGRICULTURAL PRODUCTION MODELING

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Introduction

The main objective of land evaluation and one of the objectives of production research is to indicate and elaborate options for development in agriculture. The actual development course in a given region depends not only on technical feasibilities, but also on the socio-economic situation and on politically motivated and therefore changing policies. To keep all options open as long as possible, the method of analyzing the system should be designed in such a way, that the introduction of normative concepts is postponed to the latest possible stage. In this way, entanglement with social and economic problems can be avoided in the early stages of work, the problem being already sufficiently complex without this.

Of course, all the elements of the agricultural production system are interrelated but the actual relationships are in many cases only partly understood. In order to use this partial knowledge as efficiently as possible, a hierarchical approach is adopted. In this schematized approach, the number of factors that has to be taken into account for the estimation of crop production at the highest hierarchical level is substantially reduced by assuming that constraints, that can feasibly be removed, have indeed been eliminated. At lower hierarchical levels, the factors taken into account at a higher level remain fixed and the effect of limiting factors, originally supposed to be eliminated is taken into consideration.

The analysis is elucidated with the help of a schematic presentation of the procedure followed and a more detailed discussion of the most important aspects. Finally, an application will be discussed for the synthesis and analysis of farming systems.

A Schematic Presentation

The hierarchical procedure is schematically presented in Figure 1. The rectangles in the second row represents the factors that ultimately determine the production potential. Climate and soil are fixed properties for a given region and, in combination with the level of reclamation, characterize the land quality level. The characteristics of agricultural crops may be changed by breeding, the scope for improvements in this respect being reasonably well-defined (de Wit et al., 1979). For a given land quality level, the yield potential is therefore fixed for a fairly long period of time, and it may be calculated with reasonable accuracy.

In the further analysis, the goal should not be the definition of a production function describing the relationship between the yield and all possible combinations of growth factors, since, by the nature of the agricultural production process, no unique solution to such a production function exists. Instead, a reasonable combination of growth factors should be established that will result in the yield level that is plausible in view of the present know-how. Thus, the yield level is considered concurrently as a dependent variable, determined by crop characteristics and land quality level, and as an independent variable, dictating the required input combination. This is reflected by the direction of the arrows in the diagram: towards the yield level as well as away from the yield level.

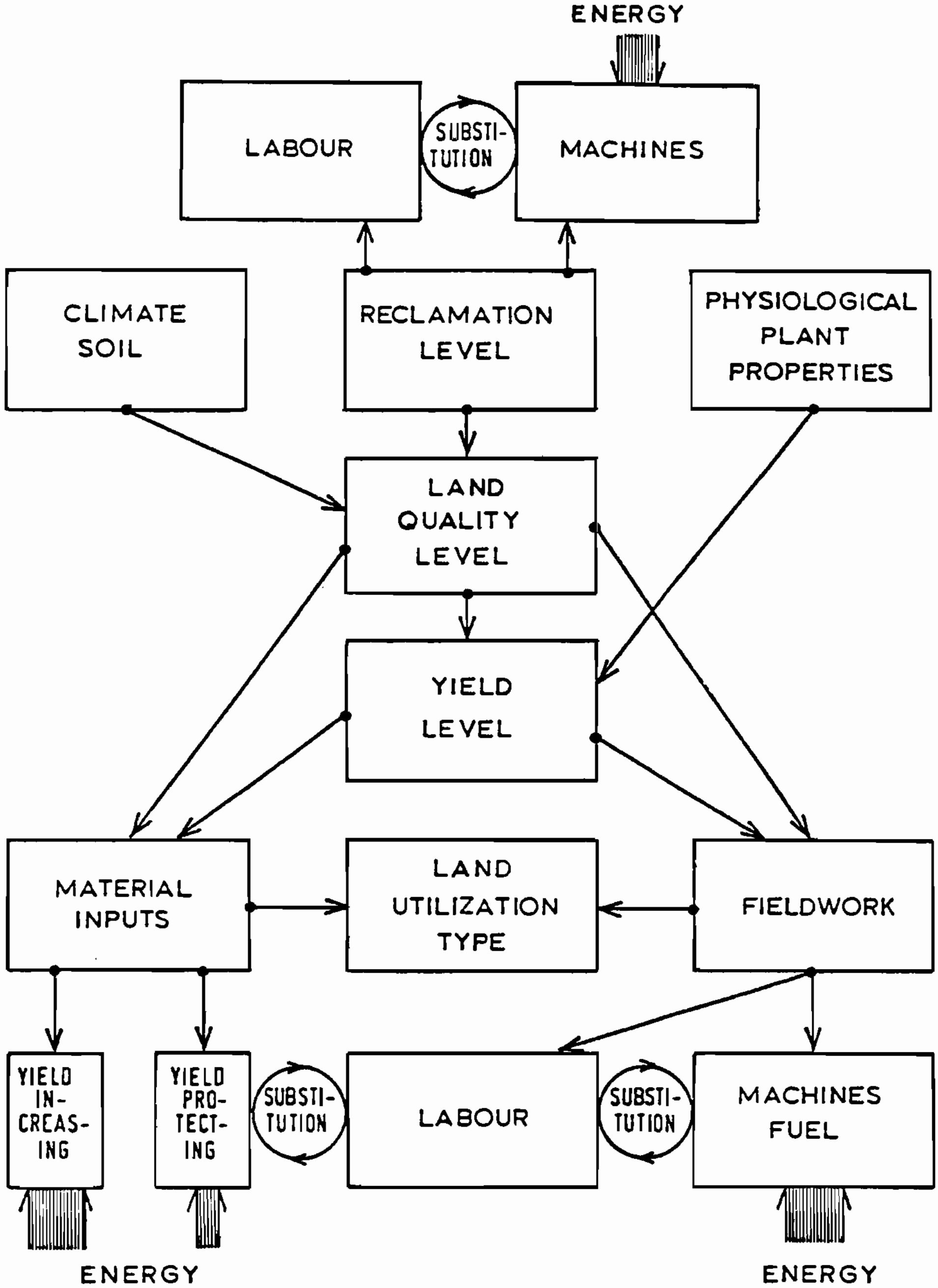

Figure 1. A schematic presentation of the analyses.

With respect to the required inputs, a distinction is made between field work and material inputs. The necessary field work can be described in physical terms, for example, frequency of plowing, harrowing, weeding, the length of supply and transport lines, etc. The time required for these activities is to a large extent independent of the required yield level as they are needed anyway. The time requirements are, however, strongly influenced by soil type and weather conditions. In performing the field work, considerable substitution is possible between manual labor and activities relying on heavy mechanical equipment and their associated fossil energy requirements.

The material inputs are further divided into yield-increasing materials, and yield protecting materials. The required amounts of yield-increasing materials, such as water, minerals and nitrogen, are directly influenced by the required yield level, soil type and weather conditions, particularly rainfall. Characteristic for these production materials is, that they cannot be substituted by labor. This is in contrast to the yield protecting materials, biocides, for which alternatives, e.g. labor-intensive weeding versus the use of herbicides and manual insect eradication versus spray-killing are possible.

The rectangle "land utilization type" indicates a preliminary synthesis of the various interacting factors which play a role in the design of crop rotations on a given acreage. Farming systems are built up from elements of different land quality levels under various types of land use. The existence of specific farming systems is not only determined by the technical feasibilities but also by the socio-economic environment. We shall return to the subject later.

Land Quality Level

The land quality level represents the integrated effect of various land qualities. It is, on the one hand, determined by intrinsic soil properties and the prevailing weather conditions and, on the other hand, by the degree of soil amelioration. In the schematized set up, four levels of soil amelioration are being distinguished.

The lowest level refers to land in an almost virgin condition and allows only cultivation with extended fallow periods. Hardly any land improvements have been carried out. Water supply is totally dependent on rainfall and flooding is avoided only if possible by simple modifications of the topography. The next level provides opportunities for more permanent use with or without fallow periods. The moisture regime is again fully dictated by weather conditions. The distinction between these two levels depends to a large extent on natural differences. The next level pertains to land where improvements have been carried out, such as leveling, simple terracing and the construction of open ditches to control excess water. The final level refers to land in a favorable condition for crop growth, well leveled, with complete water control and the necessary infrastructure. Sufficient water is available to allow unrestricted irrigation.

Apart from defining the present status of the land in a given region, it is also important to quantify the reclamation activities necessary to bring the land to another land quality level. This applies especially to the amount of vegetation and stones to be removed, number of m^4 (volume x distance), soil to be moved and the infrastructure that must be built. This aspect of the analysis is represented in the first row of the diagram in Figure 1. Reclamation can be carried out with manual labor. However, that is often only a theoretical possibility, since most of the acreage that could easily be reclaimed has already been developed, whereas the population density and hence labor availability in the remaining areas is often low. Even in China, one has come to the conclusion that it is almost inevitable to resort to the use of mechanical means. The activities to be performed are therefore analyzed for various technological levels in terms of the available equipment.

Production Level

The highest hierarchical production level can not always be achieved in practice. By definition, it is the level at which water, minerals, and nitrogen are not limiting to growth. Crop yield is then only determined by the type of crop, the prevailing level of irradiance, and the temperature regime. Simulation models to calculate the potential growth rates of healthy closed green crop surfaces are available and have been validated under a wide range of conditions (de Wit et al., 1978). These models also provide potential transpiration rates, so that the total water requirement may be obtained for any given combination of crop species and climatic conditions. Combining the above with the rainfall regime and physical soil properties also yields the irrigation requirement for optimum growth conditions. For most regions, sufficient experimental data are available to judge the feasibility of growing the major crops and to define the so-called cropping calendars: time of sowing, emergence, flowering, ripening, etc. Theoretical consideration and field data may then be combined to develop simple calculation models for the relevant crops, yielding the time course of dry matter production and transpiration, and economic yield as outputs. The model for bunded rice by van Keulen (1976) is a good example. The results of these models are directly applicable under irrigated conditions, but are also used as the basis for yield calculations in sub-optimum situations.

For the calculation of the second hierarchical production level, it is also assumed that nitrogen and minerals are optimal, but the influence of moisture availability to the crop is taken into account. The degree of water control is such, that temporary water-logging can be avoided by appropriate drainage. Water supply to the canopy is dependent mainly on rainfall and, to a limited extent, on supplementary irrigation. The physical properties of the soil and the climatic conditions are of major importance. On the basis of these data, the water balance is calculated to enable determination of periods with insufficient water supply to the canopy, resulting in reduced transpiration and consequently sub-optimum growth rates. Such calculations may be performed on a daily basis (van Keulen, 1975, Makkink and van Heemst, 1975) for periods of some weeks, up to a month (Arbab, 1972, Buringh et al., 1979). The purpose of the simulations and the degree of detail of the available data dictate the resolution of the calculations. The model is set up such, that the moisture status of the top soil is tracked separately to enable the calculation of the number of workable hours in the field: an important parameter in the farming systems synthesis.

At the third hierarchical production level, not only periods of water shortage have to be taken into account, but also periods with excess water. At this level, the possibilities of run-on and water-harvesting are also of importance. The water balance in these areas is often so complex, however, that the present models can hardly cope with the situation. Maps and photographic material, interpreted with the help of experts acquainted with the local situation, may then provide additional information, since the situation is often close to the existing one.

Yield Increasing Inputs

A fourth hierarchical production level is obtained, when in each of the above situations the availability of nitrogen and minerals is also considered. Apart from the physical properties, other characteristics of the soil, such as organic matter content, cation exchange capacity, clay content, and mineralogical composition, have to be taken into account.

Hence, as the next step, the nitrogen supply is considered, assuming that the situation with respect to minerals is still non-limiting. This special status of nitrogen is due to the amounts required, its costs and its mobility in the soil-plant-atmosphere system.

The effect of nitrogen on production is analyzed by separating the relation between yield and application into two components: yield versus uptake and uptake versus application (de Wit, 1953), as in Figure 2. The relation between yield and uptake (quadrant B) is of the well-known saturation type but the relation between application and uptake is rectilinear

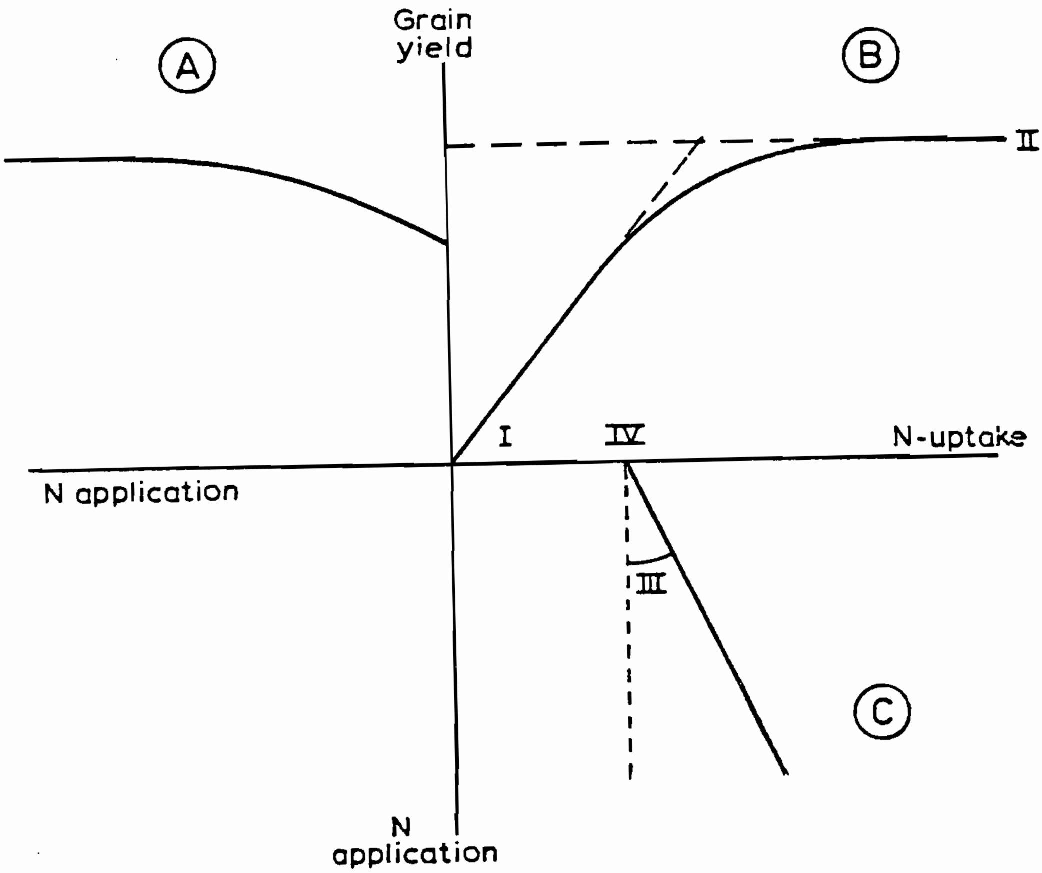

Figure 2: The relation between yield and nitrogen-application (A), desegregated in the relation between yield and nitrogen uptake (B) and nitrogen uptake and nitrogen application (C).

in the relevant range (van Keulen, 1977). Based on the presentation in Figure 2, the problem of nitrogen nutrition can be separated into four partial problems, schematically indicated by roman numerals in the graph.

The initial slope of the uptake-yield curve (I) is crop-specific and in most cases independent of soil type and weather conditions. For cereals, the value amounts to about 70 kg of seed per kg N absorbed by the crop. The maximum yield level (II), no mineral and nitrogen shortage, has been considered in the preceding section. The hierarchical build-up of the analysis requires the assumption that the water balance is independent of the nitrogen supply. This assumption is debatable, but quantitative treatment of the interaction between nitrogen supply and moisture balance is difficult and requires in most cases too much detailed knowledge of the actual growing conditions.

The moisture regime in the soil affects the processes of denitrification and leaching and, hence, the recovery of the applied nitrogen fertilizer. That is the fraction of the annual dressing taken up by the plant in its above ground parts, preferably calculated for an equilibrium situation where each year aproximately the same amount is applied. The recovery fraction of nitrogenous fertilizers may vary from a low of 0.1, when applied injudiciously or on poorly reclaimed soils to as much as 0.8 under favorable conditions and proper management.

The amount of nitrogen available from natural resources (IV) is often so low, that it may be obtained from available yield data, using slope I (van Keulen, 1977). For the time being, this is simpler and often more reliable than the use of existing models of nitrogen transformations. The grain yield of many cereal crops without any fertilizer application is around 1000 kg ha^{-1}, corresponding to a typical uptake of 14 kg N ha^{-1}. Depending on actual growing conditions, these amounts may vary by a factor or two. These differences in nitrogen availability from natural sources are negligible at the higher technological levels where chemical fertilizers are available, but they may mean the difference between food and famine in situations where these products are lacking.

For the elements Ca and Mg and to a lesser extent for P and K, the magnitude of the basic dressing is of major importance. The problem to be solved with respect to these elements can also be split up into a number of partial problems. Is a basic dressing required at the time of soil reclamation to achieve a sufficient fertility level, and what are the amounts involved? What is the magnitude of losses by fixation and leaching, how much is removed by the crop and what amounts have to be applied periodically to compensate for these losses?

Answering these questions for Ca and Mg hardly ever presents great problems but that does not imply that the fertilizer application itself is always simple: many acid soils are located at considerable distances from limestone formations. For potassium, the major criterion is the recognition of soils with high potassium fixing capacity.

Phosphate application without nitrogen fertilizer application often results in appreciable yield increases, but this leads inevitably to the withdrawal of considerable amounts of nitrogen and hence to depletion of the soil nitrogen store (Report PPS-project, 1980). Phosphate dressings should therefore be adjusted to the level of nitrogen application. In practice this is achieved with the aid of soil analyses, crop analyses and fertilizer experiments, but in prospective land evaluation studies the purpose is frequently quantification of the P requirement for land utilization types that do not yet exist. This requires a rather detailed analysis of the elements of the P cycle, as carried out by Cole et al. (1977) for organic phosphates and by Beek (1979) for inorganic phosphates. In the framework of the present study, attempts are being made to integrate these analyses in a model, but for the time being it is necessary to rely to a large extent on local experience.

Labor Requirements

During the calculation of potential yield levels, the number of workable hours is also estimated, which enables the scheduling of the crop calenders in time. It is, in general, relatively easy to indicate the activities that have to be carried out in the course of a crop growth cycle. The time required for these activities depends on the applied level of mechanization. Four such levels are distinguished: manual labor, animal traction, light two-wheeled mechanization and complete mechanization.

The task-times for recurring activities are reasonably well-established for mechanized operations (van Heemst et. al., in prep.). However, hardly any attention has been paid in agricultural research to manual labor and animal traction. At that level, data on time requirements are only approximative since they were inferred from sociological and anthropological studies.

Labor requirements at the various technological levels vary considerably. In hours per ha: 750 for spading or similar activities, 35 for ploughing with horses, 15 for ploughing with a two-wheeled tractor and 5 for ploughing with a normal tractor. One weeding with a hoe takes about 100 hours per ha but with herbicides and tractor-driven spray equipment only a few hours per ha. Pest and disease control virtually always involves biocides. The major problem here is not the estimation of the time requirements, but the estimation of the yield loss without control and hence the necessity of the operation.

In summary, it may be concluded that indicative task times are available at the four mechanization levels, but that the scatter in the basic data is such that without local knowledge, no meaningful differentiation can be made between various soil types, different levels of training and so on.

Synthesis of Farming Systems

The foregoing analysis results in tables containing the yield levels per region, per land quality level, per mechanization level and per crop, and the associated material inputs, the labor requirements in the course of the crop growth cycle, the number of workable hours and so on. This mass of data can be handled more meaningfully when summarized on the basis of farming systems. The farming systems which will develop in practice not only depend on the physical environment and the technical know-how, but also on the historically determined situation, the socio-economic environment, and the prevailing political aims. To analyze this complex situation, interdisciplinary research has been initiated, which is much more sophisticated than discussed here (Center for World Food Studies, Amsterdam/Wageningen). However, a more simplified approach, aiming at a more limited objective, may be helpful from a bio-technical point of view.

For this purpose, the analysis is limited to a family farm (a farmer, his wife, and two working children) and to four possible crop rotations with emphasis on cereals, root or tuber crops, fibre crops and seed legumes, respectively. For any given region, the specific crops that comprise the rotation are choosen on the basis of the farmers knowledge and research results obtained in the same or in comparable regions, the choice remaining partly arbitrary.

Questions that can now reasonably be answered from a biotechnical point of view are of the following type: What should be the size of the farm for maximum utilization of the available labor? During which periods in the season is labor availability a limiting factor, and can this constraint be removed by increasing the mechanization level? How much labor is idle, and during which periods, and is it possible to improve this situation by improving the land quality level or by growing more or other secondary crops? To what extent would the optimum farm size change upon variation of the ratio between the main crop and secondary crops in the rotation? Which yield increasing and yield protecting inputs are required, and in what quantities, and what should be the level of skill of the farmer? The answers should be judged, of course, in the light of the assumptions that explicitly or implicitly underlie the analysis.

In principle, 64 farming systems result from a combination of four land quality levels, four mechanization levels and four crop rotations. In practice, that number is never reached since in every region a considerable number of the combinations is not feasible for obvious reasons. Such a systematic approach enables a comparison between regions and countries. A comparison of the man/land ratio and the present levels of land quality and mechanization indicates also where feasible opportunities exist or where problems could develop. Which systems are economically feasible, or for other reasons acceptable or unacceptable, is outside the scope of this analysis.

Concluding Remarks

The present paper contains so many speculative elements that it is presented under the responsibility of only two authors. However, it would never have been completed without using the internal reports of other members of the Wageningen staff of the "Center for World Food Studies" (SOW): J.A.A. Berkhout, P. Buringh, P.M. Driessen, J.D.J. van Heemst, and J.J. Merkelijn.

Many aspects of the complex problem are actively elaborated, but the synthesis of farming systems is only in a preliminary stage. Here, the Wageningen members of the Center will have to supply the basic material for the Amsterdam members who are in charge of developing the social economic model components. At that level we are still struggling with an old problem: economists ask questions that technicians cannot answer, whereas the latter have answers to questions that are not asked by economists. But we are making progress.

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DETERMINISTIC MODELS FOR THE ECOLOGIC SIMULATION

OF

CROP AGRICULTURAL ENVIRONMENTS

by

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INTRODUCTION

Intensive agricultural activity is increasingly essential to our world today. Without these endeavors our world population cannot be properly fed and clothed. The fact that at present a large portion of the world's inhabitants does not receive an adequate diet only emphasizes the need to expand and intensify agricultural activities. Unfortunately, this development will be accompanied by negative impacts on the total physical - biological environment. Historical example has shown us time and again that these ecologic changes associated with agricultural development can be catastrophic and nearly irreversible.

The first and, therefore, most important agricultural activity in our food chain is crop production. The influence, direct and indirect, on our environment of crop production is enormous. Indirect influences, such as the removal of habitat and food sources for wild species of plants and animals, are not considered here. When the crop agricultural system is considered as a subecologic system of the total environment, we can then decompose the problem of studying the effects of agricultural development to observation and analysis of the crop ecologic system and its reciprical influences on the global environment. The influence vectors include energy and mass transfer. Crop production can change the climate and hydrologic cycle through such processes as evapotranspiration and the uptake or release of carbon dioxide. It can, as well, introduce into the global environment substances such as sediment, salts, nutrients and pesticides which stimulate or retard activities of other ecologic subsystems. An important element and the main mass transfer vector in the communication with the global environment is water. It is only with the atmosphere that gases and solids can be exchanged over the subsystem boundary without the aid of this vector.

The influence coupling of the crop agricultural system with the global environment is depicted in Figure 1. The crop system has been represented with two strongly coupled subsystems, plant and soil. This total system is quite dynamic with inputs and transfers changing continuously. Response and cycle times range from minutes to years depending on the process or influence vector considered.

The atmosphere inputs energy and carbon dioxide to the plant system and receives water vapor and oxygen in exchange. The soil system receives energy, water (precipitation), oxygen and some nutrients from the atmosphere and gives back water vapor and carbon dioxide. The airborne transfer of sediment into and out of the crop system is not depicted in Figure 1.

Man's inputs to the total system through his cultural (crop management) practicies include nutrients and pesticides to the plant system and water (irrigation), nutrients and pesticides to the soil system. He can, as well, directly manipulate the crop and soil systems through various cultivation and pruning activities. In return he harvests crops which remove mainly nutrients from the total system.

The soil and plant systems exchange nutrients and water for

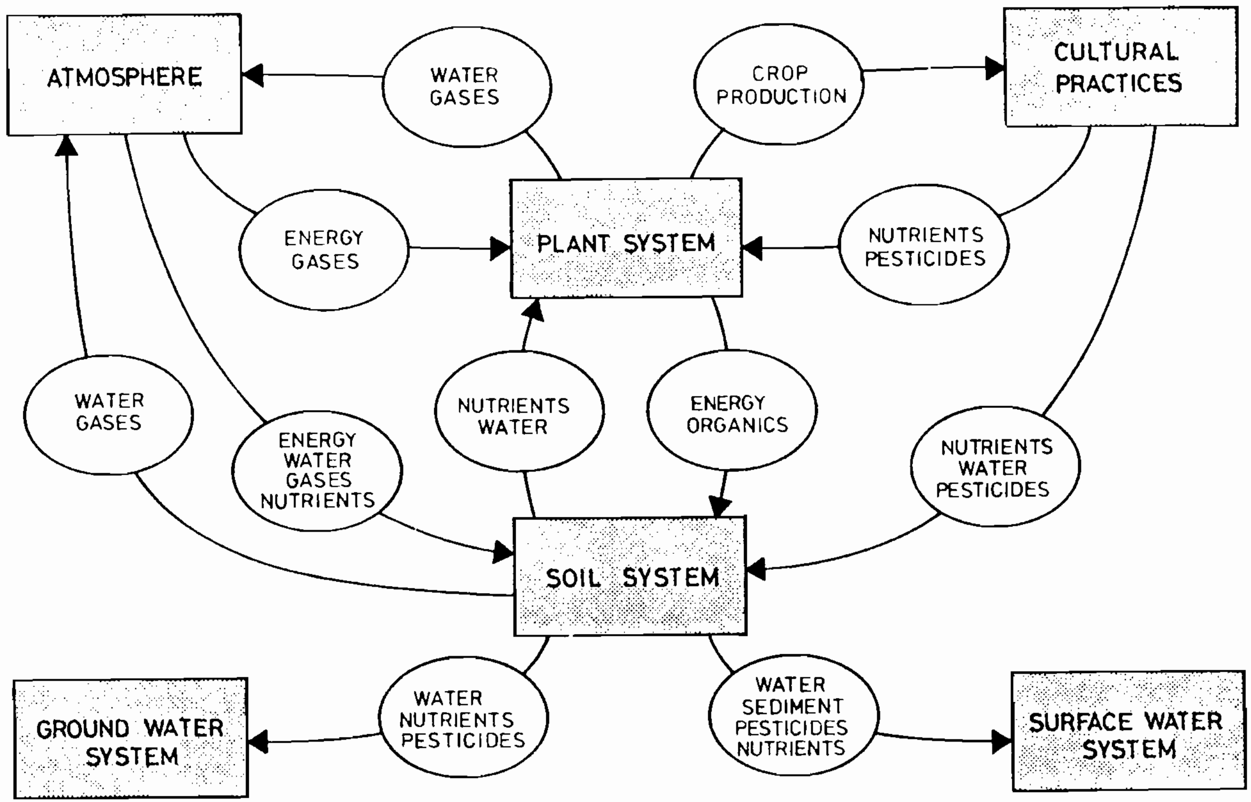

FIGURE 1. Crop system coupling with the environment.

plant energy and organic residues. Nutrients and pesticides are leached from the soil system through unsaturated and saturated flow of percolating subsurface drainage waters. Surface runoff of precipitation and irrigation water is an agent for the removal of eroded sediments, nutrients and pesticides from the soil system. Surface and subsurface discharges exist in both arid and humid climates: the relative magnitudes of each phenomenon shifts from one ecosystem to another, but each is a vector for pollutants to move into the total environment.

MODEL TYPES

The crop ecologic system can be described with single or sets of linked mathematical models. With models one can attempt to describe one or more of the coupling transfers depicted in Figure 1. Examples of traditional activities in the development of such models are applied nutrient - crop production models by agronomists or atmospheric energy - evapotranspiration and precipitation - runoff models by hydrologists. Recent research activity has expanded to include model descriptions of virtually every aspect of the crop system and its interaction with the total environment. These models can be broken into two broad classes, statistical models and causal or process-oriented models.

Statistical Models concern themselves soley with observed input and output and the significance of their correlation. Mathematical relationships are sought which simply allow for the best transfer of observed input to observed output. As these models are entirely empirical, they can only be constructed when sufficient data exists to produce mathematically significant relationships, and they cannot be extrapolated into regions where no measurement data exists. In other words, statistical models do not consider the total crop system inputs and outputs, just the strongly coupled sets of inputs and outputs of interest to the modeler. When using these models in environmental planning, the independent variables must contain those inputs which are available as planning variables. This is often a very serious problem, as in many fields we do not yet have enough quantitative experience at hand to build such relationships.

Causal or *process-oriented models* describe each significant physical, chemical or biological process which takes place within a system. Each process and its interrelationship to other processes is mathematically defined from our understanding of a system. Once the interconnected set of mathematical relationships has been set together, available measurements of inputs and outputs are used to inductively define the parameters or coefficients contained in each equation. Model calibration is rapidly becoming a recognized science unto itself (McLaughlin, 1977).

The conceptual architecture of causal models can take several forms, each of which will influence the model's internal structure and state variables. Probably the most frequently applied concepts are

- compartment analysis (Atkins, 1969; Patten, 1971),
- system dynamics (Forrester, 1961),
- energy circuit language (Odum, 1971 and 1976), and
- discrete physicochemical systems (Smerage, 1979).

Each concept, however, requires a set of functions which describe the process transformations of the model's state variables.

The process functions contained in causal models can be either empirical or deterministic. Empirical functions are based simply on measurements of inputs and outputs of single or several interrelated processes, in other words, mini-statistical ecologic system models.

Deterministic functions are the mathematical representations of accepted laws of physics, chemistry and biology. This differentiation is sometimes somewhat arbitrary. What we define today as scientific law may tomorrow just be seen as our incomplete interpretation of empirical evidence.

Deterministic ecologic models are usually seen as a set of mathematical expressions tying together the interrelationships of system processes. In reality, they usually contain a mixture of empirical and deterministic functions: the deterministic functions being those of most interest to the modeler while the empirical functions are used to tie together the loose ends of the interrelated processes where there does not exist a clear enough understanding to develop an integrated deterministic description or the modeler finds these processes to be of secondary interest or significance to his problem.

The parameters in deterministic ecologic models represent rate coefficients of natural processes. These coefficients in concept are not variable but are constants when the process descriptions are correct and all significant independent varialbles and processes have been included in the model. This allows for the extrapolation of the process functions outside of their range of calibration and for the application of deterministic models to geographic areas where no calibration data exists. Such predicitions, of course, will not be of the best quality, but they can at least be used to provide qualitative evaluations of planning alternatives.

DATA REQUIREMENTS

A significant stumbling block in the building of crop ecologic models is data. Crop systems tend to be very heterogeneous, inputs contain large random components, and it is often quite difficult to quantify certain boundary conditions which are significant: measurements of problem boundary conditions and output state variables contain large uncertainties. Measurement procedures themselves are a problem with measurement technology still in its infancy and data collection and analysis costs restrictively high.

Statistical models require measurements of the inputs deemed to be significant and of the outputs to be simulated. Experience has shown that agricultural ecologic system models require large amounts of data to achieve predicitions with an acceptable level of uncertainty. As most statistical models are for steady-state conditions, measurements must be drawn out over very long time spans to level out the transitory effects which are so strong in so many ecologic processes.

Process models require intensive, shorter term data collection programs for their calibration and verification. With these models it is also possible to use controled laboratory experiments to determine some of the model parameters (McKinion and Baker, 1979). This procedure has been used advantageously in other areas of environmental modeling. A drawback to process models is that they usually require large amounts of information on state variable boundary conditions and system inputs. This characteristic sometimes restricts the application of this type of model and dictates the use of simpler statistical models.

INTEGRATED CROP ECOSYSTEM MODEL

Causal models of crop environments based on the systems representation depicited in Figure 1 are possible with our present understanding of agricultural processes. Today's literature is full of descriptions of modelers' activities in building causal models of various parts of the total crop environment. Described briefly below are the author's experiences in developing an integrated crop ecologic model which can be used in environmental planning studies. Even if this work is incomplete, important steps forward have been made.

The development of a zero-dimensional, steady-state process-concept model to predicit waste loads originating from irrigated agriculture was initiated in 1967 (Lyons, *et al.*, 1974). The output of this early simulation model provided information on the dissolved constituents contained in deep percolation leaving the crop root zone. These predicitions were an important input to a deterministic ground water quality model which was used in studies aimed at determining the best water development and management scheme for large river basin systems (Lyons, 1977).

This steady-state crop environment model is based on several simplifying assumptions which are applied over large regional planning areas:

- constant nutrient application rates for all soil types,
- constant mix of chemicals for each applied nutrient, and
- constant crop uptake of soil solutes.

The model computes the resultant leachate additions attributable to each specific cropping unit for each planning area with uniform ion exchange and soil solubility-precipitation reactions.

During the course of this work it became apparent that while the steady-state approach is implementable on large water resource systems, it ruled out the study of certain transient effects which can be important in some areas. The model's other large drawback was that it assumed a standard plant response to weather, water and fertilizers and did not allow for a study of trade-offs in production and environmental protection. As a concequence of this need for a better analysis tool, the author developed a deterministic conceptual model of the crop environment (Water Resources Engineers, Inc., 1975). The implementation of this conceptual model into a fully operational planning tool has not yet been completed. Virtually every subsystem model in operational, but their tying together into a unified model will have to wait for a future effort.

This model does not contain all of the influence coupling depicited in Figure 1, but its structure was formulated so that it would provide the basic skeleton for future model development efforts. The elements not included are pesticides and the overland flow and erosion coupling of the soil system to the surface water system. A discrete physicochemical system representation of the crop ecosystem is used. The model is one-dimensional in the vertical direction allowing for a simulation on a unit area basis. The crop environment is broken into the following coupled component systems and subsystems:

1. Atmosphere System
    a. incoming radiation and its deposition
    b. potential evapotranspiration
2. Plant System
    a. leaf subsystem
    b. stem subsystem
    c. root subsystem
3. Soil System
    a. unsaturated flow
    b. temperature
    c. diffusion of soil gases
    d. soil microbes and the nitrogen cycle
    e. ion exchange

f. soil solutes

Individual processes are described deterministically and linked together for a simultaneous dynamic solution. In end effect, the model's structure and numerical solution scheme is very similar to existing aquatic biology models developed by the author's organization and in use in environmental planning studies (Norton, 1977). Given below is a short description of the main deterministic process functions contained in the model.

Atmosphere System

An energy balance at the soil-atmosphere interface in made. Mathematically this can be expressed as

$$R_i \cdot (1-r) + R_d - R_u - E - Q - S = 0 \qquad (1)$$

where

R_i = incoming short-wave radiation,

r = reflection coefficient of the surface,

R_d = downward flux of long-wave radiation,

R_u = upward flux of long-wave radiation,

E = evaporation energy flux,

Q = sensible heat transfer to the atmosphere, and

S = sensible heat transfer to the soil.

This equation partitions the incoming energy between the atmosphere, the plant and the soil.

The evaporative energy flux is estimated by the Modified Penman Equation,

$$E = \frac{\left(\{\frac{\Delta}{\gamma}\} H\right) + \left(\{\frac{1}{h_0}\} E_a\right)}{\{\frac{\Delta}{\gamma}\} + \{\frac{1}{h_0}\}} \quad (2)$$

where

Δ = slope of the saturation vapor pressure curve,

γ = product of Bowen's constant and ambient pressure,

H = net radiation,

h_0 = relative humidity, and

E_a = sensible evaporative heat transfer.

Analysis procedures developed previously for the temperature simulation of open water bodies are used for the evaluation of the disposition of incoming radiation (Water Resources Engineers, Inc., 1968; Tennessee Valley Authority, 1968). The sensible evaporative heat transfer is coupled to the plant transpiration through an emperical function describing the so-called stomatal resistance.

Plant System

The plant system is broken down into three connected subsystems, leaf, stem and root. Some crops require the addition of a fourth subsystem, fruit. For the purposes of this model description, however, the fruit subsystem is neglected.

The basic equation for total biomass of the plant system takes to form

$$P_T = P_L + P_S + P_R \quad (3)$$

where

P_T = total plant biomass,

P_L = leaf biomass,

P_S = stem biomass, and

P_R = root biomass.

A Michaelis-Menton (1913) representation of the plant biological system leads to a differential equation governing the growth and production of plant biomass of the following form

$$\frac{dP_T}{dt} = \mu P_L - \{\rho_L P_L + \rho_S P_S + \rho_R P_R\} \qquad (4)$$

where

t = time,

μ = the specific growth rate as defined below, and

ρ_L, ρ_S, ρ_R = the respiration rate of the leaves, stems and roots, which are temperature dependent.

The crop specific growth rate, μ, is known to coupled to the availability of required nutrients, carbon dioxide and light. The standard formulation for the specific growth is

$$\mu = \hat{\mu} \left\{\frac{N_{2,3}}{N_{2,3} + K_N} \cdot \frac{P}{P + K_P} \cdot \frac{K}{K + K_K} \cdot \frac{C}{C + K_C} \cdot \frac{\lambda}{\lambda + K_L}\right\} \qquad (5)$$

where

$\hat{\mu}$ = the crop maximum specific growth rate,

$N_{2,3}$ = the available ammonia and nitrate nitrogen,

P = the available phosphate,

K = the available potassium,

C = the available CO_2,

γ = the local light intensity, and

K_N, K_P, K_K, K_C, K_L = emperical half-saturation constants (temperature dependent).

It should be noted that Equation (5) couples crop production to available nutrient supply and thus growth rates vary in time as nutrients become available in the soil system for crop uptake. It should also be noted that the growth rate equation includes light intensity and that, other factors remaining equal, plant growth increases during daylight hours and ceases at night; respiration continues at night as indicated in Equation (4). Finally, the growth and respiration constants are temperature dependent and are formulated, along with all other temperature dependent system varialbles, according to the function described below. Experiences with the modeling of algae and higher order plants in aquatic systems has shown that the Michaelis-Menton representation given in Equations (4) and (5) can be very effectively used to simulate plant growth.

Deterministic plant growth models based on individual physiological processes in photosysthetic carbohydrate production and respiration are under development (Smerage, 1979), and in the future they could prove to provide a better deterministic representation of plant growth than a Michaelis-Menton model. The typical heterogeneousness of crop environments, however, raises the question as to their applicability in representing conditions in very diverse plant populations. These models inherently contain a large number of state variables and parameters, and one is led to ask whether it will be possible to significantly identify these model parameters given the large variability in boundary conditions and uncertanties in data on crop field conditions.

Soil System

The soil system is a complex ecosystem in itself with many interrelated physical, chemical and biological reactions occurring. Several investigators have previously developed good systems representations of the physiochemical soil reactions, see for instance Dutt, *et al.* (1972) and Reddy, *et al.* (1979). This work, however, has neglected the soil water quality - soil gases interrelationship and has only empirically tried to couple the soil system to the plant system. Similarly, soil temperature was not simulated from atmospheric data but simply supplied as a recorded input.

The simulation of soil temperature and the diffusion of soil gases is incorporated into the soil system, and the nitrogen cycle simulation reflects our experiences in this area. Each soil subsystem considered is discussed in the following paragraphs.

Unsaturated Flow

One-diemensional unsaturated flow in a porous media is described be the following diffusion equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial Z} \{K(\theta) \frac{\partial h}{\partial Z}\} - S(Z,t,\theta) - V \qquad (6)$$

where

θ = moisture content,

t = time,

Z = depth,

$K(\theta)$ = permeability as a function of θ,

h = capillary pressure head,

$S(Z,t,\theta)$ = volumetric rate of moisture absorption by the plant roots per unit volume of soil as a function of Z, t, and θ, and

V = volumetric moisture generation by soil water vapor condensation (negative for evaporation).

The plant moisture withdrawal term, $S(Z,t,\theta)$, is a macroscopic representation of root water uptake. An empirical function relating plant root density and moisture stress to water uptake needs to be used as deterministic representations presently under development have not yet satisfactorily proven themselves.

Temperature

The soil temperature phenomenon is mathematically expresses by a differential equation similar to the unsaturated flow equation,

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial Z} \left\{ \frac{k(\theta)}{C} \frac{\partial T}{\partial Z} \right\} + \frac{q}{C} \tag{7}$$

where

- T = temperature,
- t = time,
- Z = depth,
- $k(\theta)$ = thermal conductivity (bulk volume),
- C = volumetric heat capacity, and
- q = internal heat generation (or loss).

The solution technique for this equation is the same as the unsaturated flow equation. The internal heat generation or loss term, q/C, in Equation (7) is directly coupled to the evaporation-condensation term, V, in Equation (6).

Diffusion of Soil Gases

Oxygen moves from the atmosphere into the soil to satisfy the respiration demands of the soil microbes and plant roots. Carbon dioxide generated by this respiration is diffused upward to the soil surface. Carbon dioxide concentrations play an important role in the solution and precipitation of $CaCO_3$ in the soil profile. Water vapor diffuses both upward and downward according to temperature gradients, rainfall, irrigations, and plant moisture withdrawals. The movement of all three of these gases is governed by the same differential equation,

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial Z} \left\{ \frac{D}{X_a} \frac{\partial p}{\partial Z} \right\} + \frac{\beta \alpha}{X_a} \tag{8}$$

where

p = partial pressure,

t = time,

Z = depth,

D = diffusion coefficient,

X_a = fraction of air-filled pores,

β = ratio of partial pressure and mass at pressure p, and

α = production activity per unit volume of soil.

The production activity term, α, for water vapor is coupled to the previously mentioned evaporation terms of the unsaturated flow and temperature equations. Similarly, when considering oxygen and carbon dioxide α is coupled to the respiration of the plant roots and soil organic matter. Moreover, the carbon dioxide production activity term is also connected to the equilibrium reactions of soil calcium carbonate.

Nitrogen Cycle

A deterministic representation has been chosen for the simulation of soil nitrogen. In this present formulation the most important components of the soil nitrogen cycle are represented but certain reactions which are found only under special conditions have been left out, for example, the denitrofication of nitrite and nitrate.

The nitrogen cycle in the model contains three component reactions. The differential equations governing the transformations of nitrogen from one form to another are given below. The effectiveness of the mathematical relationships to represent the nitrogen cycle has been demonstrated in aquatic ecosystem models (Norton, 1977) and recently in studies of the land disposal of animal solid wastes (Reddy, *et al.*, 1979).

Ammonia Nitrogen

$$\frac{dN_1}{dt} = \beta_1 R - \beta_2 N_1 - \beta_3 N_1 - U_1 - I_1 \tag{11}$$

where

N_1 = the concentration of ammonia as nitrogen,

t = time,

β_1 = rate constant for mineralization of soil organic residue by bacterial action, temperature dependent,

R = the concentration of soil organic residue,

β_2 = rate constant for ammonia immobilization by bacterial action, temperature dependent,

β_3 = rate constant for the oxidation of ammonia by bacterial action, temperature dependent,

U_1 = crop uptake of ammonia, and

I_1 = ammonia removed by ion exchange, adsorption and volatilization.

It should be noted that β_2 and β_3 are step functions dependent on the carbon to nitrogen (C:N) ratio of the soil organic residues.

Nitrite Nitrogen

$$\frac{dN_2}{dt} = \beta_3 N_1 - \beta_4 N_2 \qquad (12)$$

where

N_2 = the concentration of nitrite as nitrogen, and

β_4 = rate constant for the oxidation of nitrite by bacterial action, temperature dependent, and

other terms as previously defined.

Nitrate Nitrogen

$$\frac{dN_3}{dt} = \beta_4 N_2 - \beta_5 N_3 - U_3 \qquad (13)$$

where

N_3 = the concentration of nitrate as nitrogen,

β_5 = rate constant for the nitrate immobilization by bacterial action, temperature dependent,

U_3 = crop updake of nitrate, and

other terms as previously defined.

The immobilization rate, β_5, is a step function similar to β_2 and β_3 dependent on the C:N ratio of the soil organic residues.

Ion Exchange

Ion exchange in the soil system of the model employs a simplified form of the statistical exchange equation to express the exchange isotherm. This equation takes the form of

$$K_{1-2} = \frac{(B_2)^{r_1} \{B_1\}^{r_2} \left(\{B_1\} + \{B_2\}\right)^{r_1 - r_2}}{(B_1)^{r_2} \{B_2\}^{r_1}} \quad (14)$$

where

K_{1-2} = exchange constant for replacement of B_2 by B_1,

$(B_1),(B_2)$ = ion activities in the solution phase of B_1 and B_2,

$\{B_1\},\{B_2\}$ = moles of ionic species in the exchange phase, and

r_1, r_2 = valences of B_1 and B_2.

This ion exchange equilibrium equation is applied to several exchange ions; Ca^{++}, Mg^{++}, Na^{+}, K^{+} and NH_4^{+}.

Soil Solutes

An equilibrium reaction in which substances A and B react to give C and D can be represented by

$$aA + bB = cC + dD \quad (15)$$

where

a,b,c,d = multiples of reactants needed to balance the equation.

For this chemical reaction the equilibrium equation of Equation (14) can be expressed as

$$\frac{\{C\}^c \; \{D\}^d}{\{A\}^a \; \{B\}^b} = K \quad (16)$$

where

$\{A\},\{B\},\{C\},\{D\}$ = effective molar concentrations, and

K = equilibrium constant.

The effective concentrations must be calculated using activity coefficients. The activity coefficients of the soil solutes can be computed by the Dobye-Hückel Theory.

The following equilibrium reactions are included in the conceptual model:

$$CaSO_4 \cdot 2H_2O \rightleftarrows Ca^{++} + SO_4^{=} + 2H_2O, \tag{17}$$

$$CaSO_4 \rightleftarrows Ca^{++} + SO_4^{=}, \tag{18}$$

$$MgSO_4 \rightleftarrows Mg^{++} + SO_4^{=}, \tag{19}$$

$$CaCO_3 + H_2CO_3 \rightleftarrows Ca^{++} + 2HCO_3^{-}, \text{ and} \tag{20}$$

$$CO_2 + H_2O \rightleftarrows H^{+} + HCO_3^{-}. \tag{21}$$

Equilibrium reactions between Ca^{++} and $PO_4^{\equiv}$ can under certain conditions also be important, and their appropriate equilibrium equations should be added when it is necessary to represent the ecologic system being simulated.

Temperature Dependence

All rate constants and other factors that are known to be temperature dependent are formulated according to the relationship

$$X_T = X_{T_s} \, \theta^{(T-T_s)} \tag{22}$$

where

X_T = the value of the variable at the local temperature, T,

X_{T_s} = the value of the variable at the standard temperature, T_s, and

θ = an empirical constant for each system variable.

This functional description of temperature dependency has proven itself in numerious ecologic models.

APPLICATIONS IN ENVIRONMENTAL PLANNING

The application of ecologic models to real world environmental planning projects is no easy task. On the other hand, the development of usable models should be one of our primary goals. The steady-state and dynamic models described above were formulated for the sole purpose of carrying out planning studies.

Crop environmental systems are normally quite heterogeneous. As a rule, there is nearly always a deficiency in data describing the total system to be studied in its present state, and predicitions of future independent variables are often quite difficult and expensive to prepare. Nevertheless, this is an important part of the use of simulation models in environmental planning. Normally a *data management system* is essential for the successful completion of environmental planning studies, but this important problem is not addressed here.

In spite of the difficulties in using simulation models in planning studies, they are being more and more frequently used and with increasing success. As an example of the information obtainable from crop environment models, Figure 2 depicits predicited additions of total dissolved solids to the environment in the Monterey Bay Region of California. This area consists of several middle size urban areas surrounded by very intensive, irrigated agriculture. The incremental waste loadings from irrigated agriculture were predicited with the above mentioned steady-state model while predicitions of the loadings from dairies & feedlots and municipal & industrial were made with other deterministic methods. A quick glance at this figure and the relative magnitude agricultural wastes can take on in relationship to urban wastes shows all the more clearly how compelling it is for us to develop more accurate and functional predicition methods for crop environmental systems.

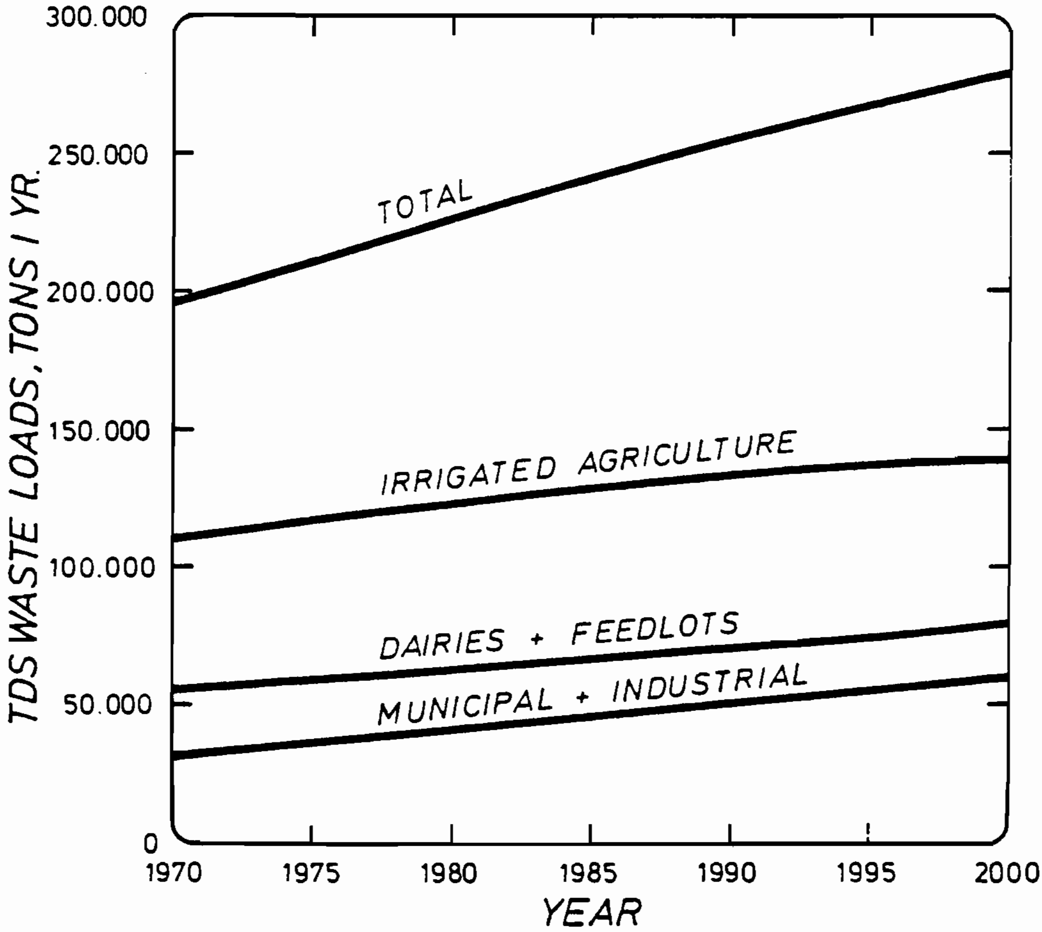

Figure 2. Total dissolved solids, incremental waste loading. Monterey Bay Region, California.

SUMMARY

Deterministic models can be used to simulate crop agricultural environments. These ecological models are in fact interwover collections of individual deterministic process models. While a sufficient theoretical basis is available for the building of deterministic models, the identification of their parameters remains a significant problem. The use of crop ecologic models in planning allows for the study of trade-offs between agricultural production and environmental protection, but their full value cannot be achieved without the support of a properly conceived data management system.

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THE MATHEMATICAL MODEL FOR THE DETERMINATION OF THE OPTIMAL CROP PRODUCTION STRUCTURES AS AFFECTED BY AGROECOLOGICAL CONDITIONS

Zsolt Harnos[1)]

During recent years, throughout the world, increasing attention has been paid toward assessing natural resources, working out possibilities for their utilization. Today this assessment includes not only the energy resources, raw materials but also the so called "biological resources". It is expecially important to be familiar with the interaction between the natural environment and plant and animal production to discover the hidden reserves in biological resources, the possibilities and limits of their utilization.

In Hungary, work on the estimation of agroecological potentials started in 1978 at the initiative of the Hungarian Academy of Sciences and was finished in the spring of this year.

At the assessment of the agroecological potential our main goal was to determine the maximal amount of plant production as a result of optimal utilization of the possibilities offered by the natural environment and to investigate the consequences of such a policy.

In concrete terms, this meant the determination of land use patterns optimally utilizing the ecological conditions that

- can be realized in principle,
- meet the requirements of the society
- and are optimal with respect to some goal.

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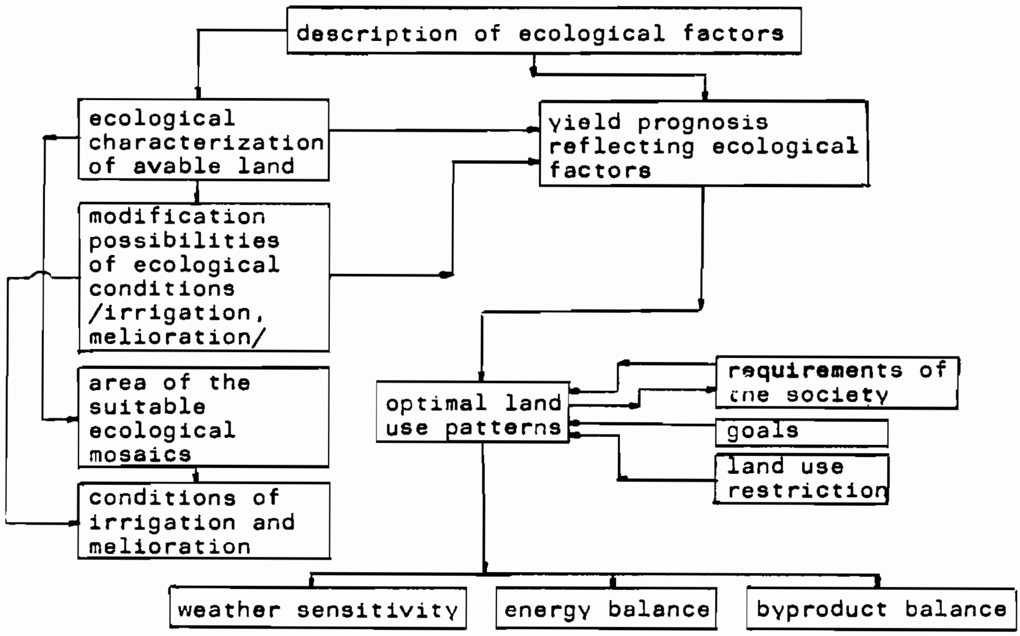
Realizability means the use of data and hypotheses in the model that can be expected by reasonable standards to be valid at the turn of the millennary.
Meeting the requirements of the society means, the capability to supply the society with all the products determined by the projected structure of consumption.
Optimality means an in some sense optimal compliance of the land use structure with the ecological conditions.
After this short introduction, the presentation of the model describing crop production follows, with the structure of the model shown in the figure below.



The first problem was to determine the attainable level of yields in 2000 given the natural environment of Hungary /precipitation, temperature, soil, relief, hydrology etc./ an the genetic potential of the species. For this end a yield prognosis was prepared, the structure of the resulting data basis is shown in Table 1.

The methodology and detailedness is described in the following papers [3] , [9] .

The model describing crop production is based on these data basis.

The main goals of the computations were :

- the assessment of production capacity of crop production under different circumstances
- the analysis of the relationships between land use patterns complying with the natural conditions and the required total production /social demand/
- the analysis of the development of land use pattern and total development of land use of the quantity and quality of available land
- the analysis of the dependence of land use patterns and total production on the amount of investments into land reclamation and on their way of realization

THE DATA BASIS AS AFFECTED BY AGROECOLOGICAL CONDITIONS

Crop : $n = 1,2,\dots,13$

Region : $k = 1,2,\dots,35$

		climatic year types 1	2 yield t/ha	3	4	area of the soil type in hectares	land suitable for melioration	irrigation	yield t/ha	rise of yield due to melioration in t/ha	irrigation in t/ha
soil types	1	$a^1_{n,k,1}$	$a^2_{n,k,1}$	...	...	$T_{k,1}$	$T^m_{k,1}$	$T^\ell_{k,1}$	$a_{n,k,1}=\sum_{i=1}^{n} a^i_{n,k,1}\,p_i$	$b_{n,k,1}$	$c_{n,k,1}$
	2	$a^1_{n,k,2}$	$a^2_{n,k,2}$	...	...	$T_{k,2}$	$T^m_{k,2}$	$T^\ell_{k,2}$	$a_{n,k,2}=\sum_{i=1}^{n} a^i_{n,k,i}\,p_i$	$b_{n,k,2}$	$c_{n,k,2}$
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
The frequency of the climatic year types		P_1	P_2	P_3	P_4						
The characteristic data of the region						$T_k=\sum_{j=1}^{34} T_{k,j}$	$T^m_k=\sum_{j=1}^{34} T^m_{k,j}$	T^L_k	$a_{n,k}=\dfrac{\sum_{j=1}^{34} a_{n,k,j}}{T_{k,j}}$	$b_{n,k}=\dfrac{\sum b_{n,k,j}T^m_{k,j}}{T^m_{k,j}}$	$c_{n,k}=\dfrac{\sum c_{n,k,j}T^\ell_{k,j}}{T^L_{k,j}}$

In the table : $0 \le T^\ell_{k,j} \le T^m_{k,j} \le T_{k,j}$; $a_{n,k,j} = b_{n,k,j} = c_{n,k,j} = 0$ if $T_{k,j} = 0$.

Where : $0 \le p_i \le 1$, $p_1+p_2+p_3+p_4 = 1$

Table 1.

- the analysis of the relationships between irrigation and land use patterns,

  etc.

The large number of crops and habitats considered resulted in about 5000 variables. This situation, in fact, determined the method; as the only solvable problem in this case is one using linear programming techniques, the same being true even after excessive aggregation.

A two level hierarchic model was constructed for the analysis of crop production.

The first, so called regional model describes the problem in an aggregated form. The so called ecological regions constitute the land units here. /See Figure 2./

The requirements of the society with respect to the production structure and land reclamation investment conditions and others are formulated in the constraints of this model.

The result gives a rough, regional allocation of the investments and land use. The global analyses of the crop production system and that of the dependence of land use and product structure on the conditions and the goals are carried out by using this model.
Detailed computations considering ecological mosaics are carried out on the other level.

The whole of the country was divided into four large regions as is shown in Figure 2., and the crop production activity in them are described by separate problems. The structure of these models is similar to that of the regional model that will be outlined in the sequel. It is the regions that are considered homogeneous in the regional model while the same is true only for the ecological mosaics in the others. The constraints of the deailed models /as far as the product structure, the allocation of land reclamation investments and even the goal function/ were formulated on the basis of the results of the regional model.

Our computations give detailed information about the land use pattern being in good compliance with the ecological conditions and about the allocation both in space and time order of land reclamation investments.

Before going into the details of the constraints of the regional model we shortly give a formal definition of the model system.

The regional model is described by a system linear inequalities parametrized in the right hand side :

$$\begin{aligned} &\underline{\underline{A}}\,\underline{x} \leq \underline{b}_0 + \lambda\left(\underline{b}_1 - \underline{b}_0\right) \\ &\underline{x} \geq \underline{0} \qquad\qquad\qquad\qquad /1/ \\ &\lambda \in [0,\ 1] \end{aligned}$$

Let us denote the set of the solutions of the above system by Ω .

Our task is to determine an $x^* \in \Omega$, with all the goal functions

$$\varphi_i(\underline{x}) = \langle \underline{c}_i , \underline{x} \rangle \qquad i \in I = \{1,2, \ldots ,\ell\}$$

reaching their optima, that is

$$\varphi_i(\underline{x}^*) = \max_{\underline{x} \in \Omega} \varphi_i(x) , \qquad i \in I .$$

This optimization problem, however, has no solution in general [4] , and for this reason we have to find special Pareto-optima, that is such $\underline{z}^* \in \Omega$ for that

$$\underline{\varphi} (\underline{z}^*) = \max \{ \underline{y} : \underline{y} = \varphi(\underline{x}) , \underline{x} \in \Omega \}$$

The maximum here is taken over $\mathbb{R}^\ell$ with respect to the ordering induced by the natural positive cone $\mathbb{R}^\ell_+$.

That is to say :

$$\underline{\varphi}(\Omega) \cap \left(\underline{\varphi}(z) + \mathbb{R}^\ell_+ \right) = \{ \underline{\varphi}(\underline{z}^*) \}$$

Two, so called compromise solution were determined from the set of Pareto optimal points.

In the first step the utopia point in $\mathbb{R}^\ell$ was determined for problem /1/.

For the i-th coordinate of the utopia point $\beta_i = \varphi_i(\underline{x}^{(i)})$ where $\underline{x}^{(i)}$ is the solution of the problem:

$$\begin{aligned} \underline{\underline{A}}\,\underline{x} &\le \underline{b}_0 + \lambda(\underline{b}_1 - \underline{b}_0) \\ \underline{x} &\ge \underline{0} \\ \lambda &\in [0,1] \\ \varphi_i(\underline{x}) &\longrightarrow \max \end{aligned}$$

We construct two new goal functions by using the utopia point,

$$\Psi_1(\underline{x}) = \sum_{i=1}^{\ell} \left(1 - \frac{\langle \underline{c}_i, \underline{x} \rangle}{\beta_i}\right)$$

and

$$\Psi_2(\underline{x}) = \max_{1 \le i \le \ell} \left(\beta_i - \langle \underline{c}_i, \underline{x} \rangle\right)$$

then we minimized them on the set Ω .
These solutions are Pareto-optimal points of the system /1/ .
The solutions of the regional model produced land use patterns on regional level. By their use, the production structure and the extent of land reclamation and irrigation determined.
Taking them as constraints and taking them corresponding goal functions, the linear programming problem describing the crop production of the four large regions were solved.

Now we arrived to the description of the main relationships and to the explanation of our choice of methodology.

The constraints can be grouped as follows :

- area constraints,
- constraints of the product structure,
- crop rotation conditions ensuring the continuity of production,
- constraints regulating the extent of land reclamation and irrigation investment.

Cropland was considered to be homogeneous in the regional model, with three kinds of possible activity :

- production corresponding the present situation
- production corresponding to the situation after land reclamation /melioration/
- production on both reclaimed and irrigated land.

The area of irrigable and reclaimed land was limited in each region.
The total area cultivated in the three possible ways had to be equal to the total croplevel in the region. The total available cropland in the regions was changed according to the amount of land under non agricultural use.

The demand that crop production had to meet consisted of two parts :

- home consumption,
- exports.

At formlulating the demand, the following points were to be considered :

- immediate public consumption,
- consumption ensuring the continuity of production and reproduction.

The public consumption is the function of the number of the population and eating habits, in the first place.

Three different consumption structures were considered consumption corresponding to the present Hungarian, West--European and physiologically right nutrition.
Thie is the point where animal husbandry is linked into the system.

The fodder needs of an appropriate stock of cattle and sowing seed for keeping production on the some level had to be reckoned with to ensure the continuity of food production, that is self-reproduction.
This consumption model served as the basis for the determination of the minimal amount of products to be produced. Upper bounds were given for crops that cannot be exported and home consumption is also limited.

The third group of constraints is for tho control of the territorial structure of the production. Is it the territorial constraints determined for each region that ensure the realizability of the rotation plan.

These are of two kinds :

- those given in the form of a limit for the ratio between the area occupied between certain crops or groups of crops respectively
- those limiting the area occupied by certain crops or groups of crops from above or below.

Similar conditions were formulated for irrigated or reclaimed land and for the ratio between irrigated and dry cultivation. All the above mentioned parameters were expressed in natural units and the same is true for the constraints, as well. There was, in fact, one single condition of a non ecological character, and this was the extent of land reclamation investments.
This is a significant means for increasing yield, but it cannot be expected that all the reclamation work will have been finished in the near future.

In the course of our investigations, more than 20 different forms of land reclamation were considered, with different investment requirements. The rise of yield due to land reclamation being known, investment costs in current prices were sufficient to determine the optimal allocation and time order of land reclamation projects. The volume of material investment was limited. The solutions under the different investment constraints gave the opportunity to determine the expedient location and time order of land reclamation projects.

The structure of the outlined model can be seen in the figure below :

$$\begin{pmatrix} & & & A_t \\ & & & A_y \\ A_1 & A_2 & \ddots & 0 \\ 0 & & & A_{35} \end{pmatrix} \underline{x} \leq \begin{pmatrix} \underline{b}_t \\ \underline{b}_y \\ \underline{b}_1 \\ \vdots \\ \underline{b}_{35} \end{pmatrix} \qquad /2/$$

$$\underline{b}_t = \underline{b}_o^t + \lambda(\underline{b}_1^t - \underline{b}_o^t)$$

$$\underline{b}_o^y \leq \underline{b}^y \leq \underline{b}_1^y$$

$$\underline{b}_o^k \leq \underline{b}^k \leq \underline{b}_1^k \qquad k = 1, \dots , 35$$

Some of the lower bounds equal to zero while some of the upper bounds may be infinite, meaning that there is no limitation. The system of inequalities means a series of problems of an ever growing size but of constant structure. The matrices A_t and A_y were the same in all cases while in the matrices A_k , relationships contolling the land use pattern were gradually extended. The solutions in the less constrained cases made great differences between the production areas of the individual crops. By the gradual extension of the conditions, however, the land use pattern reached a stable form, that is from a certain step onwards the different goals did not made the land use pattern change significantly.

significantly.

The knowledge of such stable systems is important, because the product mix can be changed without substantial modifications of the structure of the agricultural production, and hence the planning of the agricultural infrastructure can be brought into harmony with the stable - though versatile - land use pattern.

The description of the parameters serving as a basis of the production and of the main forms of the factors influencing production is herewith finished.

This is described in a concise form by the inequality system

$$\underline{\underline{A}}\,\underline{x} \leq \underline{b}_0 + \lambda\left(\underline{b}_1 - \underline{b}_0\right)$$
$$\underline{x} \geq \underline{0}$$
$$\lambda \in [0,1]$$

The possible land use patterns are represented by the solutions of this system.

The main problem here is to choose the criterion of optimality.

The usual goals in economic planning - like the maximization of net income, the minimization of costs - were not suitable as both the costs /inputs/ and the products were counted in natural units.

Hence, goals could be formulated by the way of some fictive price system, and so we used a number of comparative value systems. "Price systems", in this case, were needed only for the analysis of sensitivity of the system and not for the determination of some sort of profit.

The comparative value systems were based on some indicator of the internal content of the products like e.g. protein content, energy content, grain unit an so forth, and then the optimal product and land use structure under the different limitation levels were analized.

Obviously, because of the extreme characteristics of such value systems, an economy cannot adapt a production structure being optimal with respect to them, but the results themselves are interesting as they show the maximal possibilities in some directions.

Knowing these maximal possibilities, compromise solutions with respect to certain groups of the goal funstions or to all of them were also determined.

The product mix resulting from the compromise solutions seems to be realistic.

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STATISTICAL EVALUATION OF EXPERTS' ESTIMATES

István Vályi[1)]

In 1978, the Hungarian Academy of Sciences initiated a program for the assessment of the agroecological potential of Hungary.

With the participation of more than 30 research institutions, work was started in that year and was finished in the spring of 1980. Deputy secretary of the Hungarian Academy of Sciences, Academician István Láng gave an account of the result at the plenary session of the Academy. The present paper is aimed at presenting a solution of a certain methological problem that has arisen in the course of the work, also having general interest, by my opinion.

The aim of the project was to give a possibly detailed picture of the biological resources of the country. At the same time, to not to detach from reality, social and economic conditions also were considered, though with less emphasis. This rather comprehensive formulation contains, among others, the following problem:

> the determination of the maximal level of crop production for the year 2000 as a result of the optimal utilization of the natural resources, that is to present land use patterns, being optimal in some sense.

The structure and the main steps of the project can be seen on Table 1. For more about this subject see Zs.Harnos[1]

In order to get a correct solution of this problem, a sound and detailed data basis was required, that is we needed detailed information about the yields in 2000.

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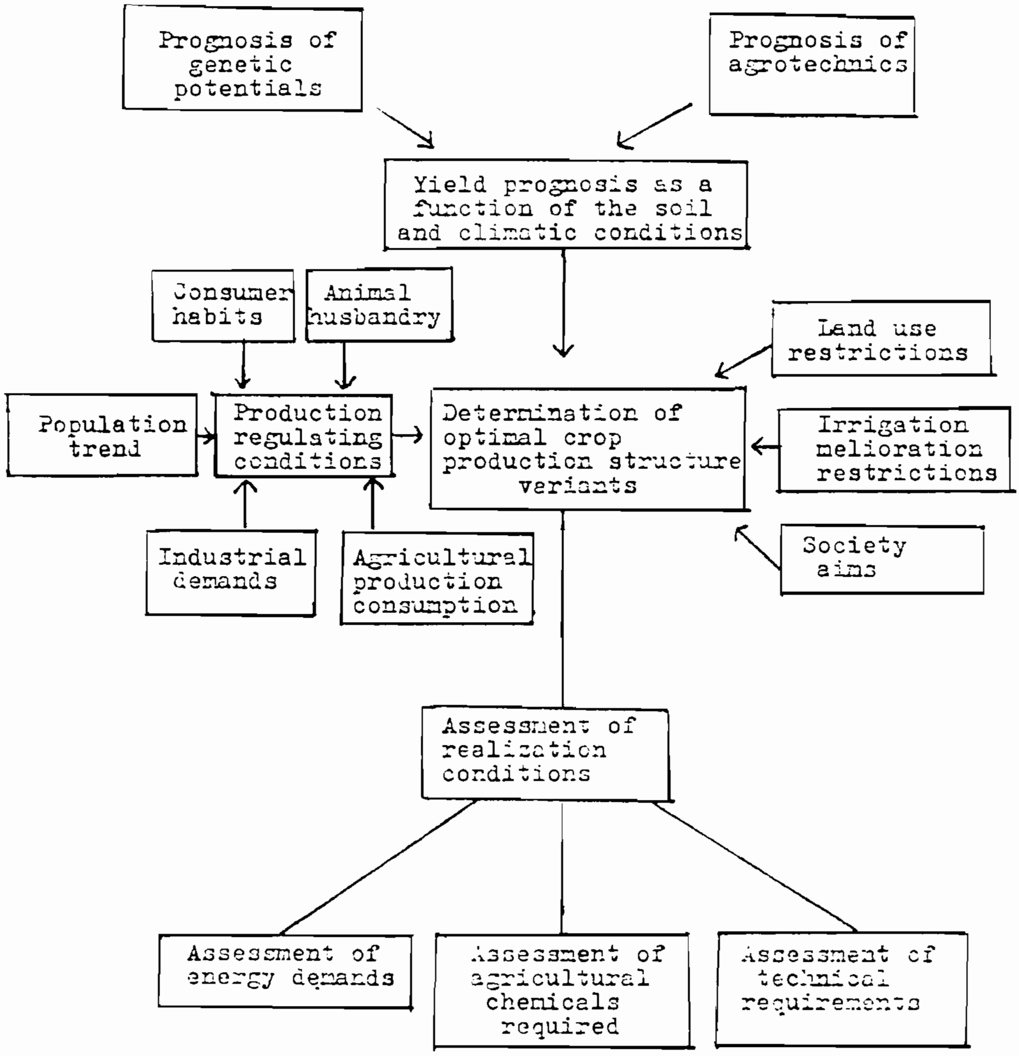
1) Bureau for Systems Analysis, State Office for Technical Development, Budapest, Hungary.

Table 1.


Prognosis of genetic potentials
Prognosis of agrotechnics
Yield prognosis as a function of the soil and climatic conditions
Consumer habits
Animal husbandry
Land use restrictions
Population trend
Production regulating conditions
Determination of optimal crop production structure variants
Irrigation melioration restrictions
Industrial demands
Agricultural production consumption
Society aims
Assessment of realization conditions
Assessment of energy demands
Assessment of agricultural chemicals required
Assessment of technical requirements

under different natural conditions.
As the presently known mathematical models describing relationships between ecological factors affecting crop production and the yields do not represent the phenomena at the required level of aggregation /are too rough or too detailed/ the use of this method had to be rejected. The alternative was to use so called soft data, that is to derive them on the basis of the unformulated knowledge of experts.
Accordingly, the yield prognosis was produced by a combined written - oral feed-back expert inquiry based on plentiful information material. This is the point where the above mentioned methodological problem arises. This kind of "soft" data was to be interpreted and checked so as to make them suitable for the input into the optimization model. This interpretation and checking was carried out by using mathematical statistics.

For each of the crops considered in the model, experts' groups were formed. The experts had to fill in questionnaires for each of the 35 agroecological regions./ See Table 2. and Figure 1./
The experts' work resulted /implicitely/ in the determination of the following function for each of the crop

$$y = f_{R,S,I} \,/\, \underline{w},\ t/$$

Where $y \in \mathbb{R}$ stands for the yield of the crop,
$R = 1, \dots 35$ for the region
$S = 1, \dots 5$ for the soil category
$I = 1, \dots 20$ for the individual expert
$\underline{w} \in R^n$ for the characteristic meteorological parameters
$t \in R$ for the time /t = 2000/

Table 2.

Estimation sheet with climatic, soil and yield information

Region Zala hills Climatic year type

		A	B	C	D
Soil category	I.				
	II.				
	III.				
	IV.				
	V.				

Soil types

Category	Soil type number	Type	%
III.	7	Clay leached brown forest soil	30
II.	8	Pseudogleyed brown forest soil	30
IV.	9	Brown forest soil	6
IV.	26	Meadow alluvial soil	3
II.	27	Meadow peat soil	4
I.	28	Lowmoor soil	6
III-IV.	31	Alluvial soil	8
		Other	3

Climatic year types

Type	precipi-tation	Heat unit	%
A	270	1270	20
B	375	1500	24
C	750	1140	4
D	450	1270	52

Yield results

Year	Sowing area as a percentage of the arable land	Average q/ha
51-57	16.3	24.5
72	17.9	33.4
73	23.2	37.3
74	23.0	36.1
75	22.1	44.3
76	19.1	36.4
77	16.6	43.2

1/ What is your estimation of the percentage of maize grown within the arable area in 2000?

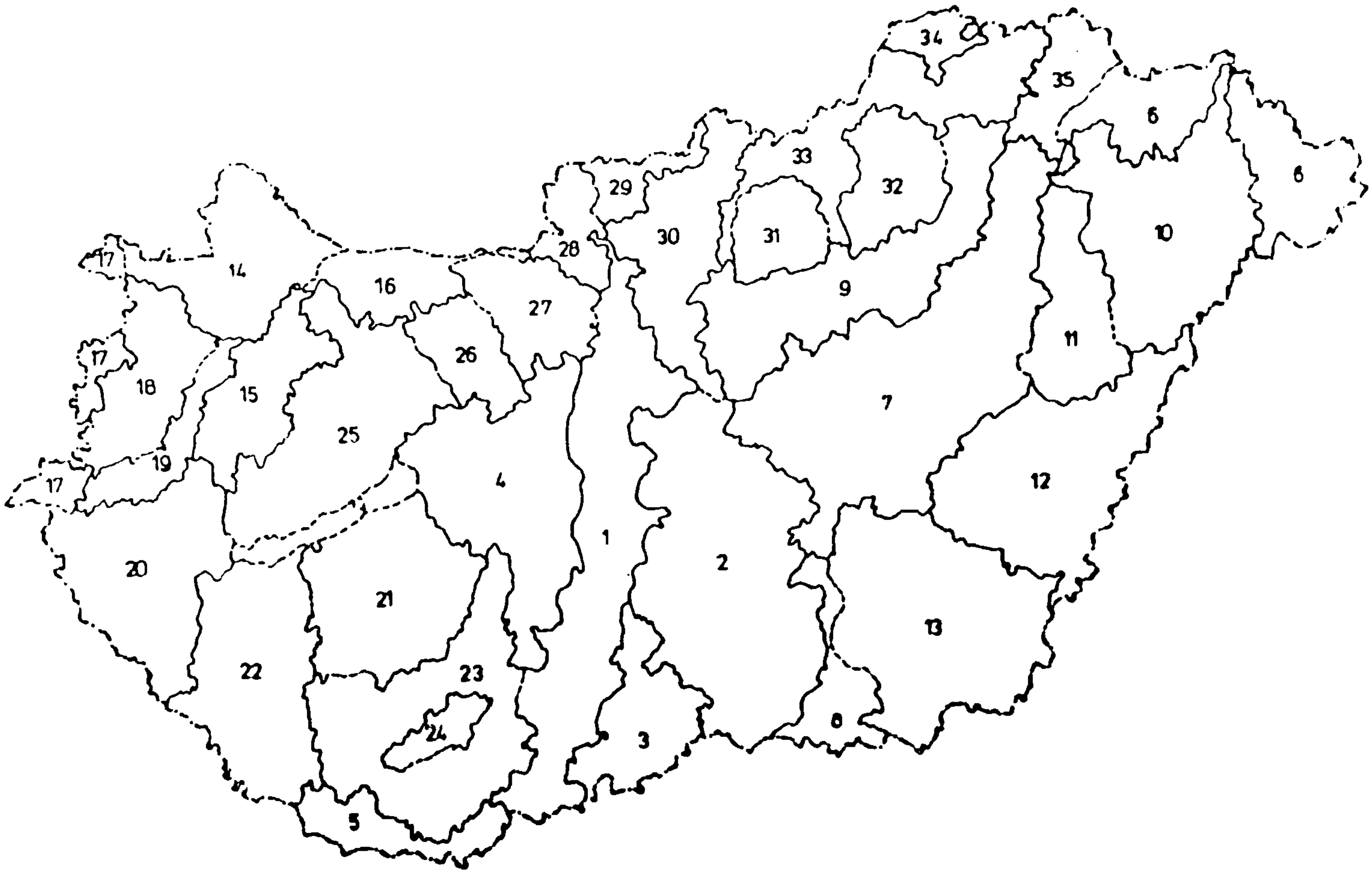


Figure 1. Ecological Regions of Hungary.

R, S and I are put into subscripts as they are measured in a nominal scale, or otherwise, they are not numbers in the common sense, but only represent individual objects.

/For a more detailed description of the climatic year types, soil categories etc. See Zs. Harnos - B. Győrffy [2] / Having this representation of the experts' estimates, the task of checking the estimates can be formulated in the following way:

let us fix all the variables but one, or consider the appropriate average , and considering y as the function of the remaining one, apply the appropriate tool of mathematical statistics.

Hence mathematical statistical investigations were carried out in five direction.

For brevity's sake investigations concerning the first three variables are described in a very sketchy way.

/1/ <u>Opinion distribution within the group of experts</u>

Investigations in this respect contained the usual analysis of the distribution of the opinions within the group. As a result, it has been established that the estimated values for the individual situations can be considered homogeneous and estimates for different ecological situations significantly differ /with probability more than 95%/.

After this step, opinion differences within the experts' group were not considered any more, and the expectation value of the opinions was taken as the data basis for further analysis.

In the sequel consider the function

$$/*/ \qquad y = E_I\left\{f_{R,S,I}\,/\underline{w},\ t/\right\} = g_{R,S}\,/\underline{w},\ t/$$

where E_I stands for the operation of taking the expectation with respect to I.

/2/ and /3/ Differences between regions and between soil categories

The dependence of the yield on the geographical situation /regions/ and on soil categories, respectively was analysed by determining a ranking between them, and also by the use of cluster analysis. See Figures 2. and 3.

Although the results reflected certain changes with respect to the present situation, they also showed that the estimates were realistic.

/4/ The anticipated dependence of the yield on meteorological parameters

As the experts estimated the yields only for the year 2000, the variable t plays no role here. Let us further fix the soil category, S.

If one supposes that soil and weather conditions completely determine the development of the crop, the subscript R /representing geographical and other factors/ could be simply left out, as well.

Then we arrive to a situation where the yield is a function of the weather parameters. At this stage we applied multivariate polinomial regression to approximate the yield estimates. This allowed us to answer two questions:

- Is the above assumption true or not /by the opinion of the experts/?

- What are the general features of the functional relationship between yield and the weather parameters?

To give an answer to these questions, polinomials with a maximal degree of three were considered. This setting allows us to detect one or two /local/ extrema.

For the interpretation of the results it is important to know, that we had about 140 observations /degrees of freedom/,

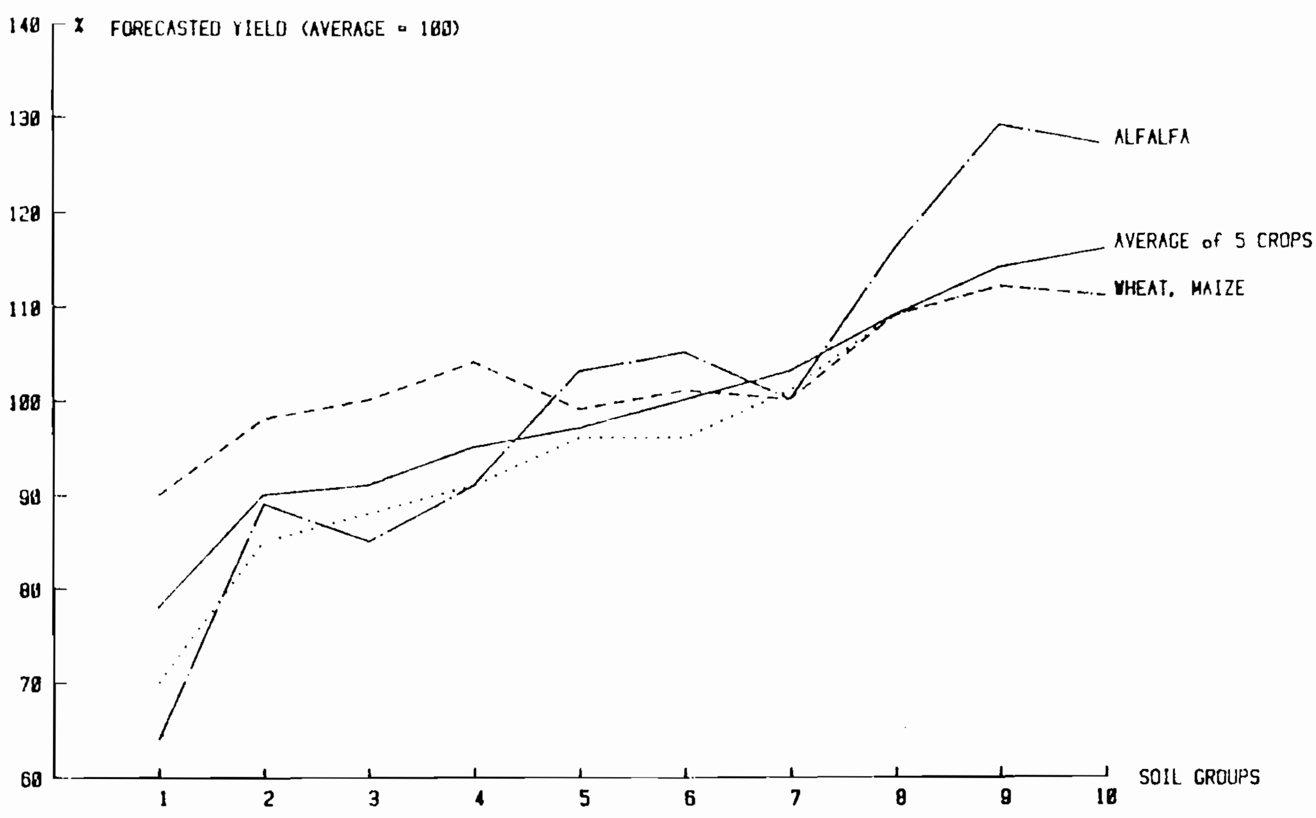


Figure 2. Evaluation of soils according to forecasted crop yields.

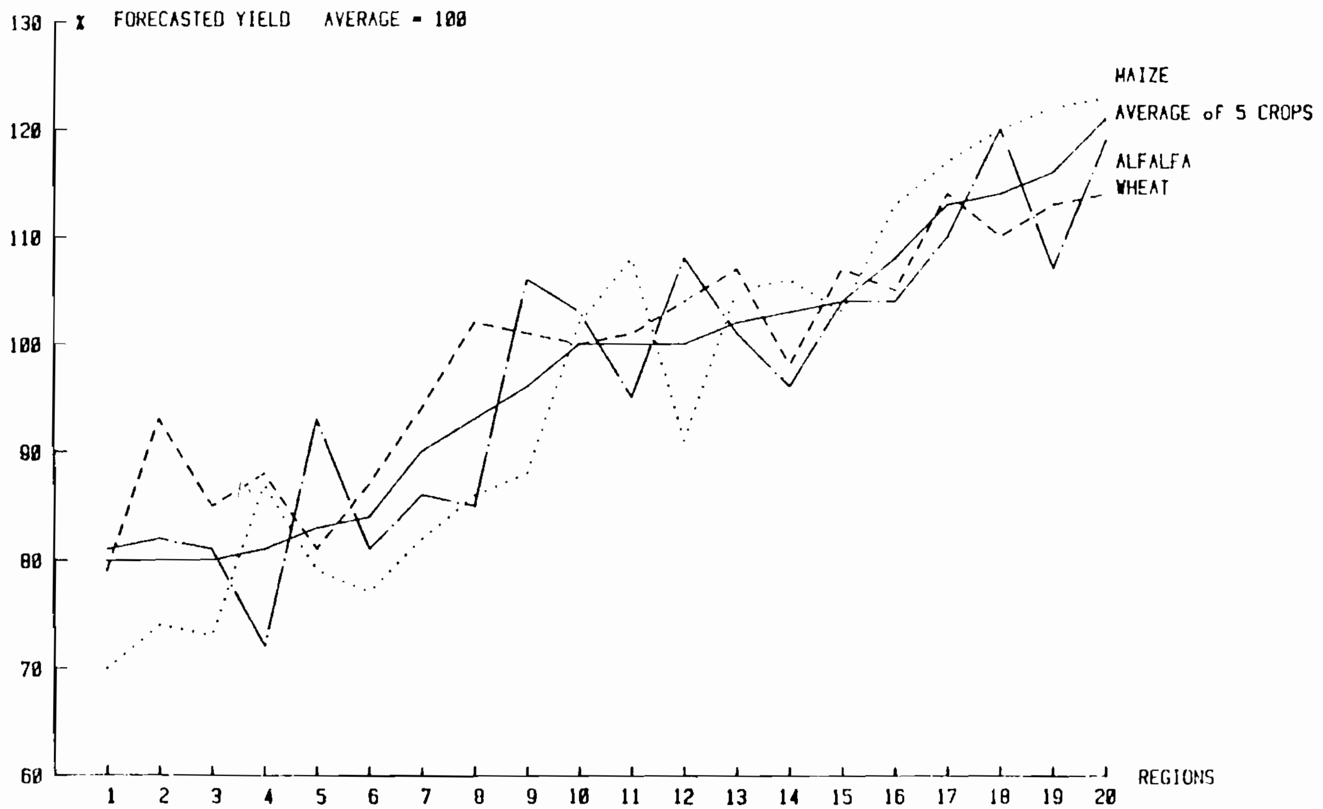


Figure 3. Evaluation of ecological regions according to forecasted crop yields.

and in many cases more than one at certain values of the explaining variables. This fact indicates that good fitting of the regressional curve cannot be expected.

In the case of wheat, the multiple correlation coefficients were between 0.5 and 0.6., and the same values for maize were between 0.6 and 0.7. Despite the above remark, this means a rather loose functional relationship.

So, the answer for the first question is negative, meaning that besides the meteorological factors listed on the questionnaire, the experts considered others, as well.

With such low correlation coefficients, the standard error of the regressional parameters was of course rather high.

But in the case of wheat, for each soil category, the regressional functions showed one global maximum within the range of the meteorological parameters. With high standard errors the place of the maximum could not be determined. Its existence, however, shows that weather was not considered as being a limiting factor for the yield of wheat. On the other hand, in the case of maize, none of the regressional equations had an extremal point within the range of the meteorological parameters. This phenomenon shows that the experts thought that weather was a limiting factor for maize.

/5/ The development of the yield in time

As was mentioned earlier, the experts' estimates are in fact not a function of time, the value of t being fixed to the year 2000. Nevertheless they can be considered as being the continuation of past results. This observation allowed the investigation of the estimates with respect to the time. Taking expectation value with respect to all variables we received one single number for each crop, the estimated average yield for the whole country.

So, the estimated yields were added to the time series of yields in the period 1900–1977.

For the development model, the following hypotheses were used:

a./ The development of the yield in Hungary is similar to that in other countries with an intensively developed agriculture and similar climatic conditions.

b./ As the data show, in the period 1900–1940. the yields generally stagnated. Later an ever accelerating growth can be observed, that after a peak slows down again. Our second hypothesis is that this development is the consequence of factors that are already present and effective. Their range of effect is however limited and the development until 2000. will take place as the result of this range extending to the whole of the Hungarian agriculture. It is also supposed, that this process will be finished in our century, and further development requires the emergence of qualitatively new factors.

All this means that our model describes the <u>safe alternative</u>.

c./ The yield in the year 2000. reaching the level estimated by the experts is also to be placed among the hypotheses.

These assumptions lead to the conclusion that the development of the yield is described by a <u>saturation process</u>.

The term is used on the basis of analogous phenomena in biology, chemistry and social sciences, phenomena succesfully described by the so called logistic function. See for instance Yao-Chi Lu[3], Nakicenovic [4] .

In mathem^ntical terms this means that:

$$y/t/ = f\ /t;\ P_1,\ P_2,\ P_3,\ P_4/ + \varepsilon_t$$

where $t = 1901, \ldots 2010$

$y/t/$ is the yield in the year t

P_1, P_2, P_3, P_4 the parameters to be determined

ε_t are independent random variables with 0 expectation and constant variance and

$$f\ /t,\ P_1,\ P_2,\ P_3,\ P_4/ = P_1 + \frac{P_2 - P_1}{1 + e^{-P_3\ /t\ -\ P_4/}}$$

For further details see Anderson [5].

Our computations resulted in

constrained development curves where the regression is taken for the period 1901 - 1977 and 2001 - 2010, in the latter y/t/. equalling to the estimated value.

unconstrained development curves where only the period 1901-1977 is considered.

In the first step, unconstrained development curves were determined for countries with developed agriculture. This, in general, showed that the logistic development model gives a realistic picture.

For the case of Hungary, based on the distribution of the experts' opinion three levels were determined, the "pessimistic", "average" and "optimistic" estimates. /The interval between the pessimistic and optimistic estimates contained about two thirds of the opinions/.

This allowed the comparison of the unconstrained development curves with the development curves under the constraint of the different experts' opinions.

In the case of wheat and maize, a remarkable coincidence of the experts' opinion and the unconstrained development curve could be observed, while in other cases like e.g. at the yield of sugarbeet, even the "pessimists" forecasted significantly higher yields, than the logistic model. Some of the results can be seen on the following Tables and Figures.

Notations: F -the relative value of the yield in 1977, between the lower and upper levels of stagnation, in percentages

P_1-the lower level of stagnation, in t/ha
P_2-the upper level of stagnation, in t/ha
P_4-the year of fastest growth

max Δ y - the growth of the yield in the year P_4
σ - the estimated variance around the development curve.

Table 3. Unconstrained development curves of the yield of wheat

	F /%/	P_4	P_1	P_2	max Δy	σ
United Kingdom	115	1958	2.2	4.6	0.09	0.22
Danemark	105	1960	2.9	5.2	0.06	0.28
Holland	100	1959	2.6	5.4	0.08	0.46
France	85	1964	1.3	4.8	0.12	0.25
/W-/Germany	80	1964	1.9	5.2	0.09	0.28
Belgium	80	1957	2.4	4.5	0.08	0.40
Czechoslovakia	70	1971	1.6	5.3	0.13	0.24
Hungary	65	1974	1.2	5.6	0.17	0.22
Austria	60	1970	1.3	5.4	0.10	0.25
Italy	50	1970	0.9	3.7	0.04	0.18

Table 4. Development curves of the yield of wheat /Hungary/

Constraint	F /%/	P_4	P_1	P_2	max Δy	σ
Pessimistic	85	1970	1.26	4.45	0.14	0.22
Average	70	1973	1.25	5.26	0.17	0.22
Optimistic	60	1975	1.24	6.06	0.19	0.22
None	65	1974	1.25	5.61	0.17	0.22

Table 5. **Unconstrained development curves of the yield of maize**

	F /%/	P_4	P_2	P_1	max ΔY	σ
France	105	1961	1.2	5.1	0.18	0.44
Austria	105	1968	1.5	6.8	0.20	0.42
USA	95	1961	1.6	5.9	0.17	0.28
Italy	80	1982	1.6	7.7	0.19	0.34
/W./Germany	70	1971	1.2	7.4	0.12	0.51
Czechoslovakia	65	1963	1.7	4.2	0.10	0.37
Hungary	65	1973	1.6	6.3	0.14	0.36

Table 6. Development curves of the yield of maize /Hungary/

Constraint	F /%/	P_4	P_1	P_2	max Δy	σ
Pessimistic	70	1971	1.56	5.82	0.13	0.36
Average	60	1974	1.54	6.79	0.15	0.36
Optimistic	50	1977	1.53	7.93	0.16	0.36
None	65	1974	1.56	6.34	0.14	0.36

Table 7. Unconstrained development curves of the yield of sugarbeet.

	F/%/	P_4	P_1	P_2	max Δy	σ
Czechoslovakia	140	1963	24.5	34.3	1.0	4.4
Austria	120	1957	22.6	44.9	1.8	5.0
Yugoslavia	110	1963	17.0	41.0	1.9	3.6
/W./Germany	100	1958	26.0	48.0	0.7	4.2
Hungary	95	1963	19.5	32.5	2.4	3.9
France	90	1961	24.7	46.3	1.5	5.0

Development curves of the yield of sugarbeet /Hungary/

Constraint	F/%/	P_4	P_1	P_2	max Δy	σ
Pessimistic	70	1966	19.3	37.8	1.2	3.9
Average	55	1970	19.4	42.5	1.0	4.0
Optimistic	45	1973	19.4	46.8	1.1	4.1
None	95	1963	19.5	32.5	2.4	3.9

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Relations between the Agro-Ecological Potential and Soil Factors

K. RAJKAI[X]

Soil is a fundamental part of natural environment, primary nutrient source of biosphere, important natural resource and basis of agricultural production. The possibilities of the increase of agricultural production and especially of crop-yields are determined - besides climatic, relief and hydrologic factors - mainly by soil conditions. Soil properties considerably influence, sometimes determine the ecological effects of the hydrologic conditions and to a certain extent, some meteorological factors, as well.

In the project of the Hungarian Academy of Sciences for the "Assessment of the agro-ecological potential of Hungary" the realizable yield of cultivated plants was prognosticated. Besides the climatic, relief, hydrologic and plant genetic factors, information on soils were collected preparing a map in the scale of 1 : 100 000. On the map the soil factors determining the agro-ecological potential of the country were indicated. The results of prognostications, based on the mentioned environmental factors, made possible (among others) to evaluate the effect of soil factors on the agro-ecological potential. Our interest was focused on two main crops; wheat and maize.

For the establishment of the relations between the realisable agro-ecological potential (crop yield) and soil factors the prognosticated yield averages were used by agro-ecological regions.

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On Figure 1. a sheet which served as a basis for our present work can be seen. On the suchlike sheets prognostications have been made regarding climatic year types (A, B, C, D) and soil categories (I-V) by agro-ecological regions. During the project of the "Assessment of the agro-ecological potential of Hungary" the country was divided into 35 ecologically different units (Fig. 2.), and the soil types were classified into 5 categories according to their suitability for crop production (Fig. 3.).

It can be seen on the figure, that the soils with extreme, unfavourable properties belong to the first soil category. For wheat these are: blown sand, peaty meadow soils and peat; for maize even solonchaks, solonchak--solonetzes, meadow solonetzes.

There are three common soil types in the second soil category for the above mentioned two crops: humous sandy soils, ameliorated peat and soils of swampy forests. Further types for wheat are, the salt-affected soils of the first category and meadow solonetzes turning in steppe formation, solonetzic meadow soils, peaty meadow soils and pseudogleys for maize. The better properties of these soils are resulted the higher colloid content in the sand, less extreme water management and lower salt content in the salt affected soils.

The third soil category contains acidic, non podzolic brown forest soils, pseudogleys and meadow soils salty in the deeper horizons for wheat, and brown forest soils, chernosems and meadow soils with less productivity for maize.

Region	Zala hills	Climatic year type			
		A	B	C	D
Soil category	I.				
	II.				
	III.				
	IV.				
	V.				

Soil types

Category	Soil type number	Type	%
III.	7	Brown forest soil with clay illuviation	30
II.	8	Pseudogley	30
IV.	9	Brown earth (Ramann brown forest soil)	6
IV.	26	Meadow alluvial soil	3
II.	27	Peaty meadow soil	4
I.	28	Peat (organic soils)	6
III-IV.	31	Alluvial soil	8
		Other	3

Climatic year types

Type	Precipi-tation	Heat unit	%
A	270	1270	20
B	375	1500	24
C	750	1140	4
D	450	1270	52

Yield results (Maize)

Year	Sowing area as a percentage of the arable land	Average q/ha
51-57	16.3	24.5
72	17.9	33.4
73	23.2	37.3
74	23.0	36.1
75	22.1	44.3
76	19.1	36.4
77	16.6	43.2

Figure 1. Estimation sheet with climatic, soil, and yield information.

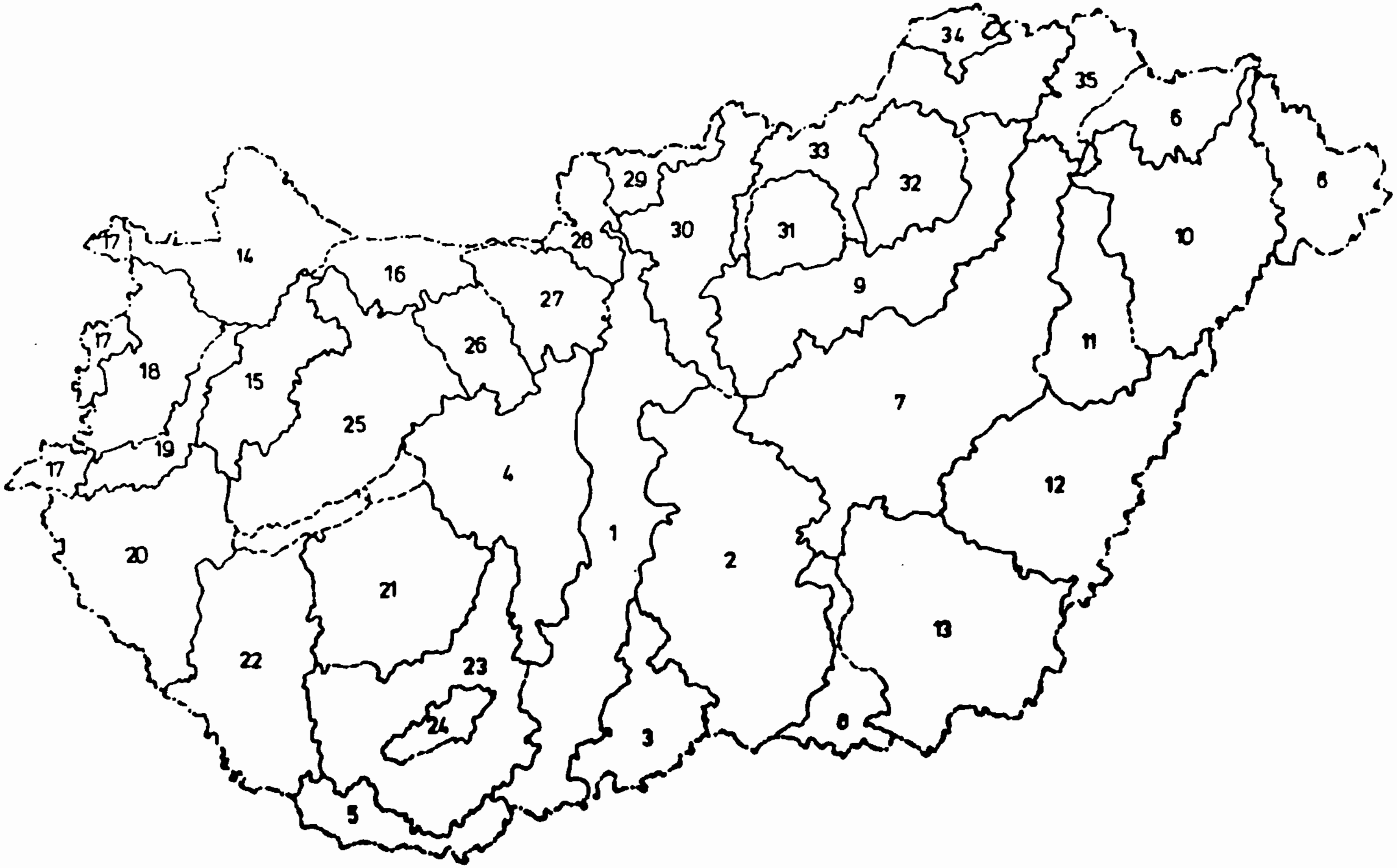

Figure 2. Ecological Regions of Hungary.

Soil category	
I	1, 2, 4, 5, 27, 28 1, 2, 4, 5, 20, 21, 22, 28
II	3, 20, 21, 22, 29, 30 3, 8, 23, 24. 27, 29, 30
III	6, 8, 23, 24 6, 7, 10, 12, 17, 18, 19,. 25, (31)
IV	7, 9, 10, 12, 17, 18, 19, 25, 26, 31 9, 15, 26, (31)
V	11, 13, 14, 15, 16 11, 13, 14, 16

Upper number for Wheat
dower number for maize

1. Stony soils
2. Blown sand
3. Humous sandy soils
4. Rendzinas
5. Erubase soils
6. Acidic, non-podzolic brown forest soils
7. Brown forest soils with clay illuviation
8. Pseudogleys
9. Brown earth
10. "Kovárvány" brown forest soils
11. Chernozem brown forest soils
12. Chernozem-type sandy soils
13. Pseudomyceliar chernozems
14. Lowland chernozems
15. Lowland chernozems with salt acc accumulation
16. Meadow chernozems
17. Meadow chernozems with salt accumulation
18. Meadow chernozems, solonetzic in the deeper layers
19. Terrace chernozems
20. Solonchaks
21. Solonchak-solonetzes
22. Meadow solonetzes
23. Meadow solonetzes turning into steppe formation
24. Solonetzic meadow soils
25. Meadow soils
26. Meadow alluvial soils
27. Peaty meadow soils
28. Peat
29. Ameliorated peat
30. Soils of swampy forests
31. Alluvial soils

Figure 3. Soil type suitability for wheat and maize.

The fourth soil category classifies suboptimal soils. These are the soils of maize in the third category and brown earths for wheat, brown earths, lowland chernozems with salt accumulation in the deeper horizons and meadow alluvial soils for maize.

The fifth soil category collects the most productive soils, the chernozem brown forest soils, lowland, pseudo-miceliar and meadow chernozems.

To establish relations between soil category and prognosticated crop yields the weighted averages of yields given to soil categories and climatic year types were generated by agro-ecological regions. The frequency of climatic year type served as bases for weighting. After this a simple statistical analysis was done to get information about the homogenity of soil categories by agro-ecological regions and the differences between them. The calculations verified the homogenity within and significant differences between the soil categories (Fig. 4.). This result confirms our concept about the soil as a determining factor of agro--ecological potential under the given conditions. The soil effect on maximum crop yield is about 25-30 %, as it can be seen on the Fig. 4. It is very interesting to compare the magnitude of the soil effect with that of climate on crop yield. According to the calculations of agroclimatologists this effect is about 25 %.

Finally the differences between the agro-ecological regions within the same soil category, the probable causes of standard deviations were analized by interpreting the

Soil category	Standard deviation in % of mean	Mean of yields prognosticated for agro-ecological regions in %
I	11,5 -	66 -
II	7,7 11,7	75 66
III	9,1 15,1	81 77
IV	10,9 14,5	89 86
V	8,1 12,5	100 100

	χ^2-test	DF	F-test	DF
Wheat	4,53	4	54,6	$\frac{4}{100}$
Maize	4,52	3	33,9	$\frac{3}{101}$

Figure 4. Statistical results of yields prognosticated for wheat and maize.

differences of soil conditions by ecological regions. The weighted averages of the prognosticated yields of climatic year types (A, B, C, D) are independent on climate. Within an soil category the variance of the weighted averages can be originated from the different soil distribution in the various agro-ecological regions. These differences which may be 0,8 - 1,0 t/ha in absolute value can be seen on Fig.5. We tried to give the explanations of some of the differences as follows.

For maize within the third soil category the 11. ecological region has the highest productivity. Within this region the prognosis regards to meadow chernozems with salt accumulation in the deeper layers and meadow soils. These soils are quite productive if the distribution of precipitation is uniform in time and space, in opposite case the quantity of yield can be reduced of oversaturation and droughsensitivity, caused by salt accumulation. Meadow soils, occuring here, mostly acidic and only smaller part of them are calcareous from the surface. Their texture are mostly clay loam. The prognosticated yields in the 6. and 10. regions regard to meadow soils instead of meadow chernozem. It takes 60-65 % of what is for 11. This can be explained by that in one-third of these meadow soils have a cemented calcium carbonate layer near to the surface. More than 60 % of these soils are heavy texture.

Soil category	Agro-Ecological Regions 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	18	21	22	29
I	95	74	71	100	-	75	-	88	-	73	77	75	-	90	87	-	-	86	82	-
	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
II	98	80	-	-	-	78	92	91	86	-	90	87	100	95	-	-	-	-	85	-
	-	-	-	-	-	64	82	80	78	72	100	80	-	81	76	-	85	-	-	-
III	-	83	-	-	-	-	90	-	89	-	95	88	100	-	-	-	83	-	84	-
	88	71	97	95	89	64	79	79	74	69	100	77	96	76	71	79	77	82	82	63
IV	91	83	95	98	96	76	92	93	87	80	99	89	100	93	87	92	83	86	82	80
	92	-	100	98	91	68	84	82	77	72	-	79	99	79	-	83	80	87	84	68
V	90	84	96	96	94	-	91	92	87	82	96	90	100	93	88	91	82	85	-	-
	90	74	99	98	90	-	82	82	77	73	100	80	99	78	72	83	80	86	-	-

Upper number for wheat
Lower number for maize

Figure 5. Forecasted relative yield averages of wheat and maize by lowland agro-ecological regions (in percentage of highest yield).

Within the fourth soil category the 13. region is the best for wheat. The prognosis regards here to meadow chernozems with salt accumulation in the deeper layers covering 25 % of the region. The precondition of maximum yield here is to keep the ground water level below the critical depth, to prevent secondary salinization. Forecasted yield in the 6. region is only 75 % of what in 13. has been. Within this region the soil condition is differing from the 13. and it means brown forest, meadow, meadow-alluvial and alluvial soils formed on sandy material. The realisable yields are also less in the 2., 10. and 18. regions. Within the 2. and 10. regions there are chernozem type sandy soils and meadow soils. Meadow soils mostly have limited depth due to calcium carbonate accumulation. In the 18. region the soils are brown earths, slightly acidic alluvial soils and meadow alluvial soils in the valleys and on the terraces of the rivers.

For maize the 3. region is the most suitable, where lowland chernozems are with salt accumulation in deeper layers, which are unfavourable in the case of too high ground water table. For growing maize the 6. region is the less suitable, where there are meadow alluvial soils and alluvial soils with strongly or slightly acidic reaction, and loam or clay-loam texture. Even productivity is limitied by flooded periods. The desintegrated and irregular shape of these soils results some difficulties in their large-scale cultivation . Within the 9. and 10. regions the lower productivity is caused by the erosion of the occuring brown forest soils.

The chernozems of the fifth soil category are the most wheat productive in the 13. region (between Körös and Maros rivers). About 90 % of this region is covered by chernozems. The lowland chernozems are calcareous generally from the surface their texture is loam and water management is the most favourable, as well as their productivity. The meadow chernozems cover the largest part (35 %) within the chernozem area. They have higher water holding capacity and higher water table related to lowland chernozems. For this reason meadow chernozems can be more deeply moistened, which property is advantageous in a drier period. Their organic matter content and natural nutrient resources are also higher. While the chernozems of the 10. region are lighter in texture (Sandy--loam, loam) and slightly acidic in the upper layers, these properties can be the causes of less productivity. In the case of 15. and 18. Transdanubian regions the smaller productivity can be related to the finding of soils on a more or less eroded undulating surface.

It can be concluded from the above analysis that various relief and soil properties as exposition, texture, pH, humus content, etc. beside soil genetic type can be important from the viewpoint of agricultural production.

The possibility to increase the agro-ecological potential is to get nearer the productivity of soils to that of the optimal soils. The differences in the productivity of the same soil category within the various agro-ecological regions can't be eliminated, because the soil conditions are relatively constant determining factors of the agro-ecological potential.

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A FRAMEWORK FOR THE STUDY OF THE DYNAMICS OF AGRICULTURAL SYSTEMS

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INTRODUCTION

Throughout history, agricultural systems have been much subject to change. While some changes have been internally generated, the majority are responses to externally-generated events and processes that occur in the physico-chemical, biological, social, economic and technological environments. Recently, a third category of change has appeared, in which changes have been forced on the farmer by a societal objection to the way that agricultural systems are degrading their environment, both external and internal. To introduce a new programme of research in the Centre for Environmental Technology at Imperial College, London, I outline here some ecological principles and methods which will be applied to agricultural systems in the hope of clarifying the basis of their dynamics. To illustrate the sort of approach that will be undertaken in selected study-sites, I present a simple model of the productivity, labour requirement, and internally-generated soil degradation of a low-technology system of shifting cultivation. The trade-offs between food production and employment generation on the one hand and environmental protection on the other will be explored.

PRINCIPLES AND METHODS

Classical approaches to the dynamics of natural ecosystems have largely addressed questions of their development from an assumed null-state, or of variations in the development path induced by different types of interference. Development (i.e. "succession") has usually been assumed to be directed towards a unique, more-or-less stable, final state. The responses of ecosystems to natural perturbations have been studied because the outcome of such natural experiments often throws light on the processes whereby succession occurs. To analyse experimentally such processes, ecosystems have sometimes been artificially perturbed using a variety of means.

Agricultural systems tend to show much smaller changes with time. Indeed, from an ecological point of view, they consist of early stages of successions which have been delayed indefinitely by harvesting activities and other forms of human control. Intensive cropping holds the succession at a very early stage, while pastoralism allows development to proceed somewhat further. Although the systems are usually managed to keep them in near-steady state, they respond to a rich variety of external stimuli. Accordingly, an early, descriptive phase of the present study will be to consider what light the published descriptions of responses to environmental stimuli throw on the dynamics of agricultural systems. Common exogenous sources of perturbations are classified in Table 1 according to whether they are physical, chemical, biological, social or economic.

In an alternative descriptive approach, perturbations can be classified according to the time-courses of change in the variable(s) involved. Considering first the source of the perturbation, a pulse or "spike"-type stimulus (Fig. 1a) is one where a driving variable external to the system shows an abrupt but short-lived extreme deviation from its normal distribution of values. Other kinds of stimulus include "step" changes where the value of the driving variable shifts abruptly to a new

Table 1. Classification of environmental events and processes causing changes in agricultural systems. The classification is based on the nature of the main underlying mechanism.

a) Physical	Drought; flood, torrential rain; tornado; hail; frost; deposition of volcanic ash; radioactive contamination; soil loss (e.g. landslide, erosion); submergence in blown sand.
b) Chemical	Volcanic emissions (e.g. SO_2); natural ozone enhancement of the air; industrial emissions (e.g. SO_2); chemical warfare (e.g. 2,4-D on crops); increase of atmospheric CO_2 content.
c) Biological	Immigrations of pests (e.g. locusts) and diseases (e.g. potato blight).
d) Social	Births, deaths and illnesses in the farm family; calls for help from neighbours; change in social status (e.g. promotion or ostracism); call-up to armed forces.
e) Economic	Supply fluctuation and therefore price variation due to conditions in other producing areas; changes in the costs of agricultural inputs (e.g. fertiliser) and of transportation; taxes; national marketing and subsidy agreements; consumer fashion; aid projects.
f) Technological	Invention and introduction of new machinery for land preparation, planting and harvesting of crops; appearance of new techniques for handling animals (e.g. automatic feeding and milking); new varieties and breed; new pesticides and fertilizers.

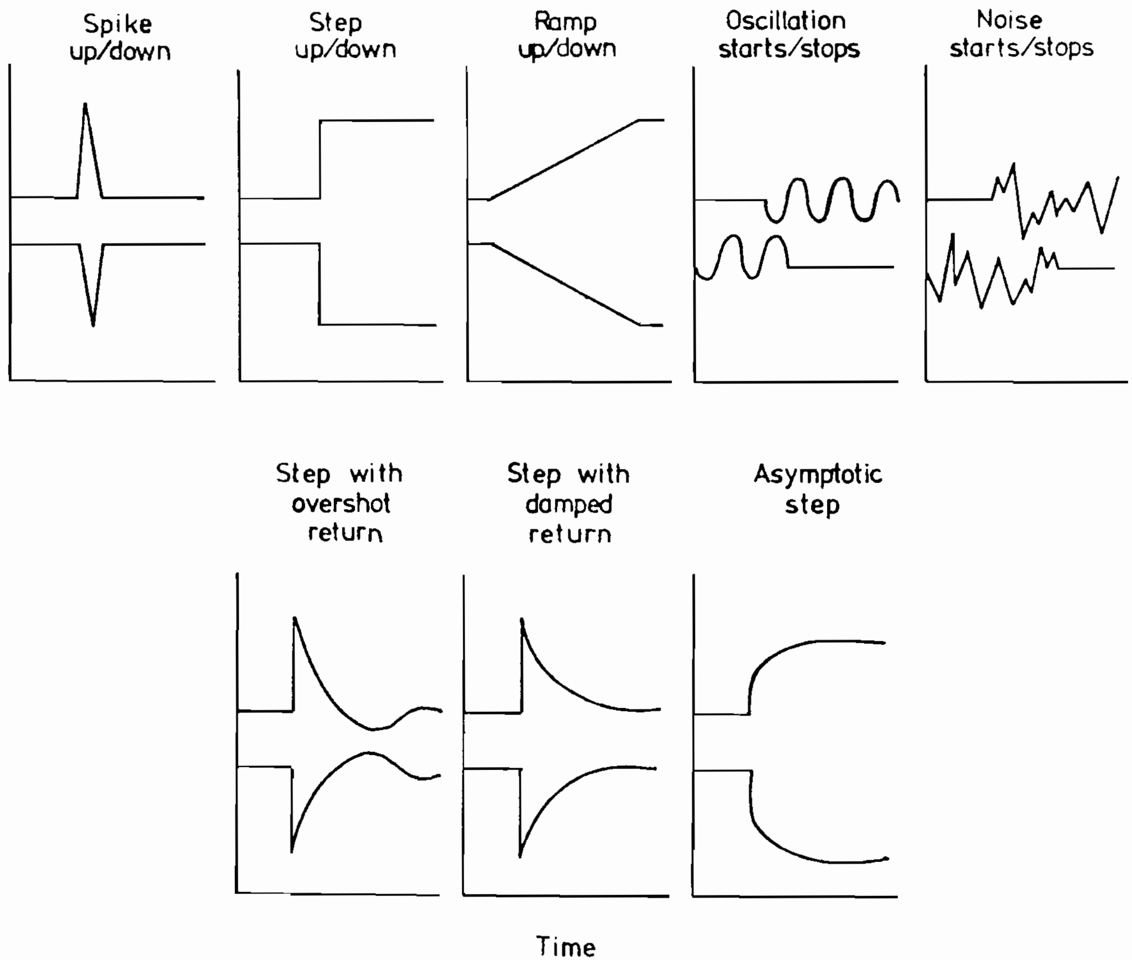

Figure 1. Common types of dynamic behaviour of variables involved in exogenous perturbations of agricultural systems: (a) stimuli and responses, and (b) responses only. For examples, see Table 2.

maintained level, "ramp" changes where there is a sustained trend over a significant period, and regular and random fluctuations that either begin or end (Fig. 1a).

The responses to these stimuli can be categorised in a corresponding, slightly extended, fashion (Fig. 1a,b) so that a range of combinations of stimulus- and response-type can be identified. A preliminary selection has been brought together in Table 2. This table suggests that: (1) only abrupt stimuli (spikes and steps) can have spike responses, (2) all stimulus types can have responses of the same type, and (3) strongly lagged responses and overshoots are possible but seem not very common.

A first comment on Table 2 is that the type of response observed may well depend on where in the hierarchy of systems from field level to world level the particular "agricultural system" is situated: while a single observed farm may respond to a certain step stimulus with a step response, an observed population of farms showing randomly lagged step responses will respond to the same stimulus with some kind of ramp. A second comment is that the exact form of the stimulus m be crucial in determining the response. Thus, a step change in an environmental variable may produce a step response while a ramp change may be gradually adjusted to within the system and so seem to produce no response at all This implies that, depending on which system variable is considered, the same stimulus may or may not be seen to produce a perturbation. A third comment parallels the second: the same stimulus applied at different times can produce different responses. For example, a rain storm soon after crop-planting on a steep slope may erode the soil catastrophically so that the land can never again support a plant cover; the same storm some weeks later may cause no irreparable damage because the land is protected by the crop canopy (Fig. 2a).

Table 2. Examples of stimulus-response combinations classified according to the time relationships of the stimulus and response involved. Names of types of time relationship are given in Fig. 1.

STIMULUS TYPE	RESPONSE TYPE			
	Spike	Step	Ramp	Damped return
Spike	Wind storm temporarily closes stomates	Rain storm erodes soil exposing unproductive rock	Establishment of trash bunds leads to terace formation and gradually decreasing runoff	Rain shower in arid zone produces short-lived burst of grass growth
Step	Law changes, and farmers organise one-day strike that halts market deliveries for a day	Rise of water level following breaching of dike stops crop growth	Farmer dies and farm productivity shows steady decline	Faced with great pest problems, farmer renounces pesticide, suffers temporary great loss, but gradually establishes alternative controls
Ramp		Falling price for product finally forces farmer to abandon farm and migrate to city	As product price rises percentage of area planted to it increases	
Oscillations start/stop		Nation starts summer daylight saving so farmer, unable to face rise in labour costs of summer milking, sells cows	Regular use of erosion-control measures started and leads to progressive rise in residue production, rainfall infiltration and yields	Water-management works lead to regular flooding. All farmers leave but as adaptation possibilities are recognised, families gradually return
Noise starts/stops		New smelter emission causes crop damage in direction depending on wind. In nearby farms, cultivation of susceptible crop ceases in the next season	Destruction of flood defences lead to irregular flooding and progressive depauperisation of farmers as consecutive crops fail	Product price becomes unstable and so progressively less of this crop is grown

Cont/

Table 2 (cont)

STIMULUS TYPE	RESPONSE TYPE: Overshot return	Step without return	Oscillations stop/start	Noise stops/starts
Spike	Flood reduces pasture growth this year but silt deposited enhances growth in next year	Intense erosion leaves so little soil that slow erosion continues till rock is reached		
Step		Irrigation introduced gives immediate yield rise which continues to plateau as utilisation skill increases		
Ramp				
Oscillations start/stop			Water management works lead to regular flooding. Farmers continue cropping but plant only at the end of a flood	
Noise starts/stops				Irregular peaks in product price attract opportunist producers able to set up fast, temporarily exploit the high price and then switch as price falls

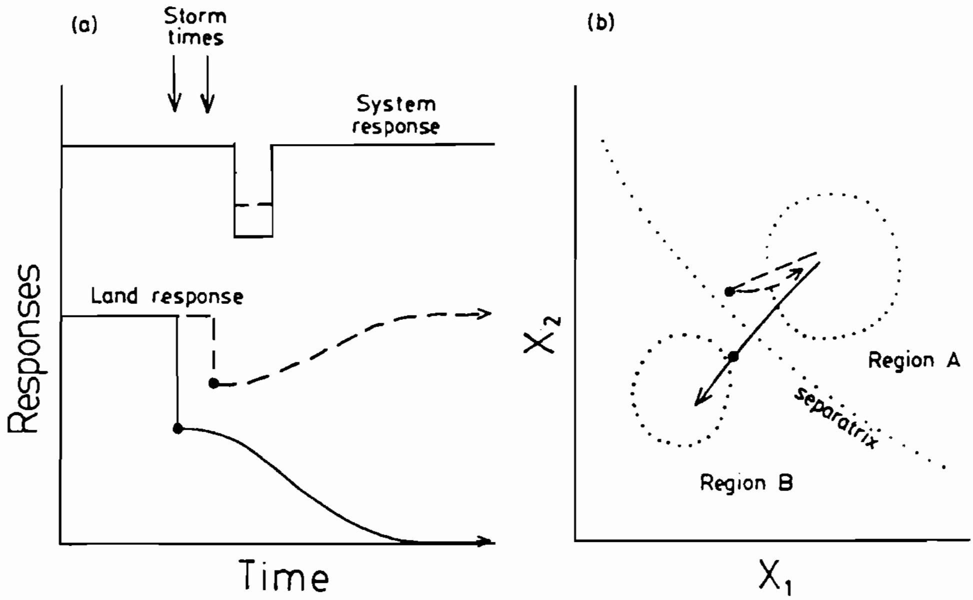

Figure 2. (a) The same storm at different times has different effects: land can be destroyed or suffer only temporary damage. In either case, the whole system may show only temporary loss of output.

(b) The configuration space of the land system showing responses to storms at different times. The regions represent locally-stable equilibria.

A situation such as just described can be represented diagrammatically in terms of two arbitrary system variables (Fig. 2b). From the point of view of the land, the system is seen to have two, alternative equilibrium regions. For the system to move from region A to region B, a specific stimulus of sufficient intensity is necessary. Since the system is so unlikely to move in the reverse direction (i.e. from almost bare rock to full soil cover), region B is effectively an absorbing state. However, as shown above, the definition of the system and choice of indicators affects the response type. Thus, from the point of view of the farmer's food-production system, the total loss of some land may only temporarily reduce food output. With unlimited forest available, alternative wild food sources can probably be found in the year of the crop loss; in succeeding years, an adjustment of the area cultivated can quickly restore the productivity of the shifting cultivations (Fig. 2a). Even if portions of land have moved in state space from one equilibrium region to another, the food-producing system as a whole remains in its original region.

For the farmer and society, a critical property of agricultural systems is their capacity to withstand perturbations (Holling 1978). If "withstanding" is seen as a near-zero response to a potentially destructive stimulus, a system showing such a response with respect to <u>configuration</u> and <u>behaviour</u> is said to be "resilient"; a system showing near-zero response with respect to <u>output</u> is "<u>stable</u>". Degrees of resilience and stability should ideally be judged by relating system response to the intensity of the stimulus. However, no wholly satisfactory way of doing this has yet been proposed. The specificity of the response to stimuli illustrated above implies that resilience and stability can only be measured with respect to particular stimuli. According to the provisional definitions proposed here, there is some necessary correlation between the two characters: although a system which bounces back to its original configuration after experiencing a potentially harmful stimulus may or may not show a temporarily reduced output, a system whose configuration is permanently changed by the same stimulus will certainly show reduced output. Only while a system is intact can its stability be assessed and so the rigorous measurement of stability depends on the definition of the intact system. In fact, given a system accepted as intact, stability can be operationally measured as the reciprocal of the coefficient of variation of some output variable. The measurement of resilience depends crucially on what constitutes an intact system, but once this is defined, the threshold intensity of a stimulus that just causes departure from intactness can be determined. An index of the resilience of the system with respect to a given stimulus is the magnitude of this critical stimulus intensity.

Because of increasing doubts as to the sustainability of present levels of food production, it is important to identify systems (or parts of systems) associated (1) with high sensitivity to harmful external stimuli or (2) with steady reductions in agricultural potential. Alternatives for such systems or system components can then be sought. If "durability" is defined as the expected time until a given system departs from intactness, then it can be predicted in case (1) by calculating the reciprocal of the sum of the probabilities of the occasions on which various stimuli attain or exceed the intensity at which destruction occurs and in case (2) by extrapolating from the time trends of the critical system variables.

The distinction made between the two types of durability introduces the distinction between system degradation due to external, and that due to internal, agencies. Exogenous degradation is often abrupt while endogenous degradation tends to be gradual. To complement Tables 1 and 2 which are concerned only with exogenous changes, in Table 3 is listed a selection of endogenous processes and events that can lead to down-grade changes in a farming system. As in Table 1, the type of process can be classified according to mechanism as physical, chemical, biological, social and economic. It must be noted, however, that where a complex of processes is involved, the choice of a single mechanism for classification purposes may be arbitrary. The Tables illustrate the range of processes and mechanisms that have on occasions been perceived as causative.

Where the system considered is the individual farm or field, much is known of the processes that determine overall changes of agricultural potential and of the rich variety of ways in which they are linked. It is at this level that process-oriented modelling will be most useful in the present programme in characterising system dynamics. At this level, human intervention is most effective and so the consideration of farmer behaviour in any models becomes vital. Since the farmer's reaction to the sorts of events and processes mentioned in Table 3 is conditioned by his perception of the farm environment (economic, physical, etc.), the within-system models will most usefully be interfaced with models of his decision-making process. In this way, the likely distribution of outcomes in any situation can be simulated as it corresponds with, say, the distribution of farm sizes and risk averseness of a population of farmers.

If the farmer's management problem were to consist only of optimising the operation of endogenous processes in a water-tight system, it would yield easily to methods of deterministic optimal control. The actual great difficulty facing the farmer is how to manage his within-farm processes (Table 3) so as to attain personal goals, not all economic, and simultaneously to minimise the farm's vulnerability to potentially-damaging environmental events and processes (Tables 1,2). The impact

Table 3. Classification of endogenous events and processes that cause changes in agricultural systems. The classification is based on the nature of the main underlying mechanism.

a) Physical	Blocking of drains leading to waterlogging; soil erosion; washing downwards of the fine soil fraction due to irrigation.
b) Chemical	Nutrient depletion because of insufficient recycling; nutrient loss through run-off and leaching; pH decline through intensive use of N-fertilisers; laterisation through lack of shade over soil surface; loss of soil organic matter through intense cultivation.
c) Biological	Build up of weeds because of, say, farmer falling ill; development of a weed flora resistant to the only available herbicide; a destructive pest becoming resistant to the last cheap pesticide; a fungus disease breaking the resistance of a staple crop.
d) Social	Departure of children to marry; discord within the farmer's family.
e) Economic	Demands of children for payment for labour causing the farm to become uneconomic; lack of monitoring of pests leading to overspending on prophylactic sprays (and other forms of mismanagement).
f) Technological	Multiplication by farmer of a mutant genotype resistant to a disease allows him to plant the crop in normally closed season; his increasing experience in cropping different fields of the farm allows the farmer to achieve steadily rising yields.

intensities of these environmental factors follow probability distributions that are often uncertain and site-specific so that immediately the problem becomes one of stochastic control. Without knowledge of the underlying parameters of his variable system, the farmer is forced according to his level of risk aversion into either a reliance on traditional methods or a more innovative strategy of adaptive control (Holling 1978). The way in which an innovative farmer trades off short-term productivity against long-term security in response to perceived threats from exogenous and endogenous factors seems to be a fruitful and important area for enquiry.

Where the system considered is more macro-scale, perhaps an agricultural region or a world-wide industry, the processes and linkages are less well understood. Nevertheless, to illustrate the ways in which dynamics vary with scale of the system, the production of just one single commodity (perhaps wheat or rice) will be examined in the present programme.

A further factor that constrains the farmer's management options arises from society's response to the working of agricultural systems. The community-at-large has drawn the farmer's attention to the leaks of sediment, nutrients, biocides and growth regulators from his systems, usually as pollutants in water courses but also as residues in marketed products. Fortunately for the farmer, societal pressure is predictable at least in the short term although its actual strength as expressed in legislation is affected by the uncertainties of government processes. From the farmer's economic point of view, the societal feed-back on his activity is nearly always negative, tending to reduce his productivity and profits.

To show the range of environmental consequences of events and processes occurring in agricultural systems, a selection of consequences is classified in Table 4 according to whether the costs or benefits are borne mostly by the farmer alone or shared with society. In western countries, society has already responded to several of the costs listed in Table 4(ii) by legislative control of the farmer. In most developing countries, productivity and profits are at present valued more highly than environmental protection. As the environmental costs of some production processes are more clearly defined, this valuation may change, but this will depend on whether the country can afford the protection measures.

MODEL OF ENVIRONMENTAL DEGRADATION ASSOCIATED WITH SHIFTING CULTIVATION

A recent visit to a University of the Philippines study site in the hills of Luzon (Nguu and Corpuz 1979) prompted a consideration of the dynamics of shifting cultivation and the ways that the farmer's decisions affect the rate of degradation of the soil's productive potential. In terms of the previous discussion, such soil degradation is largely endogenous. Its effects are partly internal (affecting future farm productivity) and partly external. The present model treats only the internal effects concerned with nutrients because a consideration of erosion awaits the results of measurements still in progress (Sajise and Raros 1978).

The model to be presented is a general one in that it is based on data from studies in a range of seasonally-dry, tropical forest areas. It seeks to illustrate the possible usefulness of a modelling approach in case a government should ever need to legislate to control the way in which shifting cultivation is practised in the hills in order to preserve the productive capacity of the soils.

In the model, the available land area A is taken to be cultivated in rotation with each part cultivated for t_c years and then abandoned to

Table 4. Events and processes that cause changes in agricultural systems classified according to whether their environmental effects are (i) internal to the system or (ii) external as well as internal. Within these categories, classification depends on the nature of the environmental effect, and on whether the event/process is itself mainly endogenous (EN) or exogenous (EX) in origin.

(i) Effects mainly internal

Physical	Soil compaction because land worked when too wet (EN); low-lying meadows waterlogged because river is in flood (EX).
Chemical	Heavy-metal content of pastures reaches level dangerous to stock through long use of slurried municipal waste (EN); some fields declared unusable because of leak from adjacent chemical factory (EX).
Biological	Infestation of perennial weed because of reliance on zero tillage and herbicides without rotation (EN); switch to keeping work horses because of rise in fuel costs (EX).
Social	Family member ill so rest of family has to work harder (EN); minimum agricultural wage raised, cost of outside labour becomes prohibitive, so farm family has to work harder (EX).
Economic	Long overdue renovation of farm buildings undertaken by farm family (EN); reassessment of rateable value of farm (EX).

Cont/

Table 4 (cont)

(ii) Major effects external as well as internal

Physical	Lack of erosion protection leads to heavy sediment loads in water draining from farm (EN); new government subsidy induces farmer to clear more land for grazing giving faster runoff and flooding down the valley (EX).
Chemical	Excessive fertilisation leads to eutrophication of nearby lake and consequent foul smell (EN); local nuclear power-station contaminates fields but contaminated milk marketed before the leak is recognised (EX).
Biological	Poor weed control in meadows leads to drift of airborne seeds onto neighbour's property (EN); locust alert induces farmer to spray his crops with anti-feedant so arriving locust swarm moves to neighbour's crops (EX).
Social	Farmer changes to strict organic farming and commune develops to provide hand labour (EN); fall in product prices forces farmer to sell up and migrate to city (EX).
Economic	Organic-grown product offered to a market wary of pesticide residues sells so well that other local growers consider switching to similar methods (EN); volcanic ash falls on area of acid soil greatly increasing productivity and farmers' incomes (EX).

fallow for t_f years. With n crops per year, nt_c crops are grown in the cropping phase. Each year, an area $a = A/(t_c + t_f)$ is cleared for cultivation. A family of 3 man-equivalents* (ME) lives on the products of the shifting cultivation; they can provide a maximum possible labour input L_{max} of 1.5 ME. Under the conditions assumed, nitrogen either as protein or as nitrate is limiting both humans and crops so that both food and soil fertility can be measured in terms of nitrogen only. The human daily requirement of about 50 g of protein (UNESCO 1978, p. 356), the size of the family (3 ME) and an assumed 6% of nitrogen in protein leads to an assumed minimum necessary food output F_{min} of 3 kg y^{-1} of (protein) nitrogen.

To provide the often-observed descending curve of yield against crop number in a sequence (Fig. 3a), it is supposed that a proportion x of a reserve of (available) soil nitrogen present at the start of crop growth is removed each year in the harvested food after which the rest is returned to the available soil pool. If, at the start of the first crop-and-fallow cycle considered, there are $N_{oc}^{(1)}$ kg ha^{-1} of (available) nitrogen in the soil, then after one crop $N_{oc}^{(1)}(1-x)$ kg ha^{-1} remain. After t_c years, i.e. when the fallow period is starting, the residual amount is $N_{oc}^{(1)}(1-x)^{nt_c} = N_{of}$ kg ha^{-1}. During these t_c years, the weight of protein nitrogen harvested will be $aN_{oc}^{(1)}(1 - (1-x)^{nt_c})$ kg. At the steady state assumed here, with areas of the size a in the 1st, 2nd, 3rd, ..., and t_c-th year of cropping, just this same amount of food will be produced from the whole enterprise in one year. This will be the annual food production F.

Considering the regenerative process under the t_f years of fallow, if

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* strictly man-equivalent-years per year

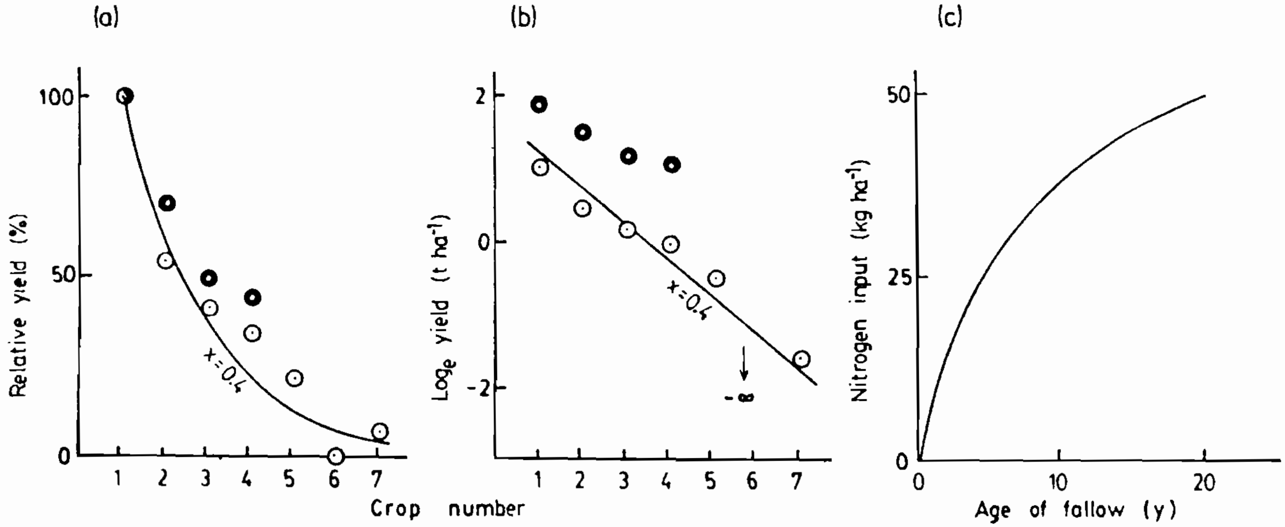

Figure 3. (a) Reduction of yield in crops grown consecutively on newly-cleared land without fertilizer. Open symbols: rice in Amazonia; filled symbols: maize in Nigeria (data of Sanchez and IITA in Sanchez 1977).
(b) The same data on a logarithmic scale. In (a) and (b) theoretical lines are drawn corresponding to a value of x = 0.4.
(c) Assumed increase with time of the input of soil nitrogen from cleared bush fallow.

there is no (available) soil nitrogen at all remaining at the start of these years, the level is taken to rise with time spent in fallow according to the curve in Fig. 3c. The decrease with time of the rate of accumulation of soil nitrogen mimics observations made on natural successions that start from bare ground (Major 1974). After t_f years, the level of nitrogen in the soil and vegetation has reached a level such that $N_{oc}^{(2)}$ would become plant-available on clearing for the start of the second cropping-and-fallow cycle. This level of available nitrogen is given by $N_{oc}^{(2)} = N_\infty t_f/(K_N + t_f)$kg ha^{-1} if the level of nutrient N_{of} at the start of the fallow was zero. Here, N_∞ is the available level obtained on clearing an infinitely old fallow and K_N is the time in years needed for the level to rise to $N_\infty/2$ if it started at zero.

If however the level of soil nitrogen N_{of} at the start of the fallow is not zero, a time t_f' must be calculated which represents the time under fallow that would have been needed for the soil to reach the level N_{of} if the starting level had in fact been zero. This time t_f' is thus the time-equivalent of the residual level of soil nitrogen left after t_c years of cropping, and is found by solving for t_f' in the equation $N_{of} = N_\infty t_f' /(K_N + t_f')$. This equation is analogous to that for $N_{oc}^{(2)}$ given above. Thus, $t_f' = N_{of}K_N/(N_\infty - N_{of})$.

Adding the time-equivalent t_f' of the residual soil nitrogen to the actual time spent in fallow t_f gives an expression for $N_{oc}^{(2)}$

$$N_{oc}^{(2)} = \frac{N_\infty(t_f + t_f')}{K_N + (t_f + t_f')}$$

in units of kg ha^{-1}.

The extent of the change in the yield potential of the soil due to one cropping-and-fallow cycle is calculated by comparing the initial and final contents of available nitrogen. The percent change is given by $100(1 - N_{oc}^{(2)}/N_{oc}^{(1)})$. Until the accumulative effects of erosion are included in the model, long-term trends cannot be usefully predicted. Hence, attention is confined to a single cycle. The difficulty of jumping directly into a steady-state rotation is acknowledged, but conceptual simplicity is pursued for the sake of illustrating the use of the model.

The labour requirement L (in ME) is calculated as the sum of a cropping cost and a clearing cost. The term for the cropping cost is ant_cP where P is the labour needed to crop unit area. The term for clearing is made proportional to the amount of material to be cleared which itself is proportional to the calculated level of soil nitrogen accumulated that would be available after slash-and-burn clearing of the fallow. The clearing cost is therefore $P_\infty(t_f + t_f')/(K_N + t_f + t_f')$ where P_∞ is the labour needed to clear virgin forest. This is consistent with the observed greater labour requirement for clearing virgin jungle than secondary forest (Ruthenberg 1971). For the assumed family, L must be less than L_{max}.

The model in full is:

$$F = aN_{oc}^{(1)}(1 - (1-x)^{nt_c})$$

$$L = a(nt_cP + \frac{P_\infty(t_f + t_f')}{K_N + t_f + t_f'})$$

$$S = 100(1 - \frac{N_\infty(t_f + t_f')}{N_{oc}^{(1)}(K_N + t_f + t_f')})$$

with

$$a = \frac{A}{t_c + t_f}$$

$$t_f' = \frac{N_{oc}^{(1)}(1-x)^{nt_c}K_N}{N_\infty - N_{oc}^{(1)}(1-x)^{nt_c}}$$

and conditions $F \geq F_{min}$ and $L \leq L_{max}$

PARAMETER ESTIMATION FOR THE MODEL

The level of plant-available soil nitrogen at the start of cropping is assumed to match the level in the partially-burned material left on the soil surface after forest clearing. Much of the nitrogen mineralised from the soil organic matter is leached at the onset of the rainy season (Chabalier 1976) and so, to compensate for this, soil organic nitrogen is provisionally ignored. The maximum initial level N_∞ is that found after clearing virgin forest, e.g. 70 kg N ha^{-1} in Amazonia (Sanchez 1977). The value taken for a standard initial level $N_{oc}^{(1)}$ assumes secondary rather than virgin forest: the labour needed to clear secondary forest in Borneo is about two-thirds of that needed for virgin forest (Ruthenberg 1971, p. 49), and so the initial nitrogen level is taken to be 70 x 2/3 = 46 kg N ha^{-1}.

The form of the nitrogen yield model proposed earlier requires that the regression of crop yield on crop number should be linear on a logarithmic scale. Near-linearity of the regressions is indeed found (Fig. 3b) in sets of data from Amazonia and W. Africa (Sanchez 1977); the slope of the longest run of points suggests a value of about 0.4 for the parameter x.

Labour requirements for cropping are based on data for a Philippine cultivator, Na Vito (Nguu and Corpuz 1979). This lady spent slightly above half her available time in a 7 month period cropping and marketing produce from slightly over 0.5 ha of annual crops on hill land. With this activity continuing throughout the year and achieving up to 2 crops y^{-1} ($n = 2$), the labour requirement is about 0.5 ME-y ha^{-1} $crop^{-1}$. Figures for shifting cultivation in Zaire are very similar (Ruthenberg 1971, p. 49).

The labour needed to clear virgin forest is based on the mid-point of a range observed in Borneo (Ruthenberg 1971). Allowing a 5-day week for this particularly arduous work, this value, 366 ME-h ha^{-1}, represents just under 0.2 ME-y ha^{-1}.

Data have not yet been found to estimate the length of bush fallow needed to attain half the maximum surface input of nitrogen. Assuming that nitrogen level in this input is proportional to total N present, data of total N from the Congo (Bartholomew et al. 1953, cited from Major 1974) are useful in showing that, as modelled, initial accumulation rate falls off significantly after 5 years. Since a run of nitrogen data at a single site is not available, the value of the "half-saturation" constant K_N was estimated as 8 years from data of basal area in Gabon (Catinot 1965, cited from UNESCO 1978, p. 541). The resulting curve of nitrogen input against time is given in Fig. 3c. According to this, a forest stand 45 years old such as described by Greenland and Kowal (1960) as "mature", would be expected to have achieved 85% of its ultimate capacity to produce a nitrogen input.

These parameter values are summarised in Table 5.

Table 5. Parameter values used in the model

N_∞	70 kg N ha^{-1}
$N_{oc}^{(1)}$	46 kg N ha^{-1}
x	0.4
P	0.5 ME
P_∞	0.2 ME
K_N	8 y
n	2 y^{-1}
t_f	10 y
A, t_c	varied

RESULTS OF THE MODEL

Three sizes of land holding are considered: 2.5 ha (the size of Na Vito's), 10 ha and 40 ha. On these holdings, the effects were calculated of taking increasing numbers of crops from any piece of land before abandoning it to fallow. The fallow period was fixed at 10 years. In Fig. 4 the results are plotted to show how food production in ME and loss of yield potential within a cycle depend on the number of crops taken. The iso-lines for labour requirement in ME are superimposed to show the area (hatched) that could be handled by the family within their labour constraint of 1.5 ME.

Bearing in mind the preliminary nature of the model, the following conclusions may be drawn from Fig. 4:

(a) As crop number increases up to 6, food production increases. Beyond 6 crops (i.e. 3 years double cropped), food production from a given area falls because excessive area is committed to low-yield crops instead of to recuperative fallow.

(b) Up to 6 crops, any rise in food production is at the expense of faster land degradation. There seems no justification possible for taking more than this (commonly found) number of crops.

(c) Labour productivity falls as the number of crops increases. Shifting cultivation of this sort generates little employment compared with intensive continuous cropping.

(d) On an area such as available to Na Vito (2.5 ha), taking a single crop only is predicted to provide 4.4 ME of protein food while taking 6 crops could provide 8.4 ME.

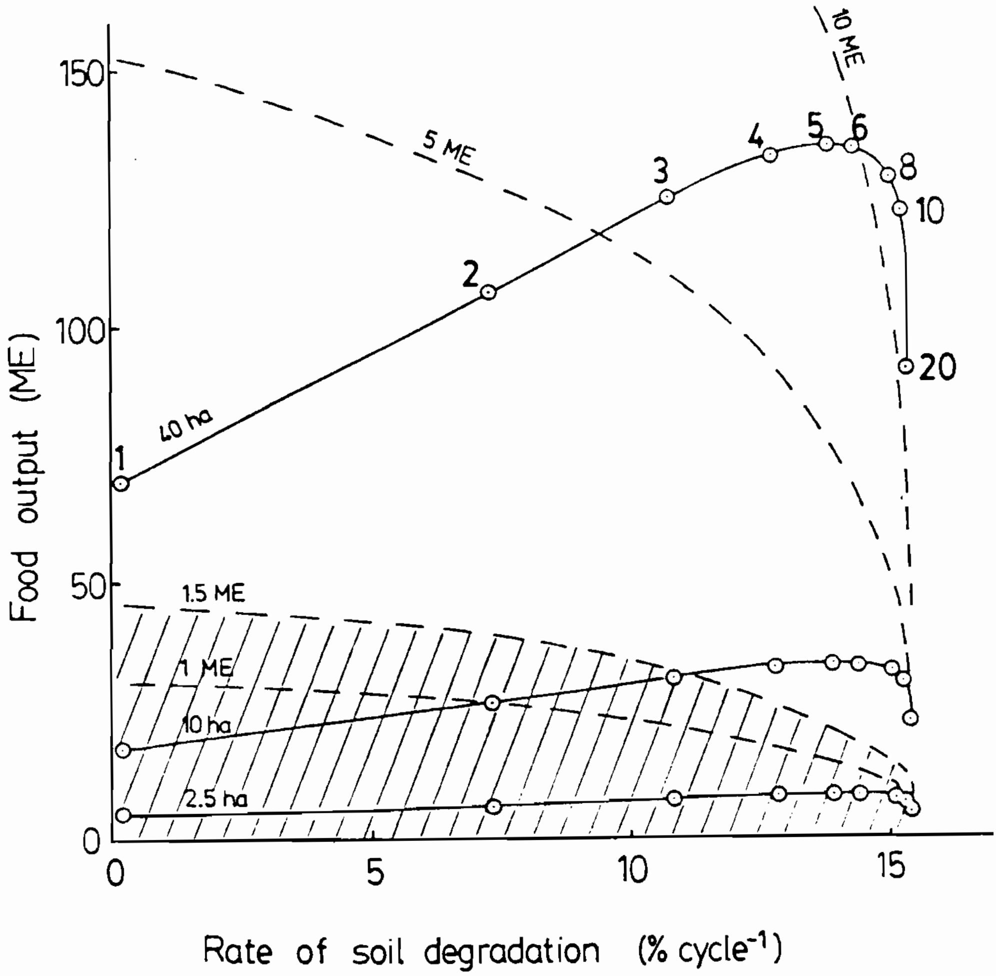

Figure 4. Relation between food output in man-equivalent-years per year (ME), rate of loss of the soil's potential, and number of crops grown before the 10-year fallow. Three sizes of available area are considered. Contours of labour requirement are given in ME. Hatching indicates the area within the labour capability of the hypothetical family of 3 man-equivalents.

(e) To just absorb the 1.5 ME of labour of the postulated 3 ME family, on 10 ha they would take 3 crops. Most profitable of all for them, however, would be taking 1 crop on 20 ha. Labour productivity is correlated with the conservation of fertility.

(f) As population pressure increases, the likely tendency is for holding size to diminish, crop number to increase, total productivity per holding and labour productivity to fall and rate of fertility depletion to rise. Future versions of the model will explore this evolutionary process.

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OVERVIEW OF THE MEETING

G. Golubev and I. Shvytov

This is a replica of the meeting's overview published earlier (CP-80-32). We are grateful to the chairmen and rapporteurs of the seesions whose reports have been used to prepare this paper.

The Opening Session

In the first part of the opening session, G. Golubev, K. Parikh and I. Shvytov outlined the main objectives of the Task on "Environmental Problems of Agriculture," of the Food and Agriculture Program and the meeting in question, respectively.

The second part of the opening session was based on two major papers: "A Hierarchical Approach to Agricultural Production Modeling," presented by C.T. de Wit and "The Modeling of Environmental Impacts of Crop Production," by D. Haith. Both papers provided information concerning current models and modeling bases. As a result of discussion of the first paper, it was concluded that simulation models describing natural processes of crop production systems should be combined with linear programming models of agricultural management. The simulation models should provide selected inputs, such as yield, nitrogen leaching, and nutrient and sediment losses for the LP models. Both simulation and LP models are linked to a "reclamation level," which is a key determinant for management options as well as feasible combinations of nutrient, water, and other material inputs. In general, the agricultural-environmental models should provide a means for analyzing a variety of crop production management problems, while allowing for potential environmental impacts.

The paper by D. Haith deals with mathematical models for analyzing nonpoint source water pollution from cropland. These models are mainly chemical and sediment loading models, but also include planning and management models, which encompass regional planning, watershed planning, and farm management models. Haith discusses four operational models developed at Cornell University and based on the Curve Number Runoff Equation of the U.S. Soil Conservation Service and the Universal Soil Loss Equation. It was recommended that the Watershed Loading Functions Model could be used to estimate chemical export in stream flow from agricultural watersheds. Both the Pesticide Runoff Model and Cornell Nutrient Simulation Model can be used to predict losses of pesticides and nutrients with runoff as well as nitrogen leaching from agricultural fields. The Farm Management Model is a simple linear programming model which can be used to maximize farm income allowing for constraints on nitrogen, phosphorus, and sediment losses from the farm.

THE NITROGEN LEACHING PROBLEM

The presentations on nitrate leaching indicated that this aspect of nitrogen behavior in the soil-plant system is adequately simulated. One of the presented models showed that nitrogen leaching can make a significant impact on the efficiency of nitrogen fertilizer use and therefore, on environmentally undesirable waste of the nitrate form of nitrogen. The model by T.M. Addiscott allows for the effects of soil aggregation, particularly the hold-back solutes. It was concluded that one needs to distinguish between nonmobile water which holds back solutes, and mobile water in the anion exclusion zone, which does not hold back solutes. There was discussion as to whether there is a real difference between the cascade model for leaching and a piston flow model. The participants agreed that the answer should depend on the relationship between the soil profile and the size of the rainfall input. It was also pointed out that allowance must be made for the nitrification, mineralization, immobilization, and denitrification of nitrogen. There are now models for nitrification, mineralization, immobilization, and denitrification, but these models have only partly been combined with models for the other processes significant for nitrogen leaching. At present, one of the main problems in the application of nitrogen leaching models for practical purposes is the absence of well defined criteria, indicating to what degree nitrate leaching is acceptable.

SURFACE LOSSES OF CHEMICALS FROM CROPLAND

Since hydrological phenomena in cropland areas constitute some of the main factors which lead to losses of chemicals, particular attention was paid to water balance processes. J. Balek discussed various limitations and constraints placed on various simulation models for describing the hydrological phenomena. It was pointed out that there is a lack of data bases for providing model parameter estimates as well as verification of model outputs and therefore, models should be built with this limitation in mind. At present, the extension of both existing hydrological models and experimental data from the field and watershed levels to the regional level poses a problem.

M. Holy presented a mathematical model of surface runoff from a uniform slope. The solution of this mathematical model enables calculation of the average velocity and height of the surface runoff at any point on the slope, as well as the total volume of runoff at the bottom of the slope. M. Holy suggested that the simulation of runoff in an entire catchment is possible by matching the runoff from several slopes within the modeled area.

S. Rao presented a state-of-the-art review of models for simulating pesticide behavior in agroecosystems. Very detailed and complex models as well as simple, physically-based models for retention, transformation, and losses of pesticides were discussed.

It was concluded that the central problem is not a lack of mathematical models but that of selecting an appropriate model and verifying it. The meeting pinpointed the problems of independently estimating the large number of parameters in complex models. The problem is associated with the variability of soil properties determining pesticide fate. It was recommended that rather than comparing average measured response, the confidence limits of simulation, as well as measurements, should be considered.

SIMULATION OF ECOLOGICAL ASPECTS OF CROP PRODUCTION ENVIRONMENT

Environmental aspects of crop production systems were discussed in connection with ecological processes studied with both simple and complex models. Special attention was given to the experience in applying these models when making management decisions. Two deterministic models of C. Lyons' for assessing the effects of meteorological conditions on crop production and the effects of the agricultural environment ecology were considered. This type of model is usually formulated as a series of equations describing physical, chemical, and biological processes. One of the problems of this type of model is that it consists of a collection of submodels, and although the individual submodels are verified, it may not be easy to do the same for the overall model. It was concluded that because of the complexity of these models and their large parameter requirements, they are designed more for understanding the situation than for making management predictions. It was recommended that O. Sirotenko's model possibly could be used for making detailed estimations of plant evapotranspiration, soil water content, and plant production. Moreover, this and similar types of models can also be used to predict the effects of additional irrigation or climatic changes on crop yield. This information could be used for making a management decision.

The simple model presented by B. Trenbath examined the stability of food producing systems in developing countries, with the objective of discovering how these systems could be more stabilized. The model allows decisions to be made concerning the value of different cropping practices and cropping systems.

Two papers dealt with statistical models which enable one to estimate potential resources for biological productivity in Hungary (K. Rajkai, I. Valyi). An approach presented by Valyi can be used to assess projected yields of wheat and maize based on the data derived from the knowledge of experts. The models of this type can be used for detailed analysis of the limiting effects of soil and climate on potential yield.

Special discussions were held about models for analyzing the economic aspects of management policies affecting the environment. The use of simple models to estimate the net social cost of imposing various agricultural management systems was illustrated by K. Frohberg, who compared the cost of various measures to limit soil erosion and water pollution. It was agreed that the problem of modeling trade-offs between environment and agricultural economics needs to be further elaborated.

COMPLEX MODEL DEVELOPMENT AND APPLICATIONS

A field scale model for Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS model) was considered as an example of a complex model. W. Knisel presented the basic components of the CREAMS model and emphasized that this model should be used to consider alternative management practices for nonpoint source pollution in field-size areas. The field was defined as an area with homogeneous soil, single management practice, single crop, and uniform weather conditions. An example of CREAMS application was given by W. Knisel. The model was used to compare erosion resulting from three management practices common in the Southern Piedmont land resource area of the United States.

G. Golubev and I. Shvytov presented in turn the results of IIASA work with the CREAMS model and its application to a number of countries. Application and status were given as shown in the following table:

Country	Problem	Status
Sweden	N-leaching	N-simulation
Czechoslovakia	N-leaching, erosion	N-simulation
Poland	N-leaching	N-simulation
GDR	N-leaching	Hydrology simulation
UK	Erosion	Simulation
USSR	Chemical losses	Hydrologic simulation
Hungary	Phosphorus loading	Data collection

The most extensive application has been in Sweden in the Western Skåne area. Nitrogen leaching simulation has been developed for potatoes and wheat with and without irrigation. Dr. Enderlein presented the results of the CREAMS model application for the Schaeffergraben basin in the GDR. Real potential evapotranspiration in this basin is about 30% higher than that computed with the CREAMS model.

The meeting discussed some problems of CREAMS application. It was noted that the main problem in the application of CREAMS is still in the estimation of parameter values. Very little data for soils, including a description of a curve number for the hydrological submodel, are available. In the discussion, it was pointed out that even the handbook does not provide good numerical descriptions for hydrological soil groups. It is yet more difficult to estimate the soil chemical and plant physiological parameters required by CREAMS.

A special discussion was held to clarify the matter of the development and application of complex models. As a result, it was pointed out that:

-- there are several current complex models in this field (CREAMS, ACTMO, APM, etc.) which it would be very interesting to compare;
-- simulation comparison of different mathematical models is very difficult to do; it is logical to begin with descriptive comparison;
-- special attention should be paid to complex models which do not need calibration;
-- a model should not be used for conditions outside the development objectives; this applies to CREAMS or other field-scale models as well as to watershed and basin models;
-- sensitivity analysis is very useful for complex models with large numbers of parameters;
-- the best way to apply the CREAMS model is to run it for "typical" or "representative" areas.

SUMMARY OF THE GENERAL DISCUSSION

G. Golubev, as chairman of the session, opened the general discussion by pointing out that models built for the analysis of agricultural-environmental processes related to crop production are commonly set up at the field scale level. But all practical problems arise on a larger scale, e.g., at the watershed, river basin, or even larger scale level. Following this observation, he concluded that the following three questions should first be discussed:

(1) How can field level results be aggregated to a larger scale level and what are the problems involved in doing this?
(2) Instead of aggregating field level results, would it be preferable to use different models for a large scale?

How could a subcomponent of the model for the analysis of the water quality of streams be an integral part of the whole model system?

(3) How can these simulation models be integrated into one model which investigates various policy options with regard to the economic effect of reducing the environmental stress related to crop production? This would be an important aid in the decision making process.

An answer given by C. Lyons to questions (1) and (2) won the consensus of many participants. He suggested that a hierarchical model system be set up. Many small-scale models would be run on the first level and their results be put into a model set up for a larger scale. In this way, one can avoid the aggregation problems mentioned in the first question. In modeling the larger scale level, one can draw on experience gained from working on the smaller scale. The results obtained from the smaller scale models will be used to enhance the performance of the larger model and hence produce more accurate values.

Many participants expressed doubt that the modeling of the diffusion of pollutants in waterways could be accomplished at a satisfactory level. Only a few attempts have been made to investigate this problem. However, it was recognized that in the future, this should be given more attention in research.

No consensus could be reached with regard to the third question. It was, however, agreed that this kind of work is needed and that cooperative work with economists should be initiated. C.T. de Wit enumerated the difficulties which arise in such cooperative work and stressed the importance of maintaining a flow of information between economists and natural scientists when building such economical-physical models. It is also of importance that the actor in the system be recognizable and that the results can be visualized. As an example, de Wit mentioned the joint modeling work undertaken by agronomists and soil scientists at the University of Wageningen and economists from the Centre for World Food Studies in Amsterdam. In their study, they used a linear programming approach as an interface system between the physical and economic aspects.

D. Haith stressed that IIASA's decision to establish a model bank was a very important step in the direction of enhancing interdisciplinary work. After mentioning the difficulties encountered in joint research among different disciplines, he congratulated I. Shvytov for his accomplishments in setting up this world bank, thus bridging some of the gaps among disciplines.

Several participants also pointed out the need for the establishment of a data base for testing and comparing models. Such a data set could either be based on real observations or on a synthetically generated set. IIASA would be the best place to establish this data base and carry out the testing procedure, as well as to compare the model's performance.

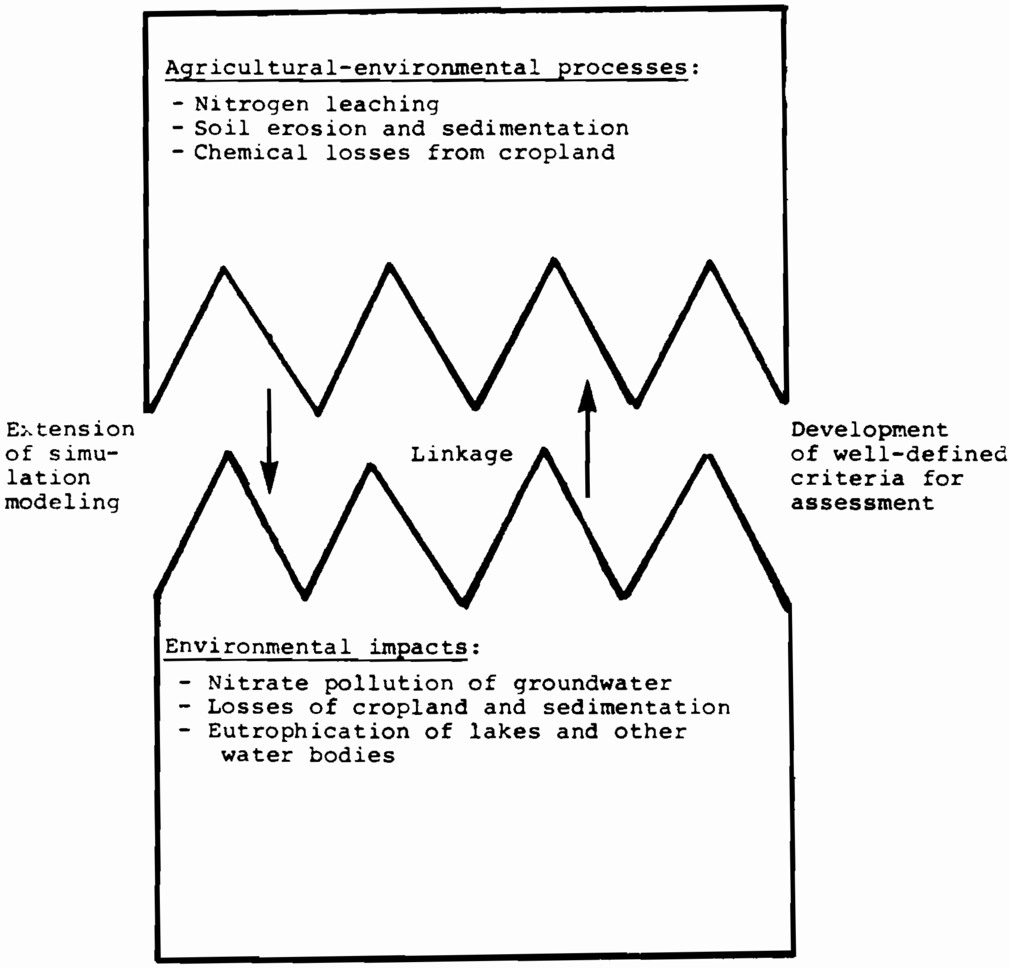

Figure 1. Linkage between environmental impacts and agricultural-environmental processes (dry farming crop production system).

CONCLUSION

We define "environmental impact" of crop production as any quantitative and/or qualitative change of environmental status due to crop production activity. Of course, all these changes of environmental status may be both "negative" and "positive" as well as having both "minor" and "major" significance. In addition, each environmental impact can have different time and space scales. Therefore, to assess these changes we need well-defined criteria indicating to what degree these changes are acceptable.

There is no universal criterion, therefore we could only concentrate on environmental impacts which have well-defined criteria for their assessment (nitrate pollution of groundwater, losses of cropland and sedimentation, eutrophication of lakes and other water bodies, pesticide pollution of water sources). In order to evaluate these impacts, one would need to have a number of simulation models having these impacts as "output" and crop production activity as "model input." Unfortunately, the majority of the currently existing models (nitrogen leaching models, soil erosion and sedimentation models, nonpoint source pollution models) describe only intermediate agricultural-environmental processes which potentially can lead to these environmental impacts. Figure 1 illustrates the present situation reflecting the necessity of linking well-modeled processes with environmental impacts needing evaluation. There are two ways to accomplish this. The first way is to extend the scope of modeling in order to cover the entire chain from crop production through the agricultural-environmental processes to the environmental impacts. Another way would be to specify the criteria for assessment of the environmental hazards on a basis of calculated outputs from a field and/or a watershed. Both approaches are viable and may be realized.

We surmise that one of the central problems in modeling the environmental impacts of agriculture is to bridge the gap discussed above.

APPENDIX A: AGENDA OF THE TASK FORCE MEETING (JUNE 2-4, 1980) ON MODELING OF AGRICULTURAL-ENVIRONMENTAL PROCESSES RELATED TO CROP PRODUCTION

<u>Monday June 2</u>

8.30 - 9.15	Registration (Conference Secretariat on First Floor)
9.15 - 10.00	Introduction (G. Golubev, Task Leader of Environmental Problems of Agriculture) (i) Opening Session (ii) General information concerning the activities and major results of the IIASA Task Environmental Problems of Agriculture
10.00 - 10.15	Aims and Approaches in Studying the Technology-Resource-Environment Interactions (J. Hirs)
10.15 - 10.45	Modeling of Environmental Impacts of Soil Fertilization (I. Shvytov) (i) Outline of the problem (ii) Objectives of the Task Force Meeting (iii) Expected results
10.45 - 11.00	COFFEE BREAK
11.00 - 11.45	A Hierarchical Approach to Agricultural Production Modeling (C.T. de Wit)
11.45 - 12.15	The Modeling of Environmental Impacts of Crop Production (D.A. Haith)
12.15 - 12.30	Discussion
12.30 - 14.00	LUNCH

THE NITROGEN LEACHING PROBLEM

14.00 - 14.30	A Critical Evaluation of a Hydrological Layer Model for Forecasting the Redistribution of Unadsorbed Anions in Cultivated Soils (I.G. Burns)
14.30 - 15.00	Review of Simulation Models for Nitrogen Behavior in Soil in Relation to Plant Uptake and Emission (M.J. Frissel & J.A. van Veen)
15.00 - 15.30	COFFEE BREAK
15.30 - 16.00	Modeling Nitrate Movement in Profiles that Contain Soil, Heavy Clay, and Chalk (T.M. Addiscott)
16.00 - 17.30	Discussion of the Nitrogen Leaching Problem

Tuesday June 3

SURFACE LOSSES OF CHEMICALS FROM CROPLAND

9.00 - 9.45	State-of-the-Art of Modeling of the Water Balance Processes in the Agricultural Field and Watershed (J. Balek)
9.45 - 10.30	Modeling of Surface Runoff Processes (M. Holy)
10.30 - 10.45	COFFEE BREAK
10.45 - 11.30	Retention, Transformation and Transport of Pesticides in Soil-Water Systems: Model Development and Evaluation (P.S.C. Rao)
11.30 - 12.30	Discussion
12.30 - 14.00	LUNCH

SIMULATION OF ECOLOGICAL ASPECTS OF CROP PRODUCTION ENVIRONMENT

14.00 - 14.20	Deterministic Models for the Ecologic Simulation of Crop Agricultural Environment (T.C. Lyons)
14.20 - 14.45	Modelling of Crop Production (O. Sirotenko)
14.45 - 15.10	Calculations of the Relationships between Soil Factors and Crop Yields (K. Rajkai)
15.10 - 15.20	COFFEE BREAK
15.20 - 15.40	Statistical Evaluation of Experts Estimates (I. Valyi)
15.40 - 17.30	Discussion (short presentations have been made by K. Frohberg and B. Trenbath)

Wednesday June 4

COMPLEX MODEL DEVELOPMENT AND APPLICATION

9.00 - 10.00	CREAMS: A Field Scale Model for Chemical Runoff and Erosion from Agricultural Management Systems (W.G. Knisel)
10.00 - 10.30	IIASA Experience in Application of the CREAMS Model (G. Golubev & I. Shvytov)
10.30 - 10.45	COFFEE BREAK
10.45 - 12.30	Discussion of the Development of Complex Models and their Applications (short presentation by R. Enderlein)
12.30 - 14.00	LUNCH
14.00 - 15.30	Closing Session - General Discussion

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APPENDIX C: LIST OF CHAIRMEN AND RAPPORTEURS

Monday June 2

Opening Session

Morning	Chairman:	Prof. G. Golubev (IIASA)
	Rapporteur:	Prof. D. Haith (USA)

The nitrogen leaching problem

Afternoon	Chairman:	Dr. M.J. Frissel (The Netherlands)
	Rapporteur:	Dr. T.M. Addiscott (UK)

Tuesday June 3

Surface losses of chemicals from cropland

Morning	Chairman:	Prof. D. Haith (USA)
	Rapporteur:	Dr. P.S.C. Rao (USA)

Simulation of ecological aspects of crop production environment

Afternoon	Chairman:	Prof. Dr. C.T. de Wit (The Netherlands)
	Rapporteur:	Dr. I.G. Burns (UK)

Wednesday June 4

Complex model development and application

Morning	Chairman:	Dr. P.S.C. Rao (USA)
	Rapporteur:	Dr. W.G. Knisel (USA)

General discussion

Afternoon	Chairman:	Prof. G. Golubev (IIASA)
	Rapporteur:	Dr. K. Frohberg (FRG)