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**ALTERRA**  
Wageningen Universiteit & Research centre  
Omgevingswetenschappen  
Centrum Water & Klimaat  
*Team Integraal Waterbeheer*

ANIMO

AGRICULTURAL NITROGEN MODEL

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## PREFACE

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The research project "Nitrogen behaviour in soil in relation to oxygen, water, and temperature", of which results are presented in this report, was initiated by the working group "Water, bodem en Lucht" of the Landinrichtingsdienst of the Netherlands. The study was carried out at the Institute for Land and Water Management (ICW) in Wageningen. The project was financed by the Dutch Ministries of Agriculture and Fisheries and of Housing, Physical planning and Environmental Hygiene. Purpose of the project was to provide possibilities to make predictions about long-term nitrate contamination of groundwater as a result of chosen scenarios in land and water use, taking into account the influences of environmental factors.

For this purpose the presented model ANIMO has been developed. During the modelling process it became clear that the completed model ANIMO would also be able to give other results, like nitrogen load on surface waters and development of organic matter properties of a soil profile, so that it can be considered as a complete (although not in every aspect detailed) model of nitrogen behaviour.

In following ICW-projects the model will be further tested and calculations will be made for selected Dutch situations. Applied on a regional scale, the model will be used as a support model in the ICW-project "Optimization of regional water use", for which the test area is the Southern Peel region.

Project leaders were ir. J.H.A.M. Steenvoorden and dr. ir. P.E. Rijtema.

We are grateful to Ir. T.J. Hoeijmakers and miss I. Akkerman, who have worked out part of the programming concerning the connection of ANIMO with the watermanagement model and the description of solute fluxes.

We thank Mr R. Looy and the other people working at the Department of Student affairs of the Technical University of Delft for the use of their printing facilities, which was a great help in completing this report in time.

## SUMMARY AND READING GUIDE

The model ANIMO simulates the behaviour of nitrogen in a soil-water-plant system, influenced by:

- soil type
- soil use
- water management
- weather conditions
- fertilizer use
- cropping history

using a one-dimensional soil system divided in a number of horizontal layers.

In its present form it can be used on a field scale; the structure of the model, however, gives the possibility of extension to regional use; this extension is being worked out.

In the model, main attention is focussed on the following subjects:

- mineralization/immobilization of N in relation to formation and decomposition of different types of organic matter (organic fertilizer, root material, root exudates, native soil organic matter)
- denitrification in relation to (partial) anaerobiosis and the presence of organic material
- transport, formation and decomposition of  $\text{NO}_3$ ,  $\text{NH}_4$  and soluble organic matter.

The model will be able to give predictions for the long term nitrate contamination of groundwater and surface water as well as for the development of organic matter qualities of the soil profile under consideration.

After the introduction in chapter 1, chapter 2 gives a short qualitative description of the nitrogen behaviour in soil and the factors influencing this behaviour.

In the chapters 3, 4 and 5 the theory of the model ANIMO is worked out:

In chapter 3 the basic structure and central transport and conservation equation is explained; in chapter 4 the modelling of moisture distribution and transport processes is described; chapter 5 gives a detailed description of the modelling of the biochemical processes, from which rate constants in the transport and conservation equation are derived.

Chapter 5 describes methods with which model parameters can be derived from literature data; these methods are worked out for some frequently occurring situations.

Chapter 7 gives some conclusions of the study and recommendations for research and further development of the model.

For the user of ANIMO information on input can be found in the appendices A and C.

For the modeller who wants to change or further develop parts of the computer program appendix B, containing a description of the computer program, is useful.

The model in its present form can be used to simulate crops which are sown and harvested during one year; in appendix E a modelling concept for grassland is given.

The model ANIMO applied on field scale, uses the results of an external watermanagement model WATBAL, which is described in another report (Berghuijs-van Dijk, 1985). Used on regio-

nal scale, it can be connected with the model FEMSAT-P (Querner and van Bakel, 1984). Combination with other water-quantity models is also possible.

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## 1. INTRODUCTION

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### 1.1. Purpose

Since the beginning of this century our surface- and groundwaters are increasingly contaminated with nitrogen species; this is a result of the growth of population, the increase of industrial activities and the intensification of agricultural fertilizer use. This contamination can have negative effects on other activities like drinking water production (maximum allowed concentration is 11 g N m<sup>-3</sup>) and preservation of natural areas (eutrophication causing deterioration of diversity of species). To prevent or reduce this contamination it is necessary to obtain a fundamental understanding of the processes causing it, and of the main ways in which the extent of leaching can be influenced. On a qualitative scale this knowledge is present; the quantification is more difficult, because of the complexity of the nitrogen cycle.

The purpose of this study was to develop a model which describes these processes and influences and which is able to predict long term nitrate contamination on surface- and groundwater as a result of chosen scenarios in agricultural land, water and fertilization management.

### 1.2. Existing models

Frissel and van Veen (1981) present a number of existing nitrogen models. Examining these, it appears that the different purposes for which scientists have developed their models, can lead to quite different models, often not useful for other than their original purpose.

If, for instance, they want to evaluate the development of organic matter in a soil profile with a known history, they will concentrate on the rootzone, consider a period of tens of years, and work with timesteps of one year. If they want to give advices for fertilization of crops, they can concentrate on the topsoil and describe periods of one growing season with timesteps of one day. If they want to have a better scientific understanding of the soil N cycle, they try to simulate their laboratory incubation experiments that took place under controlled circumstances; such a model may describe a period of some weeks and use timesteps of hours. If, however, the subject is leaching, the model will have to consider the whole soil profile at least as deep as the lowest groundwater level occurring, and describe all the important nitrogen processes, of which leaching is the result.

In our view the main processes for modelling are (see chapter 2 for explanation of terms):

- mineralization/immobilization related to the processes of the C-cycle

- denitrification related to (partial) anaerobiosis and to the presence of decomposing organic material, which implies the modelling of
  - oxygen distribution
  - transport of organic material in solution
- water management; evapotranspiration, capillary rise, fluxes to different drainage systems, watertable movement.

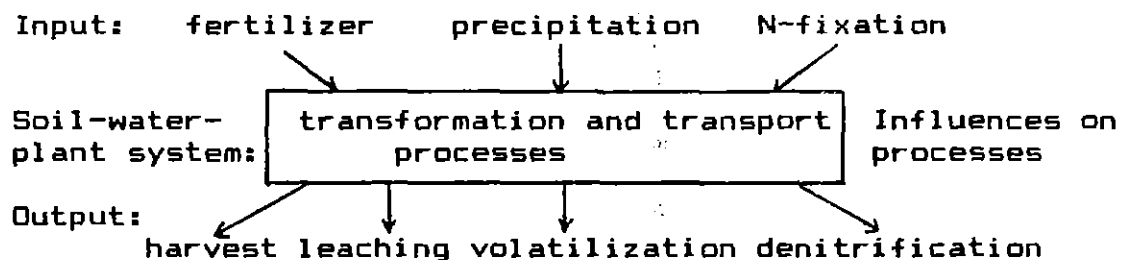
We have found no existing model describing all these processes. Especially transport of organic material in solution is often ignored due to lack of knowledge. Still it is a direct prerequisite for describing build-up of soil organic matter and denitrification below the rootzone. In the model ANIMO a first attempt is made to include this subject.

## 2. SHORT DESCRIPTION OF NITROGEN BEHAVIOUR IN SOIL

### 2.1. Nitrogen balance of the topsoil

If we consider the topsoil, the part below from the soil surface where agricultural activities concentrate, the nitrogen balance for this system can be represented as is done in fig. 2.1.

Fig. 2.1. Nitrogen balance of the topsoil



Inputs of nitrogen can originate from fertilization, anorganic or organic (manure) and soluble N-forms in precipitation. In the soil-water plant system the different forms of nitrogen can be transformed into each other, and some can be transported as solutes to deeper layers. These processes are influenced by environmental factors like temperature, moisture and pH. The processes and their influencing factors will be qualitatively described in the next two paragraphs; their modelling in the next chapters.

Nitrogen leaves the topsoil by means of harvest, leaching to deeper layers, and by volatilization (gaseous loss of  $\text{NH}_3$ ) and denitrification (gaseous loss of  $\text{N}_2$  or  $\text{N}_2\text{O}$ ).

### 2.2. Transformation processes

Nitrogen can occur in different forms in soil, which forms can be transformed into each other through the processes in the nitrogen cycle (see fig. 2.2).

To understand some of these processes it is necessary to take a look at some processes in the carbon cycle too, because of the many interdependences between organic material and nitrogen.

Fig. 2.3 gives the simplified soil organic matter or carbon cycle in soil.

Fig. 2.2. The nitrogen cycle

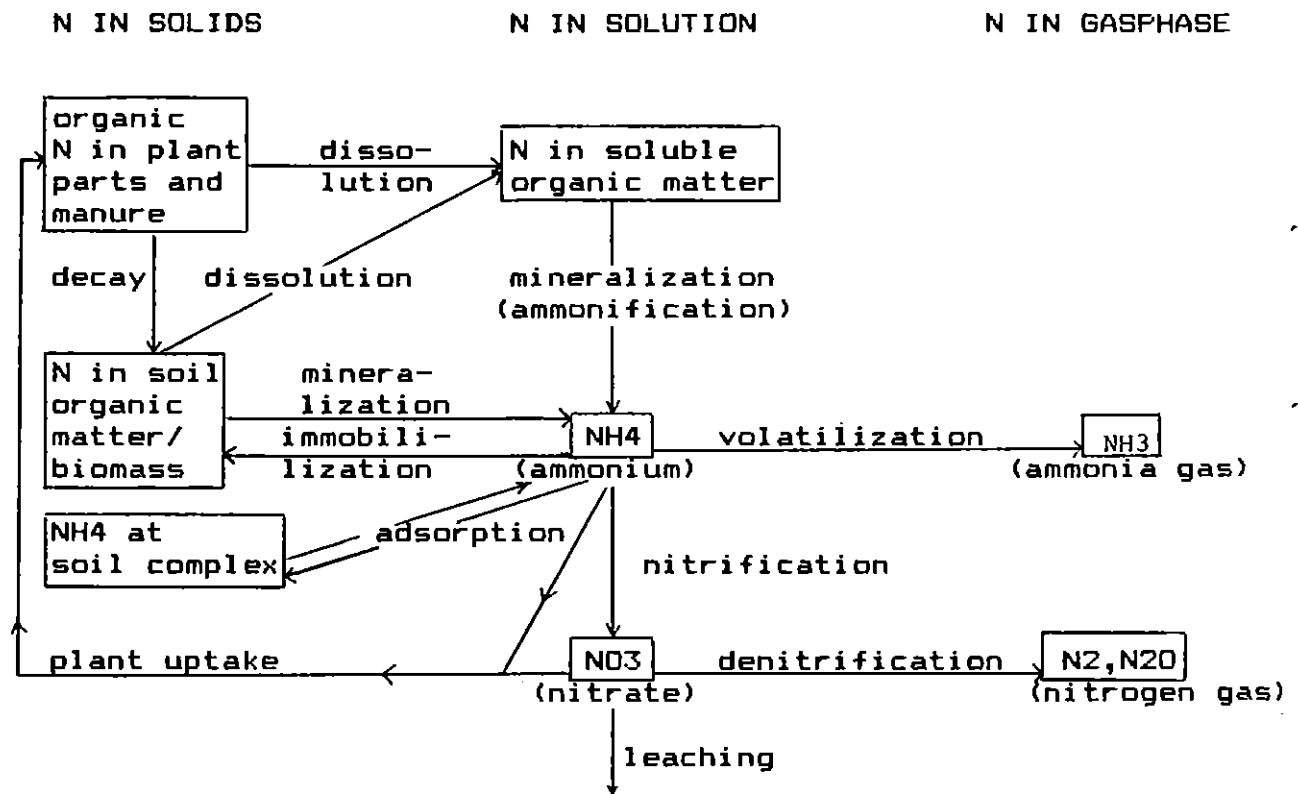
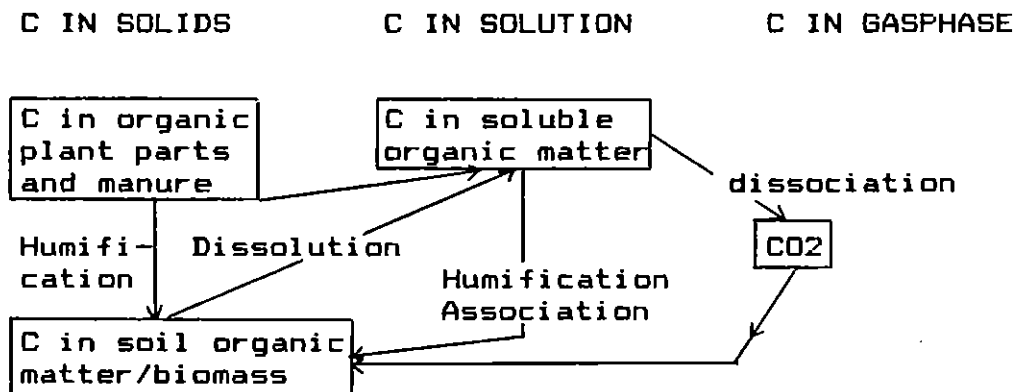


Fig. 2.3. The carbon cycle



For convenience, we shall call dead plant parts and organic parts of manure added to soil "fresh organic material". When this material starts to decompose, it is partially oxidized to CO<sub>2</sub> and H<sub>2</sub>O and partially transformed into soil organic matter or biomass. The ratio

$$a = \frac{\text{formed soil organic matter}}{\text{total amount of fresh organic material decomposed}}$$

is called the assimilation factor. At least a part of these transformation processes take place via the stage of soluble organic matter. The first step in the decomposition process when big solid molecules like cell walls are involved (cellulose, hemicellulose, pectine, lignine) is a splitting up of these molecules to smaller parts. Micro-organisms use exo-enzymes (operating outside the micro-organism cell) to perform this task. Generally spoken, the smaller the components formed, the higher their solubility is. The smaller molecules can be taken up by the micro-organism cell to be decomposed further.

The formed soil organic matter, in its turn, decomposes to CO<sub>2</sub> and H<sub>2</sub>O, but at a much lower rate than the organic plant parts. The biomass (micro-organisms) decomposes and renews itself at relatively high but often unknown rates; we can simplify and consider formation and decomposition of biomass as a one-direction overall process of the same kind as formation and decomposition of soil organic matter. Because it is quite difficult to distinguish experimentally between the small fraction of living biomass and the total amount of dead soil organic material, these two are often taken together in descriptions, as is done here. Living plant roots excrete soluble organic materials into soil solution; also, dead root cells, discarded by the plant, become available for decomposition; these products are called root exudates; they partake in the carbon and nitrogen transformation cycles too.

The different organic materials mentioned contain nitrogen as well as carbon (except CO<sub>2</sub>), so that transformations in the carbon cycle correspond with transformations in the nitrogen cycle.

The processes in the nitrogen cycle which are not directly parallel with those in the carbon cycle, will now be described shortly.

#### Decay:

Generally the formed soil organic material/biomass has a high N content as compared to plants.

#### Mineralization:

During the decomposition process of organic material mineral N may be released into soil solution in the form of the NH<sub>4</sub> ion.

#### Immobilization:

This is the process of NH<sub>4</sub> uptake from soil solution during the formation of biomass/soil organic material.

If the nitrogen content of the plant parts or soluble organic material is high and the assimilation factor is low, the

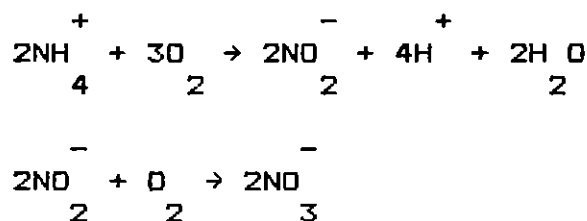
decomposing material will contain enough N to provide for the N needed to build in in the biomass/soil organic matter. The N released into soil solution is the so-called net mineralized N. If the nitrogen content of the plant parts or soluble organic material is low and/or the assimilation factor is high, additional nitrogen may be needed for the formation of biomass/soil organic matter, and this extra nitrogen is taken up from the soil solution. This process is called net immobilization of mineral nitrogen.

#### Adsorption:

The ammonium ion with its positive charge can be adsorbed at the soil complex consisting of negatively charged clay minerals and organic matter.

#### Nitrification:

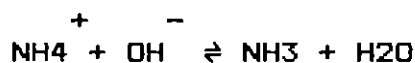
The oxidation of ammonium to nitrate is called nitrification. The process takes place in two steps, performed by different groups of micro-organisms:



Under normal circumstances the second step is much faster than the first, so that no accumulation of NO<sub>2</sub> (nitrite) will occur.

#### Volatilization:

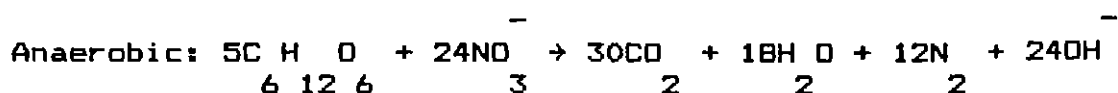
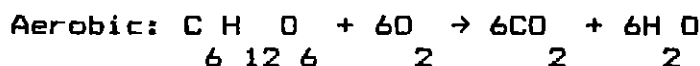
This is the process of formation of ammonia gas from NH<sub>4</sub>:



which causes gaseous losses of nitrogen from the topsoil.

#### Denitrification:

Denitrification is the process through which organic material is oxidized in the absence of oxygen. Under anaerobic conditions nitrate can be used instead of oxygen as the oxydizing agent. The nitrate itself is transformed into N<sub>2</sub> or N<sub>2</sub>O during this process. As an example the aerobic and anaerobic decomposition of glucose by Pseudomonas aeruginosa is given:



The denitrification process is another way in which nitrogen can disappear from the soil system.

#### Plant uptake:

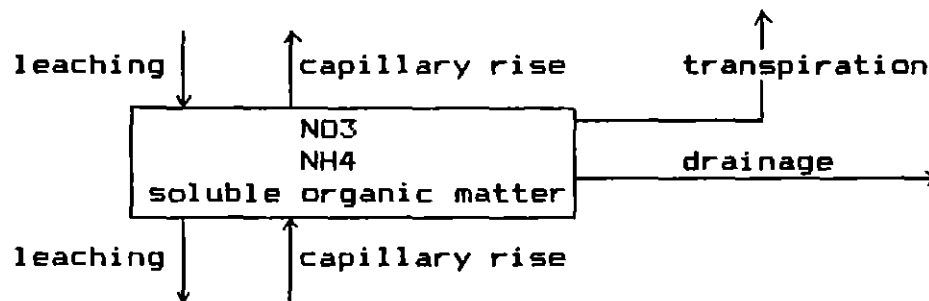
NH<sub>4</sub> and NO<sub>3</sub> can be taken up from soil solution by the plant

roots by means of the transpiration flux or through diffusion. Although generally  $\text{NH}_4$  is preferred by the plant, it is often less available than  $\text{NO}_3$  because of adsorption to the soil complex and, under aerobic conditions, because of the rapid transformation into  $\text{NO}_3$ , so that in practice the main uptake will consist of  $\text{NO}_3$ .

### 2.3. Transport processes

The soluble species considered in the N- and C-cycle,  $\text{NO}_3$ ,  $\text{NH}_4$ , and soluble organic matter, can be transported with the different occurring water fluxes (see fig. 2.4):

Fig. 2.4. Transport of soluble N forms to and from a soil layer.



Transpiration and drainage fluxes extract water and solutes from the soil system; capillary rise and evaporation are upward fluxes to and from next layers; leaching is a transport to deeper layers.

Because of its negative charge the nitrate ion is not retained by the soil complex and the whole nitrate content of a layer can be transported directly with the water fluxes; from the ammonium ion with its positive charge only the not-adsorbed part is transported.

### 2.4. Influences on processes

The main environmental influences on the transformation processes are temperature, moisture, oxygen and pH.

#### Temperature:

For chemical processes, the rate generally increases with temperature. For biological processes, often performed with enzymes, there is an optimum temperature (range) below and above which the rate decreases. Because the optimum temperature for biological processes is often around 30 °C or higher, we can say that for the temperatures occurring in soil, biological and chemical reaction rates both increase with temperature.

For some processes in the nitrogen cycle this influence has been studied especially. Van Huet (1983) gives a literature review. The reaction rates at different temperatures can be

expressed relative to the maximum rate found, or to the rate found at a certain average temperature, so that a reduction factor for other temperatures on the reaction rate can be applied in calculations.

For mineralization or mineralization combined with nitrification many of these studies exist, giving comparable results. Looking at par. 2.2 however, we must realize that the mineralization rate is first of all determined by the decomposition rates of organic materials and by their nitrogen contents. So, to get a straightforward relation for temperature influences, they should be studied relative to organic matter decomposition.

Nitrification increases with temperature; however, the process is dominated by the presence of oxygen; under aerobic conditions nitrification is so fast that ammonification is the rate limiting factor.

Denitrification increases with temperature, but this is completely due to the increase of organic matter decomposition with increasing temperature.

Summarizing we can conclude that the most important temperature influences are those on organic matter decomposition. Other temperature influences follow from these or are less important.

#### Moisture and oxygen:

These two are strongly related in soil and therefore treated together.

Micro-organisms need moisture to perform their functions. Below wilting point these are disturbed. At low moisture suction reaction rates may slow down by dilution effects or, if oxygen is needed, by absence of oxygen.

For mineralization, most authors found a relation with moisture suction showing an optimum near pF 3. If, however, they used topsoil samples for their studies, which are often aerated in field situations, the decrease in mineralization rate at low suction may be due to the necessity for adaptation of the microflora from aerobic to (facultative) anaerobic species, which adaptation in a poor growth medium as soil is, takes time. In a soil sample used to wetter conditions the decomposition rate may be equal to the optimum found at pF 3.

Also for nitrification, a relation with an optimum is found. The rate decrease at low suction is, however, determined by a shortage of oxygen.

For denitrification it is obvious that the rate of the process increases with lower moisture suction, because this implicates decrease of oxygen availability. Denitrification in unsaturated soil is a result of the presence of anaerobic soil aggregates (partial anaerobiosis). The texture of the soil plays an important role in this aspect.

Summarizing, the reduction on mineralization at low moisture suction is important, and oxygen content and distribution are important factors influencing the processes of nitrification and denitrification.

#### pH:

The influence of pH is dependent on the type of reaction and on the preference of the micro-organism involved. Measurements by several authors indicate a broad optimum pH range for mineralization, nitrification and denitrification (van Huet, 1983). The pH of most soils falls within this range. A

reaction especially pH-sensitive is volatilization, which is increased at high pH.

By combining some facts mentioned before we can get an idea of the main factors determining the extent of nitrate leaching on field scale. These are:

Presence of nitrate in solution, influenced by:

- The amount of N added by mineral fertilizers and manure: Steenvoorden(1983) showed that the higher the gift of mineral fertilizer, the higher the percentage leaching.
- The rate of formation of  $\text{NO}_3$ , which is favoured by high temperature, high N-content of organic materials added and aeration
- The rate of disappearance of  $\text{NO}_3$  from solution, favoured by high moisture conditions

Soil and water management, as expressed in:

- The presence of a crop: if a crop is present, nitrate added or formed may be taken up by the plant roots. If not, nitrate is subject to leaching. As a result, on arable land after the harvest, when the complete root material starts to decay, all the formed nitrate can be transported to deeper layers, except the part that can be denitrified. On permanent grassland this danger is less.
- The time of addition of fertilizer or manure: Additions in spring or summer are the most favourable for crop nutrition on arable land, because of direct availability of nutrients and low risk of losses by leaching and denitrification; leaching is mainly confined to wet periods (winter time).
- The rate of water transport to the subsoil: In deeply drained soils the residence time of water and solutes in the rootzone is small, and the denitrification possibilities are also small because of good aeration.
- The groundwater level: The same remark applies as for the rate of water transport. Steenvoorden(1983) found that at a average highest groundwater table of 1.5 m the amount of nitrate reaching the saturated zone may be 10 times as much as in a situation with highest groundwater table at 0.5 m; of course this is a combination of differences in storage capacities and denitrification possibilities.
- Physical soil characteristics: Examples are texture influencing partial anaerobiosis, and conductivity influencing leaching rate.
- Sprinkling

Weather conditions:

- Precipitation rate, influencing leaching rate but also denitrification rate
- Temperature, influencing production rate of  $\text{NO}_3$ .

### 3. BASIC STRUCTURE OF THE MODEL ANIMO

#### 3.1. Flow scheme

As mentioned before, the model ANIMO will be made operational both on field scale and on regional scale. The general flow scheme for the regional scale formulation is given here, because the field scale model can be considered as a part of it, a region consisting of 1 field. The flow scheme is given in fig. 3.1.

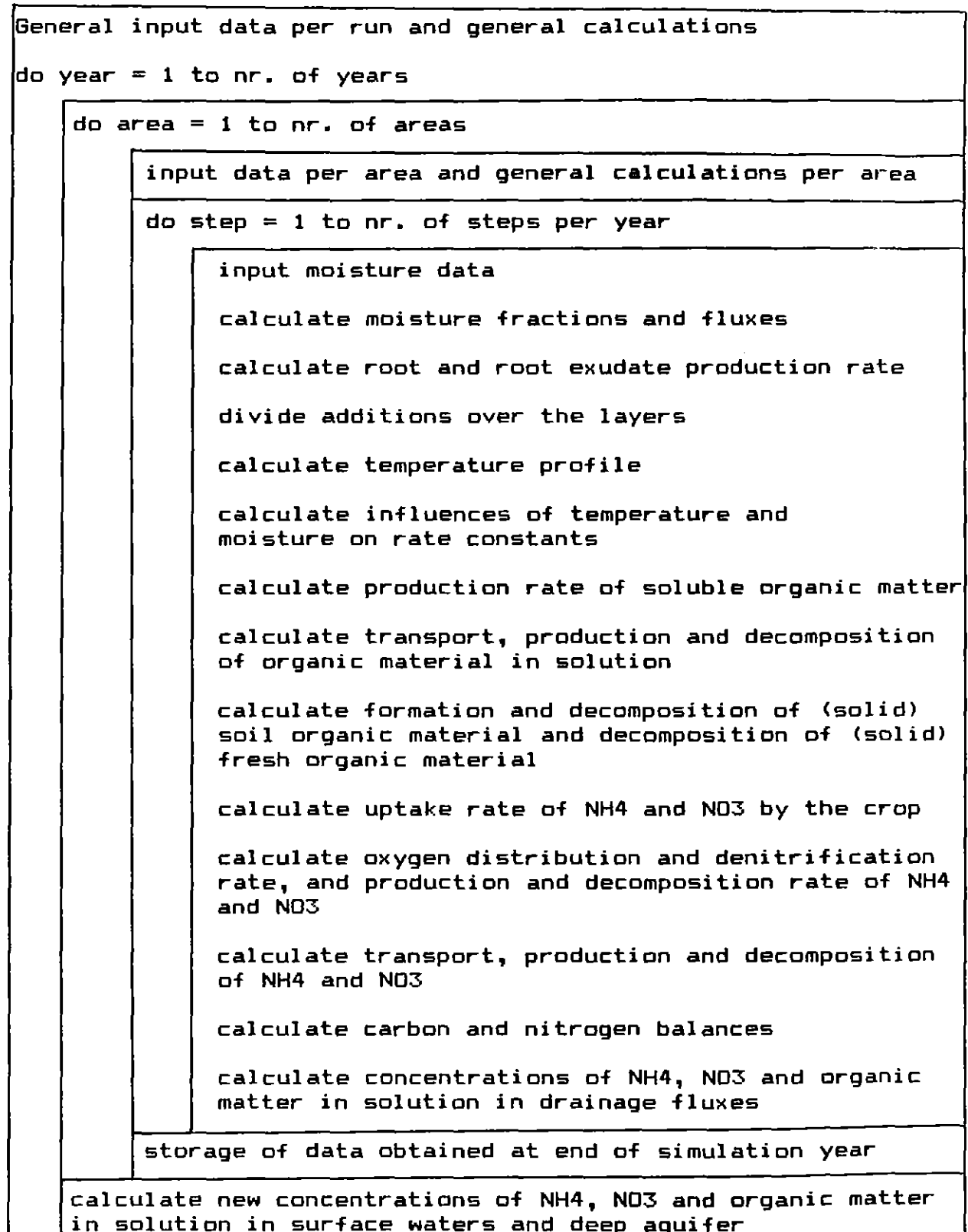
For each simulated year, calculations are made for all the subregions. This is done instead of making all the calculations per subarea for the full simulation time directly, because the chosen method makes it possible to evaluate the deep aquifer concentration after each year, by combining the deep drainage fluxes of all the areas. The new deep soil water concentration can be used in the next simulation year in case of upward seepage. The descriptions in this report will be restricted to the calculations per subarea, which form the core of the model.

#### 3.2. Geometry and time

Inside each area the model works one-dimensional. The soil is divided into a number of horizontal layers, which can differ in thickness. The water quantity models we use generally work with much less and thicker layers. These models have to supply per timestep: precipitation, evapotranspiration, drain discharges, and the height of the watertable and the moisture content of the rootzone at the end of the timestep.

From these data the water contents of all distinguished layers, the fluxes between layers and from each layer into the different drainage systems have to be calculated. Important for water quality calculations is the way in which the different drainage fluxes are divided over the layers. The timestep can be chosen according to the precision of available weather condition input data per timestep; the model can work with timesteps of one day or more (weeks, decades).

Fig. 3.1. Flow scheme of the model ANIMO



### 3.3. Transport of solutes.

A central point of the model is the transport- and conservation equation. This equation has to be used for all soluble species of importance in the nitrogen behaviour:  $\text{NO}_3$ ,  $\text{NH}_4$  and soluble organic matter. By means of this equation the new concentrations of these soluble species in all layers can be calculated after simultaneous transport and transformation processes. In fig. 3.1 the use of this equation is indicated by "calculate transport, production and decomposition of...".

The equation has the general form:

$$\frac{d\{V(n,t)*c(n),t\}}{dt} = \text{mass transport} + k_0*L + k_1*V(n,t)*c(n,t) - \frac{R_d*d\{V(n,t)*c(n,t)\}}{dt}$$

in which:

- n = layer number
- t = time (d)
- V(n,t) = moisture volume of layer n at time t (m)
- c(n,t) = concentration in layer n at time t (kg m<sup>-3</sup>)
- k<sub>0</sub> = zero-order rate constant of the species in layer n (kg m<sup>-3</sup> soil d<sup>-1</sup>)
- k<sub>1</sub> = first order rate constant for the species in layer n (d<sup>-1</sup>)
- N.B. k<sub>0</sub> and k<sub>1</sub> are positive in case of production and negative in case of decomposition.
- L = layer thickness (m)
- R<sub>d</sub> = distribution ratio: amount adsorbed/amount in solution per unit of soil system (-)

The fluxes needed in the mass transport description are calculated from the data given by the water quantity model. The next chapter gives these calculations and the solutions of the transport and conservation equation. The concentrations at t=0 follow from the previous timestep. The values of k<sub>0</sub> and k<sub>1</sub> follow from calculations on solubilization, mineralization and denitrification. These calculations are described in chapter 5.

#### 4. MODELLING OF TRANSPORT PROCESSES

For the modelling of transport processes the hydrology has been simplified. In this approach a maximum of three levels of drains is considered.

The required hydrological information for the transport processes can come from a hydrological model calculating the water balance. The output of such a model should include:

Pr	precipitation flux (m d <sup>-1</sup> )
Er	evapotranspiration flux (m d <sup>-1</sup> )
fg	discharge flux for surface runoff, field drain/trench discharge and interflow (m d <sup>-1</sup> ) (3rd order discharge)
fs	discharge flux for ditch or drain discharges (2nd order discharge) (m d <sup>-1</sup> )
fk	discharge flux for canal discharges (1st order discharge) (m d <sup>-1</sup> )
fl	discharge flux to or from the aquifer (m d <sup>-1</sup> )
Vr(t)	the moisture volume of the plant root zone at the end of the timestep (m)
h(t)	the phreatic level at the end of the timestep (m)

##### 4.1. Hydrological schematization

Considering a hydrologically homogeneous area and assuming the drains of the three different orders parallel and equidistant a cross-section between two drains of first order as given in fig. 4.1. can be made. In the example given in fig. 4.1. the density of drains/ditches (2nd order) is two times the density of canals (1st order) and the density of field drains (3rd order) is four times the density of drains/ditches. Also the stream line pattern is included in this figure (sketched). It is obvious that the longest streamlines discharge to the first-order drainage system; the intermediate streamlines discharge to the 2nd order drainage system and the shortest streamlines to the 3rd order drainage system.

For the water quality calculations the two dimensional schematization given in fig. 4.1. has been simplified to a one-dimensional schematization given in fig. 4.2. In this approach for each timestep a certain layer with specified thickness is identified for discharge to the distinguished drainage system. The differences in residence time of the water particles discharging to the respective drainage system is accounted by taking the ratio of discharge from a certain layer and its thickness proportional to the ratio of the drain distance of these drainage systems:

$$\frac{fk}{Dk} = \frac{As}{Ak} * \frac{fs}{Ds} = \frac{Ag}{Ak} * \frac{fg}{Dg}$$

in which:

Dk = thickness of layer discharging to the 1st order drains (m)

Figure 4.1. Schematic cross-section of a parallel equidistant drainage system of three different levels (shallow, intermediate and deep), with streamlines.

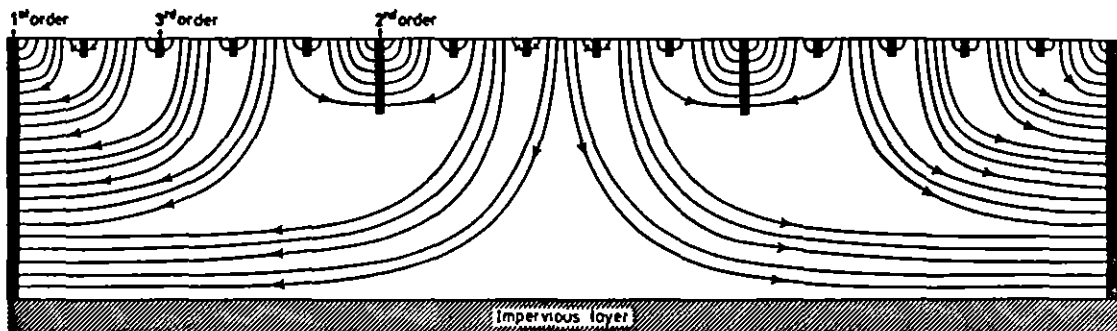
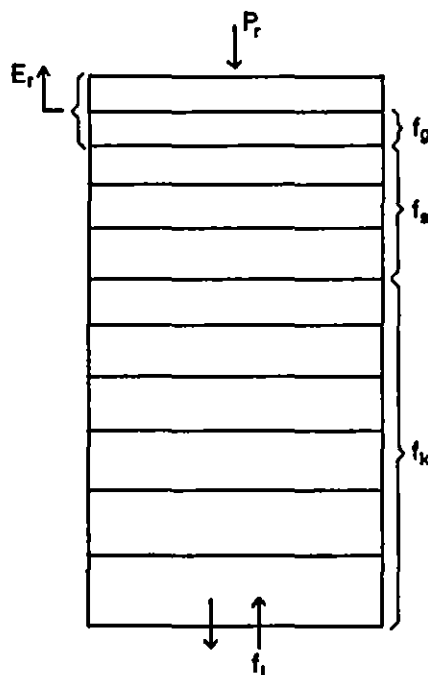


Figure 4.2. One-dimensional schematization used for the water quality calculations



- Ak = drain distance between the parallel equidistant first order drains (m)
- As = drain distance between the parallel equidistant second order drains (m), including the first order drains; see fig. 4.1)
- Ds = thickness of discharge layer to the 2nd order drains (m)
- Ag = drain distance between the parallel equidistant third order drains (m), including the 2nd and 1st order drains
- Dg = thickness of discharge layer to the third order drains (m)

For the simulation of surface runoff and interflow (3rd order drainage system) the permeability of the rootzone can be given a higher value, thereby decreasing the residence time of the water discharged by the 3rd order drainage system further.

Infiltration from the drains is treated in a similar way. If the discharge rates to the drainage system are negative infiltration is assumed.

#### 4.2. Calculation of moisture content per soil layer

Based on the data obtained from the hydrological model the moisture content of each soil layer at the end of the time-step can be calculated.

In the rootzone the moisture fraction is assumed constant with depth and in the absence of a water table in the rootzone the moisture fraction at the end of the timestep can be expressed as:

$$\theta(t) = \frac{V_r(t)}{D_r}$$

in which;

$D_r$  = thickness of the rootzone (m)

The moisture volume of the unsaturated zone below the root zone can be calculated from the hydrological input:

$$V_b(t) = V_b(0) + (\sum f_{in} - \sum f_{ou}) * t - \Delta V_r$$

in which:

- $V_b(t)$  = moisture volume below rootzone at end of timestep (m)
- $V_b(0)$  = moisture volume below rootzone at start of timestep (m)
- $\sum f_{in}$  = incoming flux (precipitation, seepage, infiltration)
- $\sum f_{ou}$  = outgoing flux (evapotranspiration, leakage, discharge to drains (m d<sup>-1</sup>))
- $\Delta V_r$  = change in moisture volume of rootzone during the timestep (m)

Below the rootzone a linear relation between moisture frac-

tion and depth is assumed in such a way that at the location of the groundwater table the moisture fraction equals saturation.

#### 4.3. Calculation of the water balance per layer

For each distinguished soil layer the water balance can be formulated:

$$(f_a - f_b - f_z - f_e) \cdot t + V(t) - V(0) = 0$$

in which:

- $f_a$  = discharge flux from the previous layer (m d<sup>-1</sup>)
- $f_b$  = discharge flux to the next layer (m d<sup>-1</sup>)
- $f_z$  = discharge flux to the drainage systems from the layer (m d<sup>-1</sup>)
- $f_e$  = evapotranspiration flux from the layer (m d<sup>-1</sup>)

For the first layer  $f_a$  equals the precipitation rate  $P_r$ . If the complete soil layer is discharging to a certain drainage system (e.g. of 2nd order) the equation for  $f_z$  is:

$$f_z = L \cdot \frac{A_s}{A_k} \cdot \frac{f_s}{D_s}$$

If only part of the layer is discharging to the 2nd order drainage system, and part to the 3rd order drainage system the equation becomes:

$$f_z = (1 - q) \cdot L \cdot \frac{A_g}{A_k} \cdot \frac{f_g}{D_g} + q \cdot L \cdot \frac{A_s}{A_k} \cdot \frac{f_s}{D_s}$$

in which  $q$  is the fraction of the layer discharging to the 2nd order drainage system.

Assuming a uniform extraction pattern for evapotranspiration, the flux  $f_e$  is given by the equation:

$$f_e = L \cdot \frac{E_r}{D_r}$$

As a result of this calculation the outflow at the lower boundary of the layer  $f_b$  is calculated. For the last layer  $f_b$  should equal the leakage or seepage term  $f_l$  that has been given as an input.

#### 4.4. Transport and conservation equation

Assuming complete mixing in each identified soil layer, the transport and conservation equation can be written:

$$\frac{d\{V(n,t)*c(n,t)\}}{dt} = \sum f_i * c_i - \sum f_o * c_o - f_e * c_e + k_0 * L + k_1 * c(n,t) * V(n,t) - \frac{R_d * d\{V(n,t) * c(n,t)\}}{dt}$$

in which:

$c(n,t)$	= concentration in layer n
$\sum f_i * c_i$	= total incoming flux of material (kg d <sup>-1</sup> )
$\sum f_o * c_o$	= total outgoing flux of material (kg d <sup>-1</sup> )
$c_e$	= concentration in evapotranspiration flux (kg m <sup>-3</sup> )
$k_0$	= production rate coefficient of order 0 (kg m <sup>-3</sup> d <sup>-1</sup> )
$k_1$	= production rate coefficient of order 1 (d <sup>-1</sup> )
$R_d$	= distribution ratio of adsorption (-)

Assuming all fluxes constant within the timestep, the moisture fraction will change linearly with time and for the moisture volume of layer n the following expression is found:

$$V(n,t) = L * (\theta_0 + HV * t)$$

in which:

$\theta_0$	= moisture fraction at the beginning of the timestep
$HV$	= change in moisture content with respect to time

The total incoming flux of material has to be identified on the basis of its concentrations: assuming these concentrations constant within the timestep gives the following expression:

$$\sum f_i * c_i = f_{io} * c(n+1) + f_{ib} * c(n-1) + f_{id} * c_{id}$$

in which:

$f_{io}$	= upward flow from layer n+1 to layer n (m d <sup>-1</sup> )
$c(n+1)$	= average concentration of layer n+1 (kg m <sup>-3</sup> )
$f_{ib}$	= downward flow from layer n-1 to layer n (m d <sup>-1</sup> )
$c(n-1)$	= average concentration of layer n-1 (kg m <sup>-3</sup> )
$f_{id}$	= infiltration flux from the drainage system(s) into layer n (m d <sup>-1</sup> )
$c_{id}$	= concentration of the infiltration water (kg m <sup>-3</sup> )

For the first layer (n = 1) the boundary condition for the incoming flux from above (layer n-1) is the precipitation rate, and for the concentration the concentration of the precipitation has to be taken. For the last layer (n = nl) the boundary condition of the incoming flux from below (layer n+1) is the seepage flux and for the concentration

the concentration in the aquifer has to be taken.  
For the mass transport from layer n the concentration is considered equal to the concentration in layer n (except for the evapotranspiration flux). For the water fluxes upward flow (to layer n-1), downward flow (to layer n+1) and to the drainage systems has to be considered:

$$\sum f_o * c_o = c(n,t) * \{f_{uo} + f_{ub} + f_g(n) + f_s(n) + f_k(n)\}$$

in which:

$$\begin{aligned} f_{uo} &= \text{downward flux to the next layer (n+1) (m d}^{-1}\text{)} \\ f_{ub} &= \text{upward flux to the previous layer (n-1) (m d}^{-1}\text{)} \\ f_g(n) &= \text{flux to 3rd order drain from layer n (m d}^{-1}\text{)} \\ f_s(n) &= \text{flux to 2nd order drain from layer n (m d}^{-1}\text{)} \\ f_k(n) &= \text{flux to 1st order drain from layer n (m d}^{-1}\text{)}. \end{aligned}$$

The concentration of the evapotranspiration flux is evaluated at each time step and considered proportional to the soil water concentration (see par. 5.4):

$$c_e = S * c(n,t)$$

in which:

$$S = \text{selectivity factor for plant uptake}$$

For nitrate and ammonium this factor can have a value  $S \leq 1$ ; for organic matter  $S = 0$ .

For the first-order production term  $k_1 * c(n,t) * V(n,t)$ , the moisture volume  $V(n,t)$  will be considered constant, and the average moisture volume  $V(n)$  is used on this place:

$$V(n) = L * \left( \theta_o + \frac{HV * t}{2} \right) = L * \theta_{av}$$

in which:

$$\theta_{av} = \text{average moisture fraction during the timestep}$$

Introduction of these relations in the transport and conservation equation gives after re-arranging the general form of the differential equation:

$$\frac{d c(n,t)}{dt} + \frac{A}{\theta_o + HV * t} * c(n,t) = \frac{B}{\theta_o + HV * t}$$

in which:

$$A = \frac{HV + f_{to}/L + S * f_e/L - k_1 * \theta_{av}}{1 + R_d}$$

$$B = \frac{f_{io} * c(n+1) + f_{ib} * c(n-1) + f_{id} * c_{id} + k_0 * L}{L * (1 + R_d)}$$

$$f_{to} = f_{uo} + f_{ub} + f_g(n) + f_s(n) + f_k(n)$$

Based on certain conditions for the parameters HV and A the following solutions of the differential equation are found:

for  $HV \neq 0$  and  $A \neq 0$ :

$$c(n,t) = \frac{B}{A} + \left\{ c(n,0) - \frac{B}{A} \right\} * \left\{ \frac{\theta_0 + HV*t}{\theta_0} \right\}^{-A/HV}$$

for  $HV = 0$  and  $A \neq 0$ :

$$c(n,t) = \frac{B}{A} + \left\{ c(n,0) - \frac{B}{A} \right\} * e^{-A*t/\theta_0}$$

for  $HV \neq 0$  and  $A = 0$ :

$$c(n,t) = c(n,0) + \frac{B}{HV} * \ln \left\{ \frac{\theta_0 + HV*t}{\theta_0} \right\}$$

and for  $HV = 0$  and  $A = 0$ :

$$c(n,t) = c(n,0) + B*t/\theta_0$$

Due to the assumption that the incoming fluxes from other layers have the average concentration of these layers also average concentrations have to be calculated. By integration over and dividing by the timestep the following solutions are found:

for  $HV \neq 0$  and  $A \neq 0$  and  $HV \neq A$ :

$$\bar{c}(n) = \frac{B}{A} + \frac{\theta_0 * \{ c(n,t) - c(n,0) \} + HV*t * \{ c(n,t) - B/A \}}{t * (HV - A)}$$

for  $HV \neq 0$  and  $A \neq 0$  and  $HV = A$ :

$$\bar{c}(n,t) = \frac{B}{A} + \frac{c(n,0) - B/A}{HV*t} * \theta_0 * \ln \left\{ \frac{\theta_0 + HV*t}{\theta_0} \right\}$$

for  $HV = 0$  and  $A \neq 0$ :

$$\bar{c}(n) = \frac{B}{A} + \frac{\theta_0}{A*t} * \{ c(n,0) - c(n,t) \}$$

for  $HV \neq 0$  and  $A = 0$ :

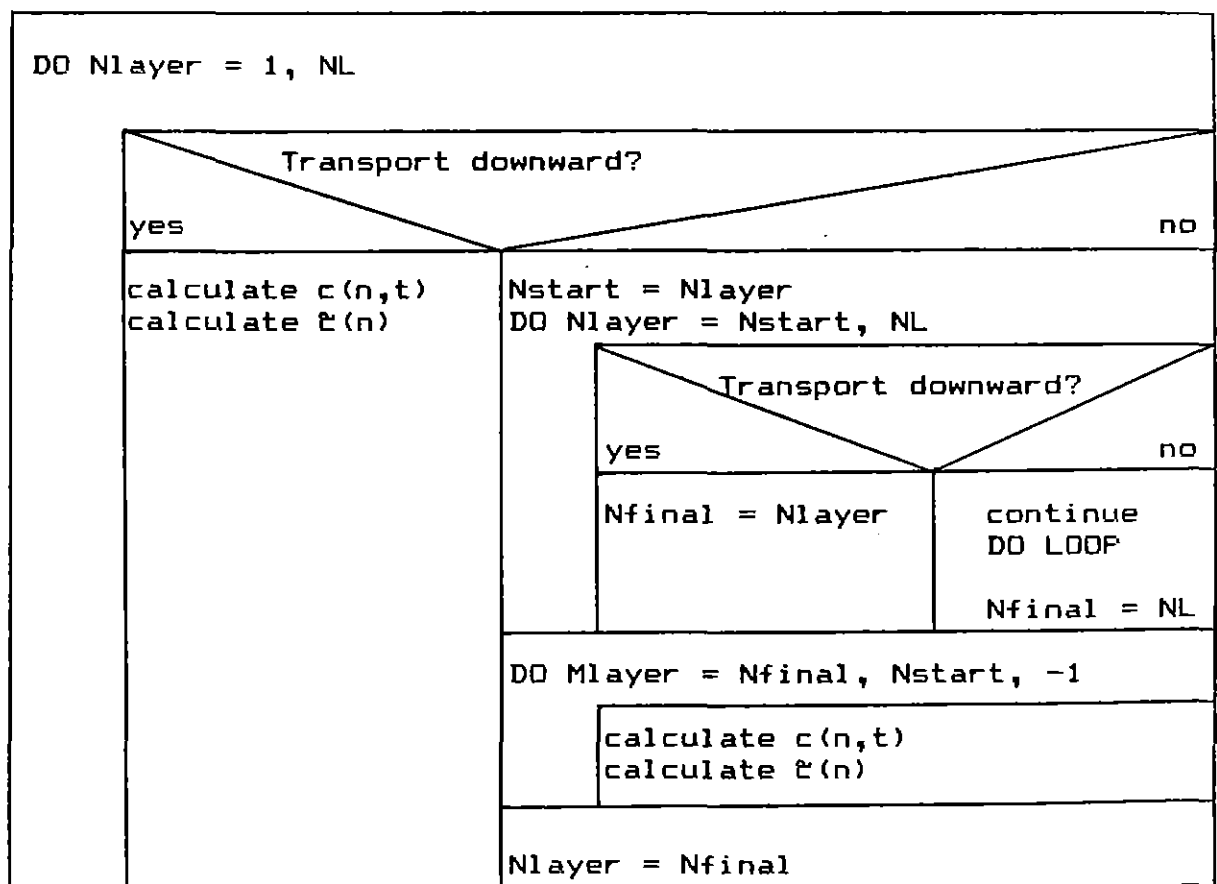
$$\bar{c}(n) = c(n,0) + \frac{B * (\theta_0 + HV*t)}{HV * t} * \left\{ \frac{HV}{B} * [c(n,t) - c(n,0)] + \frac{\theta_0}{\theta_0 + HV*t} - 1 \right\}$$

and for  $HV = 0$  and  $A = 0$ :

$$\bar{c}(n) = \frac{c(n,0) + c(n,t)}{2}$$

The calculation procedure has to follow the flow direction in the schematic column because for each layer the incoming concentration has to be known. In fig. 4.1. the calculation procedure is given. For all NL layers the direction of transport at the lower boundary is checked. If the direction of flow is upward, a search is made at which layer the direction of flow changes again (Nfinal). For the layers with upward flow the calculations for the final and average concentrations are made in reverse order.

Figure 4.1. Calculation procedure of average and end concentrations.



#### 4.5. Calculation of drainage water concentrations

For each timestep the concentration in the total discharge to each drainage system is calculated as total load of material divided by total water discharge.  
The concentration in the field drain/trench/surface runoff/interflow (3rd order) discharge as a whole is:

$$c_g = \sum_{n=1}^{n1} \left\{ \frac{f_g(n) * \xi(n)}{f_g} \right\}$$

in which:

$c_g$  = concentration in 3rd order drainage water (kg m<sup>-3</sup>)  
 $f_g(n)$  = discharge rate to 3rd order drainage system from layer n (m d<sup>-1</sup>)

Assuming that the discharges of the 3rd order drains will be transported by the 2nd order drainage system, the concentration of the drainage water of the 2nd order drains will be determined by the discharge to both systems:

$$c_s = \frac{c_g * f_g + \sum_{n=1}^{n1} \{f_s(n) * \xi(n)\}}{f_g + f_s}$$

in which:

$c_s$  = concentration in 2nd order drainage water (kg m<sup>-3</sup>)  
 $f_s(n)$  = discharge rate to 2nd order drainage system from layer n (m d<sup>-1</sup>)

Assuming that the discharges of the 2nd order drains will be transported by the 1st order drainage system, the concentration of the 1st order drainage system will be determined by the discharge to the three systems:

$$c_k = \frac{c_s * (f_s + f_g) + \sum_{n=1}^{n1} \{f_k(n) * \xi(n)\}}{f_k + f_s + f_g}$$

in which:

$c_k$  = concentration in 1st order drainage water (kg m<sup>-3</sup>)  
 $f_k(n)$  = discharge rate to 1st order drainage system from layer n (m d<sup>-1</sup>)

The concentration in the discharge to the deep aquifer is equal to the average concentration in the last layer,  $\xi(n1)$ , if leakage takes place.

## 5. MODELLING OF TRANSFORMATION PROCESSES

The calculations described in this chapter produce the rate constants  $k_0$  ( $\text{kg m}^{-3} \text{d}^{-1}$ ) and  $k_1$  ( $\text{d}^{-1}$ ) for soluble organic matter,  $\text{NH}_4$  and  $\text{NO}_3$  each, to be used in the transport and conservation equation described in chapter 4.

### 5.1. Organic matter formation and decomposition

We distinguish different kinds of organic matter, partaking in the soil carbon and nitrogen cycle. These are:

- fresh organic material. This material consists of root and other crop residues after harvesting and of the organic parts of manure. These are materials that come available stepwise, at certain clearly defined points in time.
- root exudates. These are organic products excreted by living roots, and dead root cells discarded by the plant. These products come available continuously when roots are present, and therefore their decomposition is modelled in another way. So for root material we have made the distinction between the continuously produced part and the part that comes available in one step at the harvest.
- soil organic material. This is the material formed from part of the available fresh organic material and root exudates. It consists of the dead organic soil material and of the living biomass.
- soluble organic material. As mentioned before, at least a part of the organic matter transformations passes the stage of solubilization.

Because we are uncertain which products are solubilized, we have modelled according to the following schematization:

$$\text{Fresh org. mat.} \rightarrow \text{soluble org. mat} \xrightleftharpoons{\text{CO}_2} \text{soil org. mat} \rightarrow \text{CO}_2$$

Root exudates are already partly soluble, and because it is known that they disappear very quickly, transport possibilities will be very small and there is no need to include an extra soluble stage here:

$$\text{root exudates} \xrightarrow{\text{CO}_2} \text{soil org. mat} \rightarrow \text{CO}_2$$

#### 5.1.1. Decomposition of fresh organic material

Each kind of fresh organic material is considered to consist of a few, say  $n_f$  fractions with fraction number  $f_n$ , decomposing with each its own first-order rate  $a_n$ . If we call the amount of material per fraction present at time  $t$   $O_s(f_n, t)$ , in which  $O_s$  stands for Organic material stepwise added, its

decomposition can be described as:

$$O_s(f_n, t) = O_s(f_n, 0) * e^{-a_n * t}$$

$O_s$  is expressed in kg dry material  $m^{-2}$  (unit layers of 1  $m^2$  area are taken),  $t$  in days and  $a_n$  in  $d^{-1}$ .

If different fresh organic materials are present it is convenient to be able to use the same equation for all fractions of all materials. Therefore we must define a fixed total number of possible materials  $m_n$  and possible fractions  $n_f$  (number of fractions), of which each kind of fresh organic material contains a few. This can be done by using a given matrix  $FR(m_n, n_f)$  consisting of numbers  $< 1$  that defines if and for which part a fraction  $f_n$  is present in material number  $m_n$ .

Example of this matrix  $FR$  with 5 materials and 10 fractions:

	$f_n = 1$	2	3	4	5	6	7	8	9	10
$m_n$										
= 1	0.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.0
2	0.0	0.3	0.0	0.0	0.7	0.0	0.0	0.0	0.0	0.0
3	0.0	0.0	0.4	0.0	0.0	0.6	0.0	0.0	0.0	0.0
4	0.0	0.0	0.0	0.2	0.0	0.0	0.8	0.0	0.0	0.0
5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.9

As can be seen, totals in each row are 1.0, and each fraction occurs in one kind of material only. This gives maximal freedom of material definition. If a new material is added, the division of its organic part  $AO$  (kg  $m^{-2}$ ) is simply done by calculating for all  $f_n$ :

$$\text{new } O_s(f_n, 0) = \text{old } O_s(f_n, 0) + FR(m_n, f_n) * AO$$

This rather detailed explanation is necessarily given at this place because the basic concept of the use of these fractions returns in many places in the model.

Of course these calculations are performed for each layer. In the computer program an extra dimension for the layer number is added to  $O_s$ , but here we shall not use it in this text as long as the calculations for each layer are the same.

### 5.1.2. Production and decomposition of soluble organic material

The production rate of organic material in solution,  $kO(OMS)$  (kg  $m^{-3} d^{-1}$ ), follows from the calculations in the previous paragraph:

$$kO(OMS) = \sum_{n_f} \left\{ \frac{O_s(f_n, t) - O_s(f_n, 0)}{L * t} \right\}$$

in which:

$OMS$  = organic material in solution

or

$$k_0(\text{DMS}) = \sum_{nf} \left\{ \frac{O_s(f_n, 0) * (e^{-an*t} - 1)}{L*t} \right\}$$

It will be clear that the production rate from slowly decomposing fractions will be less than that of faster decomposing fractions of fresh organic material. Once in solution, all the fractions are assumed to decompose with the same rate (see chapter 6). So for the organic material itself it is not necessary to consider these fractions separately in soluble form. However, because each fraction in the fresh material can have its own nitrogen content, it is yet necessary to distinguish them in solution, so that at their disappearance from solution the amount of mineral N released and available for soil organic matter production, can be calculated. Therefore, we use the transport- and conservation equation for each fraction, and we calculate for each  $f_n$  :

$$k_0(\text{DMS}, f_n) = \left\{ \frac{O_s(f_n, t) - O_s(f_n, 0)}{L*t} \right\}$$

$$= \left\{ \frac{O_s(f_n, 0) * (e^{-an*t} - 1)}{L*t} \right\}$$

With these the  $k_0(\text{DMS}, f_n)$  and with  $k_1(\text{DMS})$  as calculated in chapter 6, new distribution of soluble organic matter fractions is calculated with the transport- and conservation equation.

### 5.1.3. Roots and root exudates

The description of root development is important for the water quality model because:

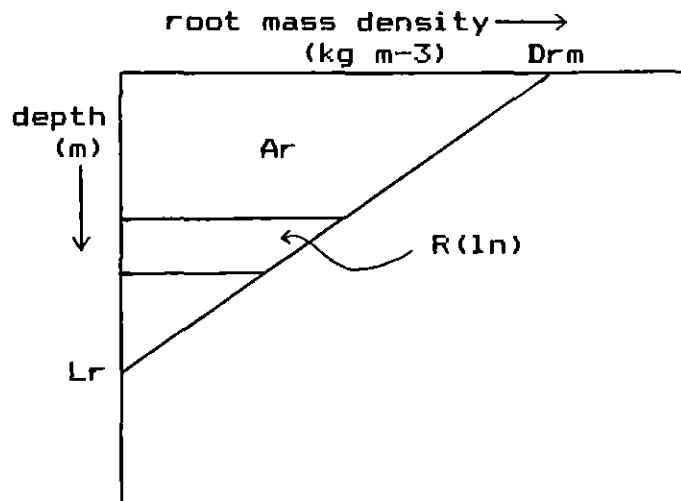
- mineral N can only be taken up from those layers in which roots are present (for arable land it will take some time before full root depth is reached).
- the root exudate production is related to root growth
- after the harvest on arable land, the formed root mass comes available for decomposition.

Development of root mass, root distribution and rooting length are functions of plant species and environmental conditions, which are very difficult to describe. Therefore we use a "standard" development per plant species, using measured data from literature.

Quantification is given in chapter 6. Between the given data we can interpolate, so that at each point of time we have a value for root length  $L_r$  (m) and amount of root material  $A_r$  (kg m<sup>-2</sup>). The distribution of root mass over the layers is modelled assuming maximal root density at the soil surface, and a linear decrease with depth to density zero at depth  $L_r$  (see fig. 5.1). The maximal density,  $D_{rm}$  is:

$$D_{rm} = 2 * A_r / L_r$$

Fig. 5.1. Schematization of root mass distribution  
(For explanation of symbols, see text)



The root mass present in each layer  $R$  ( $\text{kg m}^{-2}$ ) is equal to the density in the middle of the layer multiplied by the thickness of the layer:

$$R(t) = (D_{rm} - D_{rm}/L_r * dp) * L$$

in which  $dp$  (m) is the depth of the middle of the layer from soil surface.

In water quantity models, the so-called effective root zone is used; this is the layer containing approximately 90% of the root mass. This effective root zone  $L_{re}$  (m) can differ for different soil types. If we want to use a "standard" development of the root length in time, this difference in soil type can be taken into account as a constraint by defining:

$$L_r = \min\{L_r(t), L_{re} + 0.10\}$$

in which:

$L_r(t)$  = interpolated value for  $L_r$  from standard development data (m)

In this calculation method roots can grow to a maximum of 10 cm below the effective root zone. If  $L_r(t) > L_{re} + 10$ , the root mass  $Ar(t)$ , which is still kept the same, will be more concentrated in the top layers.

Root exudate production is generally expressed relative to root mass development. In chapter 6 we will find that a factor  $0.41 * \text{root mass development}$  is suitable. A production rate, constant during the timestep,  $k_e$  ( $\text{kg m}^{-2} \text{d}^{-1}$ ), can be calculated per layer as:

$$k_e = 0.41 * (R(0) - R(t)) / t$$

If the decomposition of exudates is described as a first-order reaction with rate constant  $a_e$  ( $\text{d}^{-1}$ ), we can write for

the amount of exudates in a layer,  $E(t)$  ( $\text{kg m}^{-2}$ ):

$$\frac{dE(t)}{dt} = k_e - a_e * E(t)$$

from which follows:

$$E(t) = \frac{k_e}{a_e} - \left( \frac{k_e}{a_e} - E(0) \right) * e^{-a_e * t}$$

#### 5.1.4. Formation and decomposition of soil organic material

In paragraph 5.1 it has been made clear that the soil organic material, according to the model, originates from two sources: the decomposition of soluble organic material and that of exudates. Although the material formed will be considered as homogenous, modelling of production/decomposition of this material will be split up in two separate descriptions, because of the different modelling in the source materials.

Soil organic material from soluble organic material fractions:

$$\frac{dH_s(f_n, t)}{dt} = a * a_s * V * s(f_n, t) - a_h * H_s(f_n, t)$$

in which:

$H_s(f_n, t)$	= Soil organic matter (humus) from soluble organic matter ( $\text{kg m}^{-2}$ ) fraction $f_n$
$a$	= assimilation factor (-)
$a_s$	= decomposition rate of soluble organic matter ( $\text{d}^{-1}$ )
$V$	= water volume of the layer (average during timestep) ( $\text{m}$ )
$s(f_n, t)$	= soluble organic matter concentration of fraction $f_n$ ( $\text{kg m}^{-3}$ )
$a_h$	= decomposition rate of soil organic matter ( $\text{d}^{-1}$ )

N.B. For the decomposition of  $H_s(f_n, t)$  no assimilation factor is used, because  $a_h$  represents a net decomposition rate to  $\text{CO}_2$  (see chapter 2).

$s(f_n, t)$  is a variable of which the change in time and the value at point of time  $t$  are calculated in the transport- and conservation equation. As can be seen in chapter 4, the equation of  $s(f_n, t)$  can have quite different forms. Therefore, we use the average value during the timestep,  $\bar{s}(f_n)$ , which is also calculated, and then the solution follows:

$$H_s(f_n, t) = \frac{a * a_s * V * \bar{s}(f_n)}{a_h} * (1 - e^{-a_h * t}) + H_s(f_n, 0) * e^{-a_h * t}$$

Soil organic material from root exudates:

$$\frac{dHe(t)}{dt} = a*ae*E(t) - ah*He(t)$$

in which:

$He(t)$  = Soil organic material (humus) from exudates  
(kg m<sup>-2</sup>)

$$\frac{dHe(t)}{dt} + ah*He(t) = a*ae*\left(\frac{ke}{ae} - \left(\frac{ke}{ae} - E(0)\right)*e^{-ae*t}\right)$$

for which the solution is:

$$He(t) = \frac{a*ke}{ah} * (1 - e^{-ah*t}) + \frac{a*(ke - ae*E(0))}{(ah - ae)} * (e^{-ah*t} - e^{-ae*t}) + He(0)*e^{-ah*t}$$

Total soil organic matter  $H(t)$  (kg) is

$$H(t) = \sum_{fn} Hs(t) + He(t)$$

## 5.2. Nitrogen mineralization and -immobilization

In this paragraph the derivation of the values for  $k_0$  and  $k_1$  for  $NH_4$  and  $NO_3$  will be described.

The principles of these calculations are:

1. The net total mineralization rate of  $NH_4$  during the timestep,  $k_0(NH_4)$ , follows from the composition/decomposition balance of the different organic materials, taking into account their diverse N contents.
2. The decomposition (oxidation) rate of  $NH_4$ ,  $k_1(NH_4)$ , has a certain basic value (following from literature data), which is reduced for (partial) anaerobic conditions.
3. The formation rate of  $NO_3$  is derived from the decomposition rate of  $NH_4$ .
4. The rate of decomposition of  $NO_3$  is determined by the part of the total decomposition of organic material that takes place under anaerobic conditions, where the oxygen demand is replaced by a nitrate demand.

Ad 1:

The total net decomposition of organic material during the timestep is calculated as:

$$Dom = \sum_{fn} \{V(0)*s(fn,0) - V(t)*s(fn,t) + L*k_0(DMS)*t + Is(fn) - Us(fn)\} + H(0) - H(t) + E(0) - E(t) + ke*t$$

in which:

$V(0)$	= moisture volume at beginning of timestep (m)
$V(t)$	= moisture volume at end of timestep (m)
$Dom$	= net decomposition of organic material during the timestep (kg m <sup>-2</sup> )
$Is(fn)$	= total amount of soluble organic matter fraction $fn$ transported into the layer during the timestep (kg m <sup>-2</sup> )
$Us(fn)$	= total amount of soluble organic material fraction $fn$ transported out of the layer during the timestep (kg m <sup>-2</sup> )

The values  $Is(fn)$  and  $Us(fn)$  follow from the transport- and conservation equation for organic material in solution.

The net release of mineral nitrogen during the timestep or ammonification,  $Mn$  (kg m<sup>-2</sup>) then follows from:

$$Mn = \sum_{fn} \{ nifr(fn) * (V(0) * S(fn,0) - V(t) * S(fn,t) + L * kO(fn) * t + Is(fn) - Us(fn)) \} \\ + nifrrhu * (H(0) - H(t)) \\ + nifrex * (E(0) - E(t) + ke * t)$$

in which:

$nifr(fn)$	= nitrogen fraction in organic material fraction $fn$
$nifrrhu$	= nitrogen fraction in soil organic material
$nifrex$	= nitrogen fraction in exudates

The rate of  $NH_4$  production is:

$$kO(NH_4) = \frac{Mn}{t * L} \quad \text{kg m}^{-3} \text{ soil d}^{-1}$$

Ad 2:

If the decomposition (oxidation) rate for  $NH_4$  under aerobic conditions is  $knh$  (d<sup>-1</sup>), the decomposition rate for  $NH_4$  under partial anaerobic conditions can be assumed as:

$$k1(NH_4) = -AE * knh \quad \text{d}^{-1}$$

in which

$AE$	= aerated fraction of the layer during the timestep considered
------	--

N.B.  $k1(NH_4)$  is negative because all the rate constants in the transport- and conservation equation are expressed in terms of production.

The calculation of  $AE$  is given in paragraph 5.3 about aeration and denitrification.

Ad 3:

The rate of production of  $NO_3$  is equal to the rate of decomposition of  $NH_4$ . Because  $k1(NH_4)$  is a first-order rate

constant and  $k_0(\text{NO}_3)$  a zero-order one, we must multiply by a concentration term, and because  $k_0(\text{NO}_3)$  is expressed in  $\text{kg m}^{-3} \text{ soil d}^{-1}$  we also multiply by the average moisture fraction:

$$k_0(\text{NO}_3) = -k_1(\text{NH}_4) * \bar{c}_{\text{nh}} * \theta_{\text{av}} = \text{AE} * k_{\text{nh}} * \bar{c}_{\text{nh}} * \theta_{\text{av}} \quad \text{kg m}^{-3} \text{ soil d}^{-1}$$

in which:

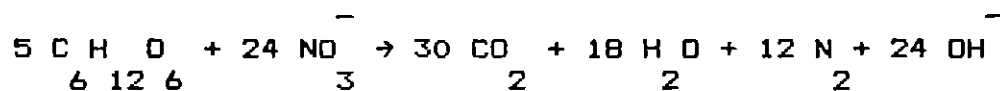
$\bar{c}_{\text{nh}}$  = average concentration of  $\text{NH}_4\text{-N}$  in solution during timestep ( $\text{kg m}^{-3}$ )

$\theta_{\text{av}}$  = average moisture fraction during the timestep

The value of  $\bar{c}_{\text{nh}}$  follows from the transport- and conservation equation applied to  $\text{NH}_4$ .

Ad 4:

If we take the anaerobic oxydation reaction of glucose by Pseudomonas aeruginosa:



as the general form in which denitrification takes place, we see that for the oxidation of each mole of carbon 24/30 mole of  $\text{NO}_3$  is needed. This means that for each kg carbon oxidized  $24/30 * 14/12$  kg  $\text{NO}_3\text{-N}$  is denitrified. If the carbon content of organic material is taken as a constant of 58% on dry weight basis, as is often done, it follows that the  $\text{NO}_3\text{-N}$  demand,  $D_n$  ( $\text{kg N m}^{-3} \text{ d}^{-1}$ ), can be expressed as:

$$\begin{aligned} D_n &= \frac{24/30 * 14/12 * 0.58 * (1 - \text{AE}) * D_{\text{om}}}{L * t} \\ &= \frac{0.541 * (1 - \text{AE}) * D_{\text{om}}}{L * t} \end{aligned}$$

As can be seen, the disappearance of nitrate as expressed here, is not a first-order process, but a zero-order process. Therefore we must combine  $D_n$  with the value derived above for the production of nitrate from ammonium, resulting in a zero-order rate constant for the net production of nitrate:

$$k_0(\text{NO}_3) = \text{AE} * k_{\text{nh}} * \bar{c}_{\text{nh}} * \theta_{\text{av}} - \frac{0.541 * (1 - \text{AE}) * D_{\text{om}}}{L * t}$$

which can be positive as well as negative. Because of this combination,  $k_1(\text{NO}_3)$  is not used in the transport- and conservation equation:

$$k_1(\text{NO}_3) = 0$$

### 5.3. Aeration and denitrification

In this paragraph the modelling of the oxygen distribution in soil air and water is described. The purpose of this modelling is to be able to determine which part of the organic matter decomposition during the timestep considered, as calculated in par. 5.2, takes place aerobically (with oxygen) and which part is oxidized with nitrate, resulting in denitrification. This partitioning is expressed in the fractions AE and (1 - AE) as used in par. 5.2.

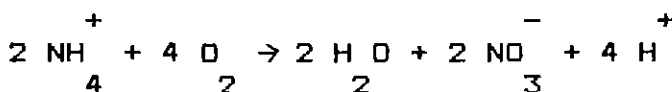
Under complete aerobic conditions, the oxygen demand can be calculated, assuming a carbon content of 58% in organic material and oxidation to CO<sub>2</sub>, so that for each mole of C, 2 mole of O (or one mole of O<sub>2</sub>) is needed:

$$Doc = \frac{32}{12} * 0.58 * \frac{Dom}{L*t} = 1.55 * \frac{Dom}{L*t}$$

in which

Doc = oxygen demand for carbon oxidation of layer considered during the timestep  
(kg m<sup>-3</sup> soil d<sup>-1</sup>)

Under these circumstances, the NH<sub>4</sub> released during mineralization and the NH<sub>4</sub> in solution and released from the soil complex will be oxidized too, according to:



resulting in an oxygen demand for nitrification of:

$$Don = \frac{128}{28} * knh * \bar{c}_{nh} * \theta_{av} = 4.57 * knh * \bar{c}_{nh} * \theta_{av}$$

in which:

Don = oxygen demand for nitrification in layer considered during timestep (kg m<sup>-3</sup> soil d<sup>-1</sup>)  
 $\bar{c}_{nh}$  = average ammonium concentration (kg m<sup>-3</sup>), here used as the value occurring under complete aerobic conditions. To calculate this  $\bar{c}_{nh}$  a separate use of the transport and conservation equation for NH<sub>4</sub> is needed.

The total oxygen demand under aerobic conditions is the sum of Doc and Don. Expressed in terms of production of oxygen, it is:

$$a = - (Doc + Don)$$

in which

a = oxygen production (kg m<sup>-3</sup> soil d<sup>-1</sup>)

If we want to express the oxygen demand in volume of oxygen gas used, we can apply the law of Boyle-Gay Lussac, which can be written as:

$$p \cdot v = m \cdot R_g \cdot (T + 273)$$

with		value
p	= gas pressure (atm)	1
v	= gas volume (l)	1
m	= number of moles	1
R <sub>g</sub>	= gas constant (l atm C <sup>-1</sup> mole <sup>-1</sup> )	0.08205
T	= temperature (C)	as occurring

we find:

$$v = 0.08205 \cdot (T + 273) \text{ l mole}^{-1} \approx 0.08205 \cdot (T + 273) / 32 \text{ l g}^{-1} \\ \approx 2.56 \cdot 10^{-3} \cdot (T + 273) \text{ m}^3 \text{ kg}^{-1}$$

With this number we can derive the total oxygen demand per unit volume of soil *b*, expressed in m<sup>3</sup> m<sup>-3</sup> soil d<sup>-1</sup> for the layer under consideration as:

$$b = -2.56 \cdot 10^{-3} \cdot (T + 273) \cdot a$$

Oxygen supply from the air into the soil system takes place mainly through the process of diffusion through the airfilled pores. According to Bakker (1965) we can write for the diffusion constant in the soil system:

$$D = D_0 \cdot p_1 \cdot \theta_g^{p_2}$$

in which:

- D<sub>0</sub> = Diffusion coefficient for O<sub>2</sub> in the atmosphere (m<sup>2</sup> d<sup>-1</sup>)
- D = Diffusion coefficient for O<sub>2</sub> in the soil gasfilled pore system (m<sup>2</sup> d<sup>-1</sup>)
- θ<sub>g</sub> = volume fraction of airfilled pores (m<sup>3</sup> m<sup>-3</sup>)
- p<sub>1</sub> and p<sub>2</sub> are empirical constants dependent on the soil type

The vertical diffusive transport of oxygen in the airfilled pores in the soil system is described by:

$$\theta_g \cdot \frac{dcp}{dt} = D \cdot \frac{d^2 cp}{dz^2} - b$$

in which:

- cp = oxygen concentration in airfilled pores (m<sup>3</sup> m<sup>-3</sup>)
- t = time (d)
- z = depth (m)

In the model we will assume a stationary situation per timestep:

$$\theta_g \cdot \frac{dcp}{dt} = 0$$

so that the diffusion equation can be reduced to:

$$D \frac{d^2 c_p}{dz^2} = b$$

Because diffusion possibility of oxygen in water is about 10<sup>4</sup> times as slow as in the air, we neglect the consumption of oxygen in the layers below groundwater level, and consider them as anaerobic.

In the model, the soil system is divided in  $n_l$  layers. Each layer  $k$  has its own thickness  $L(k)$  (m). If we keep  $D$  and  $b$  constant per layer and per timestep, expressing them as  $D(k)$  and  $b(k)$ , respectively, we can write for each layer  $k$ :

$$D(k) \frac{d^2 c_p}{dz^2} = b(k)$$

A condition that must be met in this stationary situation is that at each layer boundary the oxygen supply rate is equal to the oxygen consumption rate below that boundary. If  $Z(k)$  is the depth of the bottom of layer  $k$  from soil surface (m), and  $n_a$  is the number of aerated layers, we can express this condition according to Fick's first law, as:

$$\begin{aligned} \text{for } z = Z(k-1) \quad c_p &= c_p(k-1) \quad \frac{dc_p}{dz} = - \frac{1}{D(k)} * \sum_{n=k}^{n_a} L(n) * b(n) \\ \text{for } z = Z(k) \quad c_p &= c_p(k) \quad \frac{dc_p}{dz} = - \frac{1}{D(k)} * \sum_{n=k+1}^{n_a} L(n) * b(n) \end{aligned}$$

The boundary condition for the soil surface is:

$$\text{for } z = 0 \quad c_p = c_a$$

in which

$c_a$  = concentration of oxygen in air (m<sup>3</sup> m<sup>-3</sup>)

For each layer  $k$  we can write:

for  $Z(k-1) \leq z \leq Z(k)$ :

$$D(k) \frac{d^2 c_p}{dz^2} = b(k)$$

$$\frac{dc_p}{dz} = \frac{b(k)}{D(k)} * z + K_1$$

in which  $K_1$  is a constant.

For the boundary  $z = Z(k-1)$  we can write this as:

$$- \frac{1}{D(k)} * \sum_{n=k}^{n_a} L(n) * b(n) = \frac{b(k)}{D(k)} * Z(k-1) + K_1$$

$$K1 = - \frac{1}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) - \frac{b(k)}{D(k)} * Z(k-1)$$

resulting in:

$$\frac{dcp}{dz} = \frac{b(k)}{D(k)} * z - \frac{1}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) - \frac{b(k)}{D(k)} * Z(k-1)$$

$$\frac{dcp}{dz} = \frac{b(k)}{D(k)} * (z - Z(k-1)) - \frac{1}{D(k)} * \sum_{n=k}^{na} L(n) * b(n)$$

Integration yields:

$$cp = \frac{b(k)}{2 * D(k)} * (z^2 - 2 * Z(k-1) * z) - \frac{z}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) + K2$$

in which K2 is a constant.

For the boundary  $z = Z(k-1)$  we can write:

$$cp(k-1) = \frac{b(k)}{2 * D(k)} * ((Z(k-1))^2 - 2 * (Z(k-1)) * Z(k-1)) - \frac{Z(k-1)}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) + K2$$

$$K2 = cp(k-1) + \frac{b(k)}{2 * D(k)} * (Z(k-1))^2 + \frac{Z(k-1)}{D(k)} * \sum_{n=k}^{na} L(n) * b(n)$$

so that:

$$\begin{aligned} cp &= \frac{b(k)}{2 * D(k)} * (z^2 - 2 * Z(k-1) * z) - \frac{z}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) \\ &+ cp(k-1) + \frac{b(k)}{2 * D(k)} * (Z(k-1))^2 + \frac{Z(k-1)}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) \end{aligned}$$

or, rearranged:

$$\begin{aligned} cp &= cp(k-1) + \frac{b(k)}{2 * D(k)} * (z^2 - 2 * Z(k-1) * z + (Z(k-1))^2) \\ &+ \frac{(Z(k-1) - z)}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) \end{aligned}$$

For  $z = Z(k)$  then follows:

$$\begin{aligned} cp(k) &= cp(k-1) + \frac{b(k)}{2 * D(k)} * (Z(k)^2 - 2 * Z(k-1) * Z(k) + (Z(k-1))^2) \\ &+ \frac{(Z(k-1) - Z(k))}{D(k)} * \sum_{n=k}^{na} L(n) * b(n) \end{aligned}$$

or

$$c_p(k) = c(k-1) + \frac{b(k)}{2 \cdot D(k)} \cdot L(k) - \frac{1}{D(k)} \cdot \sum_{n=k}^{1n} L(n) \cdot b(n)$$

Now we have found a way of calculating the oxygen concentration of a layer k from that of the layer k-1, in a profile where all oxygen demands below layer k are fully met, assuming na layers are totally aerated. If, however, the oxygen demands are high and/or the diffusion process is hampered by wet conditions, the oxygen profile will show a very steep decline with depth, and for the lower layers above groundwater level negative concentrations could be calculated with the formula given above. To avoid this, we use an iteration scheme in which, starting with the toplayer, we calculate the oxygen profile for the situation that 1, 2, 3, ...etc. layers contain oxygen, stopping when first negative concentrations are calculated or the groundwater level is reached. This scheme is given in fig. 5.2.

Another complication for some layers may be that, even if some oxygen is present in the airfilled pores, the diffusion into the waterfilled soil aggregate pores may not be fast enough to make these aggregates completely aerobic. The result is that in the middle of the aggregates anaerobic conditions occur, while at the edges aerobic decomposition takes place. The soil layer is then called partially anaerobic. Because in the anaerobic parts decomposition of organic material takes place with nitrate instead of oxygen, the oxygen consumption of such a layer will be smaller than  $b(k)$ , and we have to calculate still another oxygen profile. The way of determining the reduction of  $b(k)$  will be given at the end of this paragraph. When this is done, the new reduced oxygen demands  $b'(k)$  are used in the following steps. The complete iteration scheme is given in fig. 5.3. The calculation of  $b'(k)$  for each k can be performed as follows:

If the soil pore system is considered as a number of vertical ventilation channels, the gas transport from these channels into the waterfilled soil part can be described with the equation for horizontal transport from a vertical cylinder:

$$D_s \frac{d}{dr} \left( r \frac{dc_w}{dr} \right) = -a \quad (\text{Hoeks, 1972})$$

in which:

- $c_w$  = concentration of oxygen in water (kg m<sup>-3</sup>)
- $D_s$  = diffusion coefficient for oxygen in saturated soil (m<sup>2</sup> d<sup>-1</sup>)
- $r$  = distance from centre of pore (m)

N.B. The concentration of oxygen in the soil solution at the water-air boundary  $c_w$  is, under steady state conditions, in equilibrium with the concentration in the pore air  $c_p$ . In par. 5.5 the temperature-dependent equilibrium relation used in the model is derived.  $D_s$  is obtained from the diffusion coefficient for oxygen in water  $D_w$  through multiplication

Figure 5.2. Iteration scheme for calculation of vertical oxygen distribution in airfilled soil pores

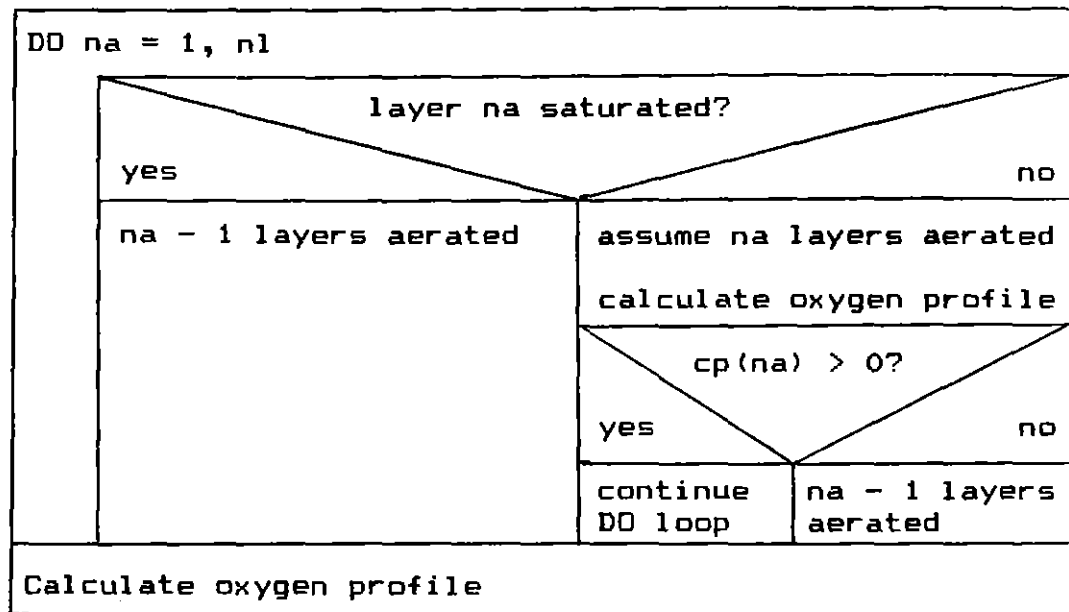
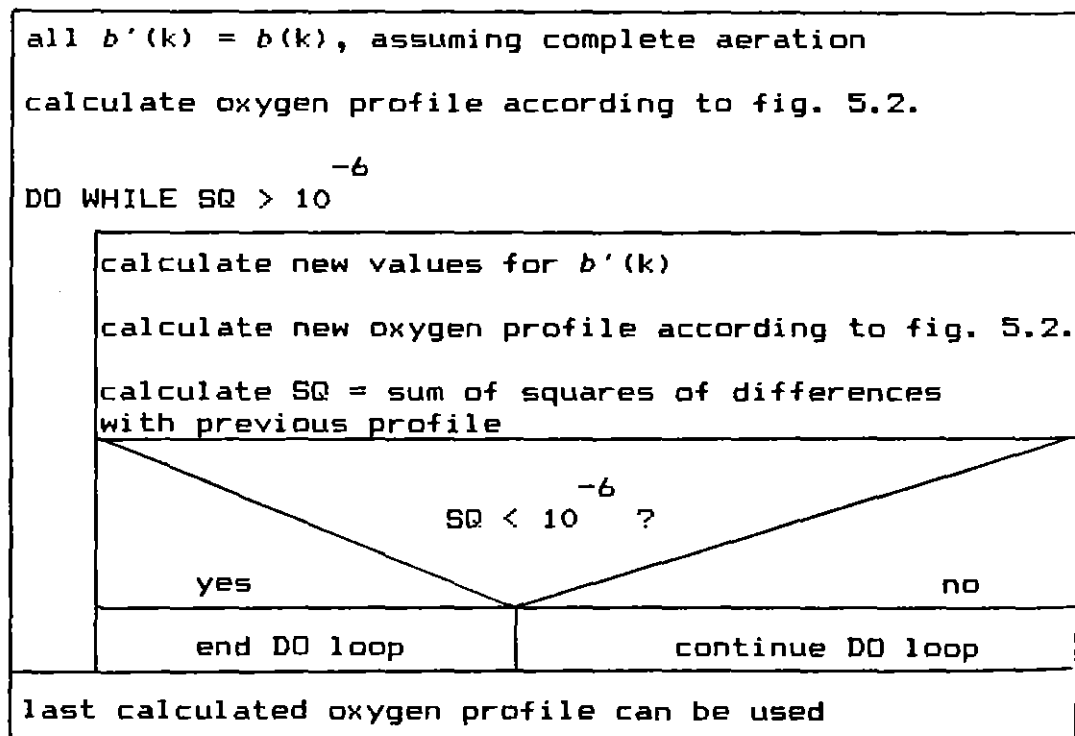


Figure 5.3. Iteration scheme for calculation of vertical oxygen distribution in airfilled soil pores, taking into account the possibility of partial anaerobiosis.



interpoleren bij bekende  $\lambda$  en  $\theta_{sat}$  →  
geometrische gemiddelden  $\lambda$  en  $\theta_{sat}$  →  $\lambda$  en  $\theta_{sat}$  →

by the volume fraction of water (in this case at saturation  $\theta_{sat}$ ), and by a labyrinth factor  $1/\lambda \approx 0.3$  representing the tortuosity of soil pores:

$$D_s = \theta_{sat} * \frac{1}{\lambda} * D_w$$

Boundary conditions for the diffusion equation are:

$$\text{for } r = r_v \quad c_w = c_{we}$$

$$\text{for } r = R \quad \frac{dc_w}{dr} = 0 \quad \text{and} \quad c_w = 0$$

in which:

- $c_{we}$  = equilibrium oxygen concentration in soil water at water/air boundary ( $\text{kg m}^{-3}$ )
- $r_v$  = radius of pore (m)
- $R$  = distance from centre of pore where  $c_w = 0$

Of course the airfilled pores in a soil layer differ in their widths  $r_v$ . If  $\Psi_2$  (cm) is the suction in the layer, the corresponding smallest airfilled pore radius  $r_2$  (m) is calculated as:

$$r_2 = \frac{0.0015}{\Psi_2}$$

$$\log r_2 = \log 0.0015 - \log \Psi_2$$

$$\log r_2 = -2.82 - \log \Psi_2$$

If the air entry point of the soil is at moisture suction  $\Psi_1$  (cm) with corresponding radius of the biggest pore  $r_1$  (m) we can estimate the average radius of the airfilled pores in the layer as the geometrical average of  $r_1$  and  $r_2$  and use this value as a generalized pore radius  $r_v$  for the whole layer:

$$r_v = \sqrt{r_1 * r_2}$$

Rewriting of the diffusion equation yields:

$$r * \frac{dc_w}{dr} = - \frac{a}{D_s} * r$$

Integration yields:

$$r * \frac{dc_w}{dr} = - \frac{a}{2 * D_s} * r^2 + K_3$$

in which  $K_3$  is a constant. Using the boundary condition

$$\text{for } r = R \quad \frac{dc_w}{dr} = 0 \quad \text{we find:}$$

$$\frac{a}{2 * D_s} * R^2 = K_3$$

$$\frac{dc_w}{dr} = - \frac{a}{2 \cdot D_s} * r + \frac{a}{2 \cdot D_s} * R * \frac{1}{r}$$

Integration yields:

$$c_w = - \frac{a}{4 \cdot D_s} * r^2 + \frac{a}{2 \cdot D_s} * R * \ln(r) + K_4$$

In which  $K_4$  is a constant

for  $r = r_v$  where  $c_w = c_{we}$  this becomes:

$$K_4 = c_{we} + \frac{a}{4 \cdot D_s} * r_v^2 - \frac{a}{2 \cdot D_s} * R * \ln(r_v)$$

So the solution for the oxygen concentration decline around an airfilled soilpore is:

$$c_w = - \frac{a}{4 \cdot D_s} * r^2 + \frac{a}{2 \cdot D_s} * R * \ln(r) + c_{we} + \frac{a}{4 \cdot D_s} * r_v^2 - \frac{a}{2 \cdot D_s} * R * \ln(r_v)$$

and for the distance  $R$  from the soil pore centre to the place where  $c_w = 0$  we can write:

$$0 = - \frac{a}{4 \cdot D_s} * R^2 + \frac{a}{2 \cdot D_s} * R * \ln(R) + c_{we} + \frac{a}{4 \cdot D_s} * r_v^2 - \frac{a}{2 \cdot D_s} * R * \ln(r_v)$$

From this equation,  $R$  can be solved by the method of Newton-Raphson iteration with

$$\begin{aligned} F(R) &= - \frac{a}{4 \cdot D_s} * R^2 + \frac{a}{2 \cdot D_s} * R * \ln(R) + c_{we} + \frac{a}{4 \cdot D_s} * r_v^2 - \frac{a}{2 \cdot D_s} * R * \ln(r_v) \\ &= - \frac{a}{2 \cdot D_s} * R * \left( - \frac{1}{2} + \ln(R) - \ln(r_v) \right) + c_{we} + \frac{a}{4 \cdot D_s} * r_v^2 \end{aligned}$$

$$\begin{aligned} F'(R) &= - \frac{a}{2 \cdot D_s} * R + \frac{a}{D_s} * R * \ln(R) + \frac{a}{2 \cdot D_s} * R - \frac{a}{D_s} * R * \ln(r_v) \\ &= - \frac{a}{D_s} * R * (\ln(R) - \ln(r_v)) \end{aligned}$$

according to the iteration scheme

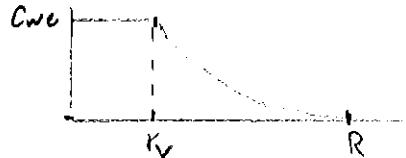
$$R(n+1) = R(n) + \frac{F(R(n))}{F'(R(n))}$$

By calculating in advance the  $R$ -values for extreme values of  $a$ ,  $D_s$  and  $r_v$ , and interpolating between these  $R$  values with the current  $a$ ,  $D_s$  and  $r_v$ , a suitable starting point  $R(0)$  can

be found.

The aerated area in horizontal direction  $ae$  (m<sup>2</sup>) for each pore is:

$$ae = \pi(R^2 - r_v^2)$$



If the volume of a pore over a layer thickness of 1 m is estimated as  $\lambda * \pi * r_v^2$  and the moisture difference between the suctions  $\Psi_1$  and  $\Psi_2$  is  $\theta_+$ , we can approximate the number of airfilled pores as:

$$N = \frac{\theta_+}{\lambda * \pi * r_v^2} = \frac{\theta_+}{10.47 * r_v^2}$$

If all airfilled pores would be regularly distributed the whole aerated soil fraction in the layer considered  $AE$  (m<sup>3</sup> m<sup>-3</sup>) would be

$$AE = N * ae$$

but the distribution of the pores is a random one, so that the aerated volume of soil will not increase linearly with the number of airfilled pores. If we define the chance that a new airfilled pore interferes with an already aerated soil part proportional to that aerated soil part, the total aerated soil volume with  $N$  airfilled pores is equal to:

$$AE = 1 - (1 - ae)^N \approx 1 - e^{-ae \cdot N}$$

and the reduced oxygen production and demand rates are calculated as:

$$a'(k) = -AE * a(k) \text{ (kg m}^{-3} \text{ d}^{-1}) \quad ? \text{ klopt dit wel.}$$

and

$$b'(k) = AE * b(k) \text{ (m}^3 \text{ m}^{-3} \text{ d}^{-1})$$

As a summary of the complex and interrelated processes described in the paragraphs 5.2 and 5.3, the logical order in which the calculations explained take place, is clarified by the scheme given in fig. 5.4.

During short-term heavy rainfall periods it is possible that the rootzone is temporarily saturated with water, and anaerobic conditions occur. In a model that uses steady state average weather conditions during timesteps of more than one day, these periods will not be described. However, due to the relative abundance of organic material in the topsoil, denitrification during such short periods cannot be ignored. Therefore we must make an estimate of the period and the depth over which the topsoil layers are saturated, during the timestep considered. This can be done as follows:

If the precipitation surplus  $P_s$  (m) of the timestep is considered as a vertical column of water with area

$$\theta_{sat} - \theta_{av}$$

Figure 5.4. Scheme for the calculation of  $k_0$  and  $k_1$  values for  $\text{NH}_4$  and  $\text{NO}_3$

<p>Total amount of decomposition of organic material and N-contents of organic materials</p> <p>calculate <math>k_0(\text{NH}_4)</math> for all layers</p> <p>calculate oxygen demand under complete aerobic conditions for all layers:</p> <div> <p>assume temporarily <math>k_1(\text{NH}_4) = -k_{nh}</math></p> <p>calculate <math>\bar{e}_{nh}</math> under aerobic conditions using the transport- and conservation equation for <math>\text{NH}_4</math></p> <p>calculate oxygen demand resulting from org.mat. decomposition and nitrification</p> <p>calculate maximal oxygen production and demand <math>a</math> and <math>b</math></p> </div> <p>calculate oxygen profile under aerobic conditions (see fig. 5.2)</p> <p>calculation of oxygen profile and AE under partial anaerobic conditions (see fig. 5.2 and 5.3) by iteration</p> <p>definitive values for AE for all layers</p> <p><math>k_1(\text{NH}_4) = -AE \cdot k_{nh}</math></p> <p>real <math>\bar{e}_{nh}</math> with transport and conservation equation for <math>\text{NH}_4</math></p> <p><math>k_0(\text{NO}_3) = f(\bar{e}_{nh}, AE, \text{Dom})</math></p>
--

$$AE = 1 - \exp\left\{-\frac{\pi(R^2 - r_v^2)}{\lambda \cdot \pi \cdot r_v^2} \theta^+\right\} = 1 - \exp\left\{\frac{\theta^+}{\lambda} \left(\frac{R^2}{r_v^2} - 1\right)\right\}$$

$\lambda$  (cm): weegverlengingsfactor in relatie tot vochtgehalte en kleifraction.

In kleigronden is de weegverlengingsfactor bij gelijk vochtgehalte, veel groter dan in andere gronden.

$f_c$ : clay fraction = eigengevoerde parameter (volume aandeel)

literatuur: 0.3

Zandgronden: 0.05

veelgronden: 0.02

the height  $h$  (m) of this column is

$$h = \frac{P_s}{\theta_{sat} - \theta_{av}}$$

the relative duration  $t$  of this temporary anaerobiosis caused by saturated transport of such a column of water is

$$t = h/k_s(1)/t$$

in which:

$k_s(1)$  = saturated conductivity of layer 1 (m d<sup>-1</sup>)

$t$  = fraction of timestep with anaerobiosis in toplayer or -layers

The number of layers partaking in this temporary anaerobiosis can be estimated as all those layers with  $Z(k) < h$ .

Now this extra denitrification process has to be combined with the scheme given above. This can be done easily, because both  $t$  and  $(1 - AE)$  have been defined as a fraction, although the first is expressed as a fraction of the timestep and the second as a fraction of the layer volume. Both can be expressed as a fraction of the total amount of organic material decomposed, that is the fraction decomposed anaerobically. So, for the layers under consideration:

$AE$  becomes  $AE - t*AE = AE*(1 - t)$  and

$(1 - AE)$  becomes  $1 - AE + t*AE = 1 - AE*(1 - t)$

and this calculation must take place just after the definitive  $AE$  following from oxygen distribution calculation is used in determining  $k_1(NH_4)$  and  $k_0(NO_3)$  (see fig. 5.4)

#### 5.4. Uptake of mineral N by plants

In this paragraph the calculations leading to the parameter S, the selectivity constant for uptake of soluble species by plant roots, used in the transport- and conservation equation, will be explained.

In the model, only mineral N is taken up in the form of nitrate or ammonium. Therefore, for soluble organic material, the value of S is always zero.

It is assumed that the mineral N requirement of the crop is related to the growth rate, which, on its turn, is related to the amount of evapotranspiration realized. A maximal crop production will be realized in a warm year with optimal N supply. If the total evapotranspiration realized during the growing season in such a warm year is  $E_{pot}(m)$ , and the total maximal N uptake is  $N_{max}(kg\ m^{-2})$ , we can define a optimal mineral-N concentration  $C_{opt}(kg\ m^{-3})$  in the evapotranspiration flux as:

$$C_{opt} = \frac{N_{max}}{E_{pot}}$$

Because the nitrogen requirement in the first part of the growing season is often higher than in the second part, we shall distinguish two periods in this respect:

$$\text{first period: } t_0 - t_1 \text{ with } C_{opt1} = \frac{N_{max1}}{E_{pot1}}$$

$$\text{second period; } t_2 - t_3 \text{ with } C_{opt2} = \frac{N_{max2}}{E_{pot2}}$$

$t_0$  is the time of year (d) when the crop starts to grow

$t_1$  is the time when the mineral N need decreases

$t_3$  is the end of the growing season.

If the evapotranspiration during the growing season is reduced, the total N requirement of the plant will decrease. The cumulative realized nitrogen uptake for the layers of the rootzone, which must be corrected for the N excreted via root exudates, can be calculated as:

$$N_{re}(i) = N_{re}(i-1) + \sum_{n=1}^{nr} \{S(i) * [fe(n,i) * \bar{c}_{ni}(n,i) + \bar{c}_{nh}(n,i)]\} \\ - \sum_{n=1}^{nr} \{nifrex * ke(n,i) * t\}$$

in which:

$N_{re}(i)$  = realized cumulative N uptake by crop roots ( $kg\ m^{-2}$ )

$i$  = timestep number from  $t_0$

$S(i)$  = selectivity constant for this timestep

$n$  = layer number

$nr$  = number of layers in the rootzone

$fe(n,i)$  = realized evapotranspiration flux from layer  $n$  (m)

$\bar{c}_{ni}(n,i)$  = average concentration of nitrate-N during timestep

$\bar{c}_{nh}(n,i)$  = average concentration of ammonium-N during timestep  
in layer n (kg m<sup>-3</sup>)

The maximal N uptake would be:

(with  $C_{opt} = C_{opt1}$  for  $t_0 < t < t_1$  and  $C_{opt} = C_{opt2}$  for  $t_2 < t < t_3$ )

$$N_m(i) = N_m(i-1) + \sum_{i=1}^{nr} f_e(n,i) * C_{opt}$$

in which:

$N_m(i)$  = maximal cumulative N uptake (kg m<sup>-2</sup>)

If for the timestep under consideration  $N_{re}$  would be greater than  $N_m$ , the selectivity constant for the next timestep can be approximated by:

$$S(i+1) = \frac{N_m(i)}{N_{re}(i)}$$

If  $N_{re} \leq N_m$  then

$$S(i+1) = 1$$

And of course if no crop is present, then

$$S(i+1) = 0$$

This procedure of evaluation of the last timestep, correcting afterwards and proceeding in spite of too much uptake during a timestep is followed because otherwise endless iteration procedures would be involved.

## 5.5. Influence of temperature

When the model is used for prediction purposes, the course of temperature in the future years is not known; in this case we use a simple sinus-wave model for the air temperature, with a damping effect for depths below the soil surface. The description of soil temperature at a certain depth  $z$  (m) from soil surface and at a certain day of the year  $t$  according to such a model is (Van Wijk, 1963):

$$T(z,t) = T_a + A_0 * e^{-z/D_m} * \cos(w*t + \varnothing - z/D_m)$$

in which:

$T(z,t)$  = temperature at depth  $z$  and time  $t$  (°C)

$t$  = time of the year (d)

$T_a$  = average yearly temperature (°C)

$A_0$  = amplitude of temperature wave (°C)

$D_m$  = damping depth (m)

$w$  = frequency of temperature wave (rad d<sup>-1</sup>)

$\varnothing$  = phase shift (rad)

For the yearly temperature wave the frequency is:

$$w = \frac{2\pi}{365} = 0.01721 \text{ rad d}^{-1}$$

The damping depth is the depth where the amplitude of the sinus wave is reduced to  $A_0/e$ .  $D_m$  can be calculated from:

$$D_m = \sqrt{2a/w}$$

in which:

$a$  = thermal diffusivity ( $\text{m}^2 \text{d}^{-1}$ )

The value of  $a$  is a measure for the rate with which temperature differences are levelled; it is dependent on the thermal conductivity  $\lambda$  ( $\text{cal m}^{-1} \text{d}^{-1} \text{C}^{-1}$ ) and the specific heat  $c$  ( $\text{cal m}^{-3} \text{C}^{-1}$ ) of a soil:

$$a = \lambda/c$$

The parameter  $a$  is not a constant for a certain soil type; it changes with moisture content. In the model a constant value for  $a$  is used, which has to be estimated from average yearly moisture data (See Van Huet, 1982).

Van Duin (1956, in: Van Huet, 1982) showed that the yearly temperature wave is  $\pi/4$  behind the heat flux wave at soil surface. If the minimum of the heat flux is on the 22nd of december, the minimum of the temperature at soil surface is at the 7th of february. This is accomplished by taking

$$\Phi = -3.7721 \text{ (from: } \cos(w*t + \Phi) = -1)$$

When a certain extreme temperature-scenario must be calculated, the values of  $T_a$  or  $A_0$  or  $a$  can be adapted.

When the model is used for evaluating processes in the past, and temperature measurements have been made, these can be used in the calculations. To derive a temperature course from a limited number of data, the method of Fourier analysis is used (see van Wijk, 1963). If 52 weekly measurements, numbered  $i$  ( $i = 1 \dots 52$ ) of air temperature  $T(0,i)$  at day numbers of the year  $t(i)$  are known which must be equidistant in time, the model describes:

$$T(z,t) = T_a + \sum_{n=1}^6 \{A(n) * \exp(-z\sqrt{n}/D_m) * \sin(n*w*t + \Phi(n) - z*\sqrt{n}/D_m)\}$$

in which the Fourier coefficients  $A(n)$  and  $\Phi(n)$  ( $n$  from 0 through 5) are calculated as follows:

$$\Phi(n) = \arctg(a(n)/b(n))$$

$$A(n) = b(n)/\cos(\Phi(n))$$

$$a(n) = \frac{2}{52} * \sum_{i=1}^{52} \{T(0,i) * \cos(n*w*t(i))\}$$

$$b(n) = \frac{2}{52} * \sum_{i=1}^j \{T(0,i) * \sin(n * w * t(i))\}$$

and

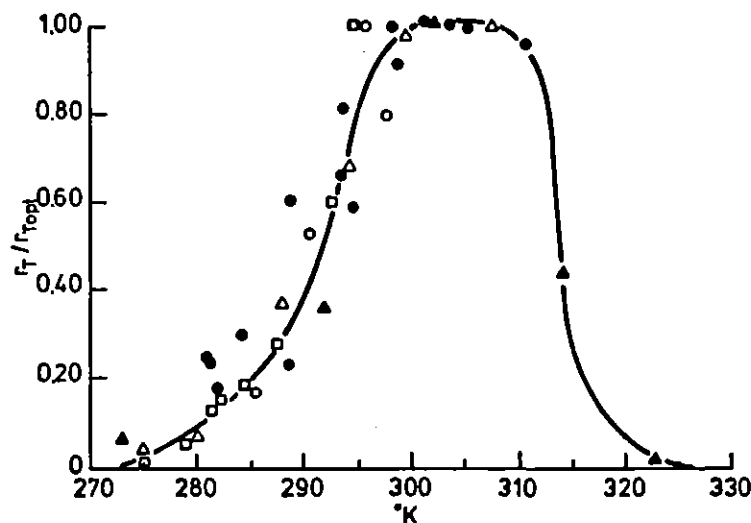
$T_a$  =  $a(0)/2$  is the average of the temperature data given (C)

The average temperature of each layer during the timestep can be calculated with one of these models by using for  $z$  the depth of the middle of the layer from soil surface and for  $t$  the day number at the middle of the timestep.

Then the temperature influences on the different processes can be calculated:

The reaction rate for biological decomposition processes is temperature dependent. Rijtema (in: Lammers, 1983) presents data collected by Kolenbrander (personal communication), as shown in fig. 5.5.

Figure 5.5. Relation between temperature and relative microbiological activity (Lammers, 1983).



A maximum rate occurs between temperatures of 26-36 C. For temperatures from 0 to 26 C this curve can be described by the Arrhenius equation:

$$r(T) = Z * \exp(-a/Rg * T)$$

in which:

$r(T)$  = rate at temperature  $T$  (here  $T$  expressed in K)  
 $Z$  = a constant  
 $a$  = a constant

If we want to express the rate relative to that at average year temperature  $T_a$ , we get (with  $T$  in C and  $a/Rg = 9000$ ):

$$\frac{r(T)}{r(T_a)} = \exp\left(-9000 * \left(\frac{1}{T + 273} - \frac{1}{T_a + 273}\right)\right)$$

For temperatures below 0 C, we take

$$\frac{r(T)}{r(T_a)} = 0$$

The factor  $r(T)/r(T_a)$  can be calculated for each layer. By multiplying  $a_e$ ,  $a_s$ ,  $a_h$ ,  $k_{nh}$  and each  $a_n$  (see 5.1.2, 5.1.4 and 5.2) with this factor, separate rate constants for all these processes for each layer are obtained.

Influence of temperature on the diffusion coefficient for oxygen in air:

The diffusion coefficient  $Da(0)$  of oxygen in air at a temperature of 0 C is  $0.1758 \text{ cm}^2 \text{ s}^{-1}$ . If we assume no changes in the partial pressure of oxygen in air (0.21 atm), the relation with temperature can be calculated as (Bakker, 1965):

$$Da(T) = Da(0) * \left( \frac{273 + T}{273} \right)^{1.75} \text{ cm}^2 \text{ s}^{-1}$$

$$\text{so } D_0 \text{ (see 5.3)} = Da(T) * 10^{-4} * 3600 * 24 \text{ m}^2 \text{ d}^{-1}$$

So for each layer and timestep a different  $D_0$ , dependent on temperature, is used.

Influence of temperature on the solubility of oxygen in water:

The solubility of oxygen decreases when temperature increases. From solubility data given by (Dorzaken, wezen en gevolgen van waterverontreiniging, 1974) a linear relationship for the temperature range of 0 to 15 C for the equilibrium concentration at the air/water boundary was derived:

$$c_{we} = (69.03 - 1.404 * T) * 10^{-3} \text{ kg m}^{-3} \text{ water at 1 atm O}_2 \text{ in air}$$

The solubility is proportional to the partial  $O_2$  pressure at the air/water boundary, so:

$$c_{we} = (69.03 - 1.404 * T) * 10^{-3} * c_p \text{ kg m}^{-3} \text{ water}$$

Influence of temperature on diffusion coefficient for oxygen in water:

For this influence the model interpolates between the following data:

Temperature (C)	$D_w \text{ (m}^2 \text{ d}^{-1})$
	-5
0	$8.64 * 10^{-5}$
	-4
10	$1.38 * 10^{-4}$
	-4
20	$1.64 * 10^{-4}$

and calculates  $D_w$  for each layer.

## 5.6. Influence of moisture

The influence of suboptimal moisture contents on the same rate constants as mentioned in par. 5.5, is described by multiplication of these rates with a reduction factor dependent on the pF. The relation used was derived from the measured influence of moisture on mineralization rate of soil organic nitrogen in a field trial on grassland at Ruurlo during several years. For each layer the pF must be determined from average moisture fraction during the time-step and the pF curve. Then the reduction factor can be found by interpolation using the following data:

pF	reduction factor
$\leq 2.4$	1.00
2.7	0.57
2.9	0.36
3.2	0.32

Reduction in some process rates due to high moisture contents is assumed to take place only if anaerobic oxidation is hampered by lack of nitrate for denitrification.

## 5.7. Additions to the soil and ploughing

At the start of each timestep additions to the soil can be simulated: the properties of the added materials must be specified in the input data. The additions can exist of:

- inorganic fertilizer
- manure or animal slurry
- plant roots
- other organic materials

Specifications needed per material added are:

Composition of standard materials, defined at beginning of the run:

- fraction of the material which is organic
- N fraction in the organic material fractions
- decomposition rates for different fractions in the organic material (see par. 5.1.1)
- fraction  $\text{NH}_4$
- fraction  $\text{NO}_3$

Way of addition:

- depth of incorporation of the material (number of layers)
- number of layers that are ploughed

The material is equally divided over the layers of incorporation. Only when plant roots are "added", that is when the crop is harvested, the distribution of roots as calculated, is adopted. In case of a tuber crop the harvested tuber material is subtracted and the root rests are divided over the top 10 cm of soil.

N.B. If crop residues other than roots are to be incorporated in the soil this should be defined separately as an addition at harvest time.

The simulation of ploughing in the model means the equal redistribution of all species and fractions present in the participating layers over the layers for which ploughing is desired.

## 5.8. Other processes

### Volatilization:

One important process in the nitrogen cycle has only been incorporated roughly in the model. Volatilization of  $\text{NH}_3$ , formed from  $\text{NH}_4$ , is a process strongly dependent of short-term weather conditions. When  $\text{NH}_4$ -containing material is added on top of the soil and the weather is dry and warm, a major part of it may get lost through volatilization. If, however, the material is incorporated in the soil or precipitation falls directly after application, the major part will be saved. Because these weather conditions cannot be foreseen, modelling of volatilization is done as follows:

- For additions on top of the soil: a certain percentage, defined beforehand, of the  $\text{NH}_4$  applied is immediately lost: for grassland 30-40%, for arable land ca. 20%.  
Addition of the remaining material to layer 1.
- For additions incorporated in the first (few) layer(s): no volatilization

### Adsorption of $\text{NH}_4$ :

The  $\text{NH}_4$  ion may be adsorbed to the soil complex, consisting of the negative surfaces of clay particles and humic compounds. The distribution ratio  $R_d$  is the ratio amount adsorbed : amount in solution, both expressed in  $\text{kg m}^{-3}$  soil system:

$$Q = R_d \cdot c_{nh} \cdot \theta$$

in which:

$Q$  = amount of  $\text{NH}_4$  adsorbed ( $\text{kg m}^{-3}$  soil system)

The amount adsorbed in a certain soil layer is:

$$q_{nh} = L \cdot Q$$

in which:

$q_{nh}$  = amount adsorbed in a soil layer ( $\text{kg m}^{-2}$ )

The total amount of  $\text{NH}_4$  present in a layer is:

$$c_{nh} \cdot \theta \cdot L \cdot (R_d + 1)$$

The value of  $R_d$  is dependent of the cation exchange capacity (C.E.C.) of a soil and of the composition of the complex and the solution.

Organic matter decomposition in the subsoil:

Soil organic matter present in the deeper layers of the subsoil can have a very slow decomposition rate, in the order of 0.3% per year (Steenvoorden, 1983) and possibly originates from other sources than the organic material in the topsoil. Therefore the possibility is given in the model to attribute an extra reduction factor to the rate constant  $a_h$  for deeper layers.

Nitrogen fixation is not included in the model.

## 5.9. Mass balances

After all the transformation- and transport processes have taken place, at the end of the timestep the amounts of carbon and nitrogen left can be checked by making mass balance calculations.

Mass balance for organic material:

Per layer the following equation should be met:

$$B01 = B02$$

in which:

$B01$  = Disappearance of organic material + amount influx - amount outflux (kg m<sup>-2</sup>)  
+ amount of exudates formed

$B02$  = transformation of organic material into CO<sub>2</sub> (kg m<sup>-2</sup>)

$$\begin{aligned} B01 &= \sum_{fn} \{V(0)*s(fn,0) - V(t)*s(fn,t)\} + k_0(DMS)*L*t \\ &+ \sum_{fn} \{I_s(fn) - U_s(fn)\} + H(0) - H(t) \\ &+ E(0) - E(t) + k_e*t \end{aligned}$$

$$= Dom$$

$B02$  = amount transformed into CO<sub>2</sub> from:  
DMS  
Soil organic material ( $H_s$  and  $H_e$ )  
exudates

$$\begin{aligned} B02 &= \sum_{fn} \left\{ \int_0^t ((1-a)*a_s*\mathcal{B}(fn)*V) dt \right\} \\ &+ \sum_{fn} \left\{ \int_0^t (a_h*H_s(fn,t)) dt \right\} + \int_0^t a_h*H_e(t) dt \\ &+ \int_0^t (1-a)*a_e*E(t) dt \end{aligned}$$

$$\begin{aligned}
 B02 &= \sum_{fn} \{ (1-a) * a_s * S(fn) * V * t \} \\
 &+ ah * \sum_{fn} \int_0^t \left\{ \frac{a_s * a_s * V * S(fn)}{ah} * (1 - e^{-ah*t}) dt + \int_0^t Hs(fn,0) * e^{-ah*t} dt \right\} \\
 &+ ah * \int_0^t \left\{ \left( \frac{a * ke}{ah} * (1 - e^{-ah*t}) + \frac{a * (ke - ae * E(0))}{ah - ae} * (e^{-ah*t} - e^{-ae*t}) \right) \right. \\
 &\quad \left. + He(0) * e^{-ah*t} \right\} dt \\
 &+ (1-a) * ae * \int_0^t \left\{ \frac{ke}{ae} - \left( \frac{ke}{ae} - E(0) \right) * e^{-ae*t} \right\} dt \\
 &= \sum_{fn} \{ (1-a) * a_s * S(fn) * V * t \} \\
 &+ \sum_{fn} \left\{ a * a_s * V * S(fn) * \left( t + \frac{e^{-ah*t} - 1}{ah} \right) - Hs(fn,0) * (e^{-ah*t} - 1) \right\} \\
 &+ a * ke * \left( t + \frac{e^{-ah*t} - 1}{ah} \right) + \frac{a * ah * (ke - ae * E(0))}{ah - ae} \\
 &\quad * \left\{ \frac{e^{-ae*t} - 1}{ae} - \frac{e^{-ah*t} - 1}{ah} \right\} - He(0) * (e^{-ah*t} - 1) \\
 &+ (1-a) * \left\{ ke * t + \left( \frac{ke}{ae} - E(0) \right) * (e^{-ae*t} - 1) \right\}
 \end{aligned}$$

The deviation in the mass balance for organic material, BO(%) is now defined as:

$$BO = \frac{B01 - B02}{TOOM} * 100\%$$

in which TOOM = total amount of organic material present at the end of the timestep (kg m<sup>-2</sup>)

$$TOOM = \sum_{fn} Os(fn,t) + H(t) + E(t) + \sum_{fn} s(fn,t) * V(t)$$

Mass balance for mineral nitrogen:

Per layer the following equation should be met:

$$BN1 = BN2$$

In which:

BN1 = amount of mineral N disappeared from solution plus total influx of mineral N minus total outflux of mineral N plus net amount mineralized (kg m<sup>-2</sup>)

BN2 = amount of nitrogen denitrified and taken up by plant roots plus increase in amount adsorbed (kg m<sup>-2</sup>)

N.B. Plant uptake = plant uptake of mineral N, here not corrected for exudate-N production as was done in par. 5.4., because the balance is for mineral N in solution and exudate-N is organic N.

$$\begin{aligned} BN1 &= V(0) * (c_{nh}(0) + c_{ni}(0)) - V(t) * (c_{nh}(t) + c_{ni}(t)) \\ &+ I_s(NH_4-N) + I_s(NO_3-N) - U_s(NH_4-N) - U_s(NO_3-N) \\ &+ k_0(NH_4) * L * t \end{aligned}$$

$$\begin{aligned} BN2 &= 0.541 * (1 - AE + t * AE) * Dom \\ &+ f_e * t * S * (c_{nh} + c_{ni}) \\ &+ Q(t) - Q(0) \end{aligned}$$

N.B. The uptake of mineral N can be written in this form for all layers, because for those layers not belonging to the rootzone,  $f_e = 0$ .

The derivation in the mass balance for N, BN(%), can be expressed as:

$$BN = \frac{BN1 - BN2}{TON} * 100\%$$

in which TON (kg) is the total amount of mineral N present in the layer at the end of the timestep.

$$TON = V(t) * (c_{nh}(t) + c_{ni}(t)) + Q(t)$$

## 6. CALCULATION OF STANDARD PARAMETER VALUES

### 6.1. Organic material formation and decomposition

Parameter values for description of the long term organic matter- and organic N-behaviour, needed in the model ANIMO, must be chosen in such a way that the results obtained correspond to a number of relevant observations in practice:

1. Kolenbrander (1969) collected literature data on long-term net decomposition of different organic materials added to soil or on top of soil in field trials.  
In fig. 6.1 the decomposition curves are given.  
The parameters for decomposition of fresh organic material,  $a_n$ , combined with the decomposition rate of humus,  $a_h$ , and the decomposition rate of organic material in solution,  $a_s$ , must produce about the same results for all these materials. The influence of the parameter  $a_s$  in this aspect is that the smaller  $a_s$  is, the more OMS leaches to deeper layers, and the smaller the real net decomposition of organic material in the trials, because then the disappearance measured will be due to leaching as well as to decomposition.
2. Janssen (1984) showed that not only the amount of organic material present determines the decomposition rate, but also the nature and age of this material. In other words: the cropping history of a soil profile is an important factor to be taken into account when the decomposition rate of the soil organic material is determined.
3. The decomposition rate for "soil organic material" (the net decomposition rate of all the decomposing organic material present in soil) on the long term must be 1.5 to 2% per year (Kortleven 1963). This means that  $a_n$  and/or the smallest  $a_n$  per material must be of this order.
4. Steenvoorden (1983) measured Total Organic Carbon (TOC) profiles in solution in a lysimeter experiment where heavy gifts of animal slurry were added to soil. The parameter  $a_s$  must be chosen in such a way that these results can be approximated.
5. If heavy gifts of animal slurry are applied, build-up of soil organic material must take place not only in the rootzone or the zone to which fresh organic material is added, but also in the layer below that zone (see McGrath, 1981). The only way in which this can be reached in a model is by simulating transport of organic material in solution, which material has a decomposition rate not too high for this effect to occur, and by applying a lower decomposition rate for soil organic material.
6. The distribution of nitrogen over the organic material fractions in cattle slurry must be such that in the first year after application approximately 50% of the organic N is mineralized. (Van Dijk and Sturm, 1983).

Figure 6.1. Net decomposition of different organic materials adapted from Kolenbrander (1969).

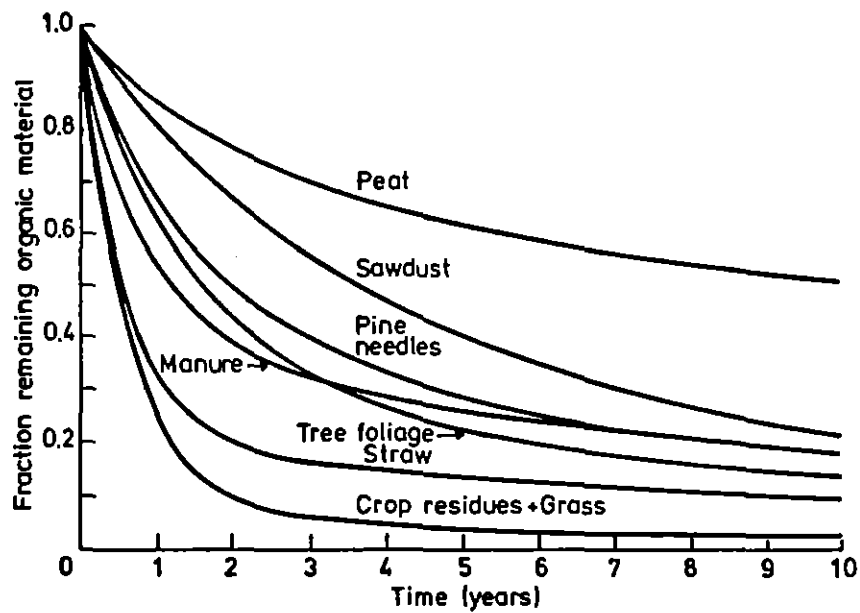
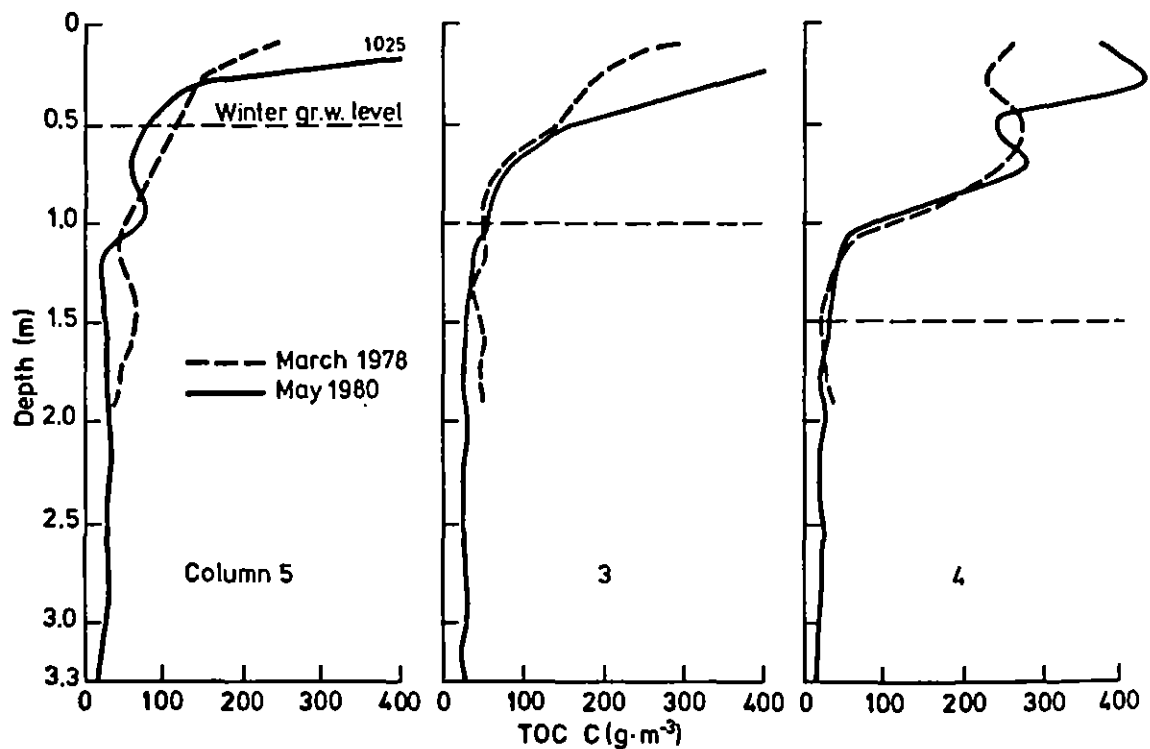


Figure 6.2. TOC profiles in a lysimeter experiment with yearly application of high rates of pig slurry in november (Steenvoorden, 1983).



The parameters to be determined for use in the model ANIMO are:

1. The fraction FR(fn) and the decomposition rate an(fn) of each fraction fn in each kind of organic material
2. The production and -decomposition rate of exudates, ke and ae
3. The production- and decomposition rate of OMS, kO(OMS) and k1(OMS)
4. The decomposition rate of humus, ah
5. The nitrogen contents of all these materials, nifr(fn), nifruhu, nifrex
6. The fraction of organic material which already is in solution when the material is applied (mainly of interest for animal slurry).

For the parameters under numbers 2 and 4 and some of those under 6 we shall use directly estimated values. For the other parameters we shall derive the values from a simplified simulation model, because they are so strongly interrelated.

Ad 2.

Root exudates consist of many different materials; carbohydrates, amino acids, organic acids, and others. Most research is done on carbohydrates and amino acids; the impression is given that these are the main components. Barber and Gunn (in: Russel, 1977) found a ratio of 9:1 of these components in the exudates of young barley plants. If the average C/N of carbohydrates is put at 100 (%N = 0.68) and that of amino acids at 3.5 (%N = 19), the average N content of the exudates can be estimated at

$$\text{nifrex} = 0.9 \cdot 0.0068 + 0.1 \cdot 0.19 = 0.025$$

This number corresponds with an average N-content of root material.

The amount of exudates excreted is an entity difficult to determine under natural circumstances, because the produced material is rapidly decomposed by micro-organisms. Measurements under sterile circumstances, however, show a too low excretion of exudates, because it is known that the presence of microflora stimulates exudation.

Exudate production rate is often expressed as relative to plant growth. Several sources named in Russell(1977) give the results of their calculations, varying from less than 1% of the dry weight increase of the plant to 9% of the root mass increase under sterile circumstances. Shamoot e.a. (1968) found that 25 to 49 g organic material originating from roots per 100 g harvested root material stayed behind in the soil after the harvest. When the fact that during the growing season much of the produced exudates is already oxidized is taken into account, it might even be that total exudate production during a growing season is of the same order as root production.

Merckx e.a. (1985) measured distribution of <sup>14</sup>-C over plant parts, soil and soil-root respiration, after growing wheat plants in a <sup>14</sup>-CO<sub>2</sub>-atmosphere. Some results of their experiments are given in table 6.1. The soil respiration can be estimated as half of the soil-root respiration.

From these data we calculate the data given in table 6.2,

The total amount of exudate decomposed during a time interval  $t_1$  to  $t_2$ , expressed as  $^{14}\text{C}$  activity, can be estimated as:

$$\frac{3}{2} \cdot \text{soil respiration activity } (t_2 - t_1)$$

assuming an assimilation factor of  $1/3$ .

The total amount of exudate formed during a time interval (expressed as  $^{14}\text{C}$  activity) can be estimated as

$$\text{cum soil resp. act. } (t_2 - t_1) + \text{soil residue act. } (t_2 - t_1)$$

and we can define for each time interval  $t_2 - t_1$ :

$$\begin{aligned} \frac{\text{exudate production}}{\text{root production}} &= \text{relative exudate production rate} \\ &= \frac{\text{cum soil resp. act. } (t_2 - t_1) + \text{soil residue act. } (t_2 - t_1)}{\text{cum root activity } (t_2 - t_1)} \end{aligned}$$

The average value for relative exudate production calculated from these data is 0.41. In the model we use this value:

$$k_e = 0.41 \cdot (R(\ln, t) - R(\ln, 0))$$

It must be stressed that this number is derived from only one experiment with one plant species in one growth stage. In reality, exudate rates and the composition of exudates is dependent on plant species and age, but there are not enough data to model these effects.

The parameter  $k_e$  is calculated per timestep and per layer in the rootzone.

Looking at the last two columns of table 6.2 we can see that the calculated exudate decompositions are sometimes higher than the calculated exudate productions. This can be a result of the assumptions about the assimilation factor and the ratio soil respiration : root respiration. At any case it will be clear that the decomposition must have been very fast. The remaining soil residue consisted of humus-like material. In the model we shall use a very high decomposition rate:

$$a_e = 1.0 \text{ d}^{-1}$$

so that in practice, little or no exudates will remain in solution.

Table 6.1. Distribution of  $^{14}\text{C}$ -activity (kBq) after growth of wheat plants in 2 different soils in a  $^{14}\text{CO}_2$ -atmosphere with specific activity of 5-6 kBq  $\text{mg}^{-1}\text{C}$ . (Merckx, 1985).

Days after germination	Soil-root respiration (cum)	Soil residue (cum)	Roots (cum)	
				Sandy soil
21	196	40	463	
28	1616	393	2301	
35	4940	421	7663	
42	9441	583	14377	
				Silty clay loam
21	12	7	?	
28	204	58	260	
35	858	265	1501	
42	1993	684	4295	

\* Prior to growth in the  $^{14}\text{C}$  atmosphere the plants were grown in a normal atmosphere for 10 days.

Table 6.2. Calculation of exudate production rate from the data of table 6.1. For calculation method see text.

Days after germination	Relative exudate production	Exudate activity formed (kBq)	Exudate activity decomposed (kBq)	
				Sandy soil
28	0.58	1063	1065	
35	0.32	1690	2493	
42	0.36	2413	3377	
				Silty clay loam
35	0.43	534	491	
42	0.35	987	852	
	average			
	0.41			

Ad 4. The decomposition rate of humus:

From the analysis results by Stanford and Smith(1972) of 39 different topsoils it can be derived that these soils had an average C/N quotient of 11; this number does not change if the average of fallow, unfertilized soils is calculated or that of cropped and fertilized soils. From this we conclude that the bulk of the organic material present in these soils was of the same nature; because of the low C/N quotient it must have been humus. Therefore a humus decomposition rate of 0.02 j-1 was used in the following calculations, and the decomposition rates of all fractions in the fresh organic materials should be greater than 0.02 j-1.

[ When solubilization and transport of organic material in solution are not taken into account, some of the curves of fig. 6.1 can be fitted relatively simple to the following concept:

Decomposition of fresh organic material:

$$\frac{dO_s(fn)}{dt} = O_s(fn) \cdot \exp(-a_n \cdot t) \quad (\text{the same as in ANIMO})$$

Formation and decomposition of soil organic material:

$$\frac{dH(fn)}{dt} = -a \cdot \frac{dO_s(fn)}{dt} - a_h \cdot H(fn)$$

Resulting in a direct formulation of the total amount of organic material present at time t after the addition at t=0:

$$O_s(fn,t) + H(fn,t) = a \cdot \frac{O_s(fn,0) \cdot a_n}{fn \cdot a_h - a_n} \cdot \left( \frac{e^{-a_n \cdot t}}{a_n} - \frac{e^{-a_h \cdot t}}{a_h} \right)$$

It appeared that with this formulation and using  $a_h \approx 0.02$  j-1 and  $a \approx 0.33$ , no parameters for  $fr(fn)$  and  $a_n$  could be found which described the curves for the faster decomposing materials in fig. 6.1; the reason for this is that even with very high values for  $a_n$ , the fresh material is transformed for 1/3 part into slowly decomposing humus. If we hold to  $a_h = 0.02$  j-1, it means that transport of soluble organic material plays an important role. ]

For the nitrogen content of soil organic material/biomass a factor  $nifrh_u = 0.048$  was fixed, corresponding with a C/N ratio of 14 if the C-content of this material is 0.58.

Ad 1, 3, 5 and 6

Before the simplified model with which the other parameters are derived, is presented, we shall first make some estimates of the rate constants involved.

In fig. 6.2. the TDC-profiles given by Steenvoorden (1983) are given. Pig slurry was added at a rate of 300 t y-1 to lysimeter columns with different winter groundwater tables. Except for the first, which was in spring 1977, all additions were fall additions, starting in the fall of 1977. From these profiles it can be concluded that:

- there is a kind of basic TDC concentration of about 30 g

m-3 in all columns, which cannot originate from the slurry additions, because in column 5 the water front from the precipitation surplus has not reached the bottom of the column after the 3 years of experimentation. We shall ignore this low concentration, probably consisting of a slowly decomposing material.

- The formation of OMS continues after the first year of addition of slurry, because the TOC concentrations in the top layers are higher after 4 gifts than after 2 gifts, although, certainly in column 4, the yearly precipitation surplus reaches a much greater depth than the rootzone where the slurry was worked in.
- The production of OMS in the first year per addition is greater than in the following years, otherwise the TOC fronts would show a much greater increase in concentration through the years.

The total amount of organic matter per addition was 1350 g m<sup>-2</sup>. Oosterom and Steenvoorden (1980) give the COD (Chemical oxygen demand) of cattle slurry before and after centrifugation. The COD is proportional to the TOC. After centrifugation, 40% of the COD was still in solution. If the same applies to pig slurry, it means that at least 40% of the organic matter will be solubilized during the first year (936 g). After one winter, the precipitation front in column 3 will have reached a depth of about 1.5 m (300 mm precipitation surplus, moisture fraction about .2). The organic material content of this layer in solution is about 150/0.58\*0.2\*1.5 g = 77.4 g. If the 936 g would be all the OMS production of the first winter after an addition, we can be calculated from:

$$\begin{aligned} \text{OMS}(t) &= \text{OMS}(0) * e^{-as*t} \\ -as*t &= \ln\left(\frac{77.4}{936}\right) = 2.49 \quad \text{and} \quad as = 1.36*10^{-2} \text{ d}^{-1} = 4.97 \text{ j}^{-1} \end{aligned}$$

for the winter period. When temperature effects are considered, and when more than 40% of the organic matter solubilizes, as will be greater.

If the 40% organic matter would not immediately be available for decomposition in pig slurry, but produced during the first half year, the rate constant as would even be higher. If we assume that 40% organic matter comes available in solution at a constant rate of production k, we can derive:

$$\begin{aligned} \frac{d\text{OMS}}{dt} &= k - as*\text{OMS} \\ \text{OMS} &= \frac{k}{as} * (1 - e^{-as*t}) = 77.4 \text{ g} \\ \text{with } k &= \frac{936}{183} \quad \text{we find } as \approx 0.066 \text{ d}^{-1} = 24.1 \text{ j}^{-1} \end{aligned}$$

From these two calculations we estimate as in the order of 15 j<sup>-1</sup>.

From fig. 6.1. we see that the net decomposition of manure during the first year is about 50%. When no solubilization would have taken place, and all the material would directly be transformed into either CO<sub>2</sub> or soil organic matter, this would mean a decomposition of the fresh organic material of

$$Dom = \frac{3}{2} * 50\% = 75\% \text{ when the assimilation factor would be } \frac{1}{3}$$

Because solubilization has taken place, it means that the 50% loss is caused by both decomposition and transport from the topsoil. The experiments of which Kolenbrander (1969) reports, mainly concern analysis of the top 10 to 20 cm of the soil. So the total net decomposition may be less than 50%, due to humus production in deeper layers, in which case also the decomposition of fresh organic material would be less than 75%. At 75% decomposition, a first-order decomposition rate would be 1.39 j<sup>-1</sup>. If several fractions in the organic material are distinguished, their separate decomposition rate constants can vary around this number for manure. Johnen (1974) gives decomposition rates of pure organic materials in the soil:

cellulose	1.39 j <sup>-1</sup>
hemicellulose	2.30 j <sup>-1</sup>
lignine	0.639 j <sup>-1</sup>

These materials are the main organic components in plant material. The slowest decomposing organic material mentioned by Johnen (1974) in this context was

phenols	0.105 j <sup>-1</sup>
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Therefore we shall choose values for the parameters  $a_n$ , meeting the criterium:

$$a_n \geq 0.1 \text{ j}^{-1}$$

Because we have more data about manure than about the other materials in fig. 6.1., we shall derive the value of  $a_s$  with the simplified model using the available data and constraints for manure:

$$a_h = 0.02 \quad a_s \approx 15 \quad a_n \geq 0.1 \quad \text{and} \quad \sum_{f_n} O_s(f_n, t=1 \text{ y}) < 75\%$$

The simplified model has the name HISTOR. It calculates the decomposition of fresh organic material to organic material in solution, and to soil organic material plus the N mineralization following from these transformations, according to the same principles as the model ANIMO, but in a less detailed way. Denitrification is not included.

The basic structure and concepts of this model are:

- 5 layers of equal thickness
- fixed water content per layer, equal to the contents at the beginning of april or the beginning of october when normally the transition from precipitation surplus to evapotranspiration surplus takes place
- the precipitation surplus of the whole year falls during the winter in a steady state flux

- timesteps of half a year (a summer step and a winter step)
- additions of organic material to layer 1 at the beginning of summer or at the beginning of winter
- production, transport and decomposition of OMS in layer 1 and transport and decomposition of OMS in the other layers during the winter period
- production and decomposition of OMS (no transport) in all layers during the summer period
- continuous soil organic matter formation and decomposition and N mineralization in all layers
- rate constants for organic matter transformation processes are reduced in the wintertime and increased during the summertime as compared to their yearly average values.

Reasonable estimates of parameter values should be obtained by the following iteration process:

1. Choose parameter values
2. Simulate the lysimeter experiments of Steenvoorden (1983) with HISTOR
3. Simulate the decomposition of manure with HISTOR
4. Comparison of TOC profiles measured and calculated in step 2.
5. Comparison of total organic material content of layer 1 calculated in step 3 with the values of the decomposition curve given by Kolenbrander (1969)
5. Check if the amount of N mineralized in the first year is about 50% of the mineral N present in manure.
6. If necessary, choose other parameter values and continue with step 2.

The values fixed for  $a_h$ ,  $a_e$ ,  $n_{frhu}$ ,  $n_{frex}$  and the formation rate of exudates and the parameter  $a_s$ , found in the process described above, should also be applicable to the other materials of fig. 6.1., and for those materials we only have to find the parameters  $a_n(fn)$  and  $n_{fr}(fn)$ .

The description of the processes in the model HISTOR, based on the concepts described above, is (layer indices are omitted unless otherwise indicated):

- \* Decomposition of fresh organic material for layer 1 during summertime:

$$\frac{dO_s(fn)}{dt} = -a_n * O_s(fn)$$

$$O_s(fn, t) = O_s(fn, 0) * e^{-a_n * t}$$

- \* Formation and decomposition of OMS for layer 1 during summertime:

$$\frac{ds(fn)}{dt} = \frac{1}{L * \theta} * \frac{dO_s(fn)}{dt} - a_s * s(fn)$$

$$s(fn, t) = \frac{a_n * O_s(fn, 0)}{(a_s - a_n) * L * \theta} * (e^{-a_n * t} - e^{-a_s * t}) + s(fn, 0) * e^{-a_s * t}$$

- \* Exudate production and decomposition during summertime: as in par. 5.1.
- \* Soil organic material production and decomposition for layer 1 during summertime:

from DMS:

$$\frac{dH_s(f_n)}{dt} = L \cdot \theta \cdot a \cdot s \cdot s(f_n) - a_h \cdot H_s$$

$$H_s(f_n) = \frac{a_n \cdot D_s(f_n, 0) \cdot a \cdot a_s}{a_s - a_n} \cdot \left\{ \frac{e^{-a_h \cdot t}}{e^{-a_s \cdot t}} - \frac{e^{-a_n \cdot t}}{e^{-a_h \cdot t}} \right\} + \frac{L \cdot \theta \cdot a \cdot a_s \cdot s(f_n, 0)}{a_h - a_s} \cdot (e^{-a_s \cdot t} - e^{-a_h \cdot t}) + H_s(f_n, 0) \cdot e^{-a_h \cdot t}$$

from exudates: as in par. 5.1.

Total soil organic matter layer 1:

$$H(t) = \sum_{f_n} H_s(f_n, t) + E(t)$$

- \* Decomposition of DMS for the other layers in summertime:

$$\frac{ds(f_n)}{dt} = -a_s \cdot s(f_n)$$

$$s(f_n, t) = s(f_n, 0) \cdot e^{-a_s \cdot t}$$

- \* Formation and decomposition of soil organic matter for the other layers during summertime:

$$\frac{dH_s(f_n)}{dt} = L \cdot \theta \cdot a \cdot a_s \cdot s(f_n) - a_h \cdot H_s$$

$$H_s(f_n, t) = \frac{L \cdot \theta \cdot a \cdot a_s \cdot s(f_n, 0)}{a_h - a_s} \cdot (e^{-a_s \cdot t} - e^{-a_h \cdot t}) + H_s(f_n, 0) \cdot e^{-a_h \cdot t}$$

Total soil organic matter other layers:

$$H(t) = \sum_{f_n} H_s(f_n)$$

- \* Nitrogen mineralization layer 1 during summertime:

$$M_n(1) =$$

$$\sum_{f_n} \{ n_{ifr}(f_n) \cdot (D_s(f_n, 0) - D_s(f_n, t) + L \cdot \theta \cdot s(f_n, 0) - L \cdot \theta \cdot s(f_n, t)) \} + n_{ifrhu} \cdot \{ H_s(0) - H_s(t) + H_e(0) - H_e(t) \}$$

$$+ \text{nifrex} * \{E(0) - E(t) + k_e * t\}$$

- \* Nitrogen mineralization other layers during summertime  
(with layer index i):

$$Mn(i) = \text{nifrh} * \{H(0) - H(t)\}$$

$$+ \sum_{fn} \{ \text{nifr}(fn) * (L * \theta * s(fn, 0) - L * \theta * s(fn, t)) \}$$

- \* Decomposition of fresh organic material in layer 1 during  
wintertime : the same as for the summertime

- \* Formation and decomposition of OMS in layer 1 during  
wintertime:

$$\frac{d s(fn)}{dt} = - \frac{1}{L * \theta} * \frac{d O_s(fn)}{dt} - a_s * s(fn) - \frac{f}{L * \theta} * s(fn)$$

$$s(fn, t) = \frac{a_n * O_s(fn)}{L * \theta * (a_s + f/L/\theta - a_n)} * (e^{-a_n * t} - e^{-(a_s + f/L/\theta) * t}) + s(fn, 0) * e^{-(a_s + f/L/\theta) * t}$$

- \* Decomposition of exudates during wintertime:

$$E(t) = E(0) * e^{-a_e * t}$$

- \* Formation and decomposition of soil organic matter in layer  
1 during wintertime:

from OMS:

$$\frac{d H_s(fn)}{dt} = a * a_s * L * \theta * s(fn) - a_h * H_s$$

$$H_s(fn) = \frac{a * a_s * a_n * O_s(fn, 0)}{a_s + f/L/\theta - a_n} * \left\{ \frac{e^{-a_h * t} - e^{-(a_s + f/L/\theta) * t}}{a_h - a_s - f/L/\theta} + \frac{e^{-a_n * t} - e^{-a_h * t}}{a_h - a_n} \right\} + \frac{L * \theta * a * a_s * s(fn, 0)}{a_h - f/L/\theta - a_s} * (e^{-(a_s + f/L/\theta) * t} - e^{-a_h * t}) + H_s(fn, 0) * e^{-a_h * t}$$

from exudates:

$$\frac{dH_e}{dt} = a \cdot a_e \cdot E(t) - a_h \cdot H_e(t) = a \cdot a_e \cdot E(0) \cdot e^{-a_e \cdot t} - a_h \cdot H_e(t)$$

$$H_e(t) = \frac{a \cdot a_e \cdot E(0)}{a_h - a_e} \cdot (e^{-a_e \cdot t} - e^{-a_h \cdot t}) + H_e(0) \cdot e^{-a_h \cdot t}$$

Total soil organic matter layer 1:

$$H(t) = \sum_{f_n} H_s(f_n, t) + E(t)$$

\* The average OMS-concentration of layer 1 during the winter is:

$$\bar{s}(f_n) = \frac{f}{P_s} \int_0^t s(f_n) dt$$

in which:

$f$  = steady state percolation flux during wintertime (m d<sup>-1</sup>)

$P_s$  = precipitation surplus (m)

$$\begin{aligned} \bar{s}(f_n) &= \frac{f}{P_s} \frac{a_n \cdot O_s(f_n)}{L \cdot \theta \cdot (a_s + f/L/\theta - a_n)} \\ &\quad \cdot \left\{ \frac{1}{a_n} \cdot (1 - e^{-a_n \cdot t}) - \frac{1}{a_s + f/L/\theta} \cdot (1 - e^{-(a_s + f/L/\theta) \cdot t}) \right\} \\ &\quad + \frac{f}{P_s} \frac{s(f_n, 0)}{a_s + f/L/\theta} \cdot (1 - e^{-(a_s + f/L/\theta) \cdot t}) \end{aligned}$$

\* Formation and decomposition of OMS in the other layers during the winter (with layer indices i):

$$\begin{aligned} \frac{ds(f_n)}{dt} &= \frac{f}{L \cdot \theta(i-1)} \cdot \bar{s}(f_n, i-1) - \frac{f}{L \cdot \theta(i)} \cdot s(f_n, i) - a_s \cdot s(f_n, i) \\ s(f_n, i, t) &= \frac{f/L/\theta(i-1) \cdot \bar{s}(f_n, i-1)}{a_s + f/L/\theta(i)} \cdot (1 - e^{-(a_s + f/L/\theta(i)) \cdot t}) \\ &\quad + s(f_n, i, 0) \cdot e^{-(a_s + f/L/\theta(i)) \cdot t} \end{aligned}$$

\* The average OMS-concentrations of the other layers i during wintertime is:

$$\bar{s}(f_n, i) = \frac{f}{P_s} \int_0^t s(f_n, i) dt$$

$$g(fn,i) = \frac{f \cdot f/L/\theta(i-1) * g(fn,i-1)}{P_s \quad a_s + f/L/\theta(i)}$$

$$* \{ t + \frac{1}{a_s + f/L/\theta(i)} * (e^{-(a_s + f/L/\theta(i)) * t} - 1) \}$$

$$+ \frac{f \cdot s(fn,i,0)}{P_s \cdot a_s + f/L/\theta(i)} * (1 - e^{-(a_s + f/L/\theta(i)) * t})$$

\* Exudate decomposition during wintertime:

$$E(t) = E(0) * e^{-a_e * t}$$

\* Formation and decomposition of soil organic material other layers during wintertime:

from OMS:

$$\frac{dH_s(fn)}{dt} = L * \theta(i) * a * a_s * g(fn) - a_h * H_s$$

$$H_s(fn) = \frac{L * \theta(i) * a * a_s * g(fn)}{a_h} * (1 - e^{-a_h * t}) + H_s(0) * e^{-a_h * t}$$

Total soil organic matter other layers:

$$H(t) = \sum_{fn} H_s(fn)$$

\* Nitrogen mineralization layer 1 during wintertime:

$$Mn(1) = \sum_{fn} \{ nifr(fn) * (O_s(fn,0) - O_s(fn,t) + s(fn,0) - s(fn,t)) \}$$

$$+ nifrrhu * \{ H_s(0) - H_s(t) + H_e(0) - H_e(t) \}$$

$$+ nifrex * \{ E(0) - E(t) \}$$

$$- \sum_{fn} \{ nifr(fn) * f * g(fn) * t \}$$

\* Nitrogen mineralization other layers during wintertime:

$$Mn(i) = \sum_{fn} \{ nifr(fn) * (s(fn,0) - s(fn,t) + f * t * (g(fn,i-1) - g(fn,i))) \}$$

$$+ nifrrhu * \{ H_s(0) - H_s(t) \}$$

From some orienting runs with HISTOR it appeared that the results concerning leaching of organic material were influenced largely by:

- water management, as translated in: groundwater level and precipitation surplus realized

- choice for a spring or a fall addition.

Two of the literature references of Kolenbrander (1969) were checked: they concerned fall additions to very shallow lysimeters in field situations, and contained no data on water management or influence of the groundwater table. Therefore in the other runs we chose for fall additions and for column 4 with its winter groundwater table at 1.5 m and precipitation surplus of 0.330 m j-1.

Application of the model HISTOR to manure decomposition:

First it was necessary to adapt the decomposition curve for manure for the probable presence of straw in the material used, because nowadays in the animal slurry there is no straw present, and this applies, in any case, to the lysimeter experiments of Steenvoorden (1983).

According to the Handboek voor de Rundveehouderij (1980), the stable-manure production is 5000 kg per cow per 180 days, including the approximately 1.5 kg straw added per day. The organic matter content of this manure is 14%. This means that the straw content in the organic material is

$$\frac{1.5 \cdot 180}{5000 \cdot 0.14} = 0.386 \text{ or } 54 \text{ kg}$$

Table 6.3 gives the results of the correction.

Because we chose for fall addition, the lowest possible curve and not the average one like in fig. 5.1, was drawn through the measurements presented by Kolenbrander (1969) for animal slurry.

Table 6.3. Conversion of the decomposition curve of stable manure to that of faeces.

Years after addition	Remaining amount per 1000 kg manure or 140 kg organic matter				
	Org. mat. %	Org. mat. kg	Straw kg	Faeces kg	Faeces %
0	1.000	140.0	54.0	86.0	100.0
1	0.49	68.6	19.0	49.6	57.7
2	0.36	50.4	11.1	39.3	45.7
3	0.33	46.2	8.9	37.3	43.4
4	0.30	42.0	7.9	34.1	39.7
5	0.25	35.0	7.3	27.7	32.2

The results of the parameter fitting are presented in table 6.4.  
Remarks about this table:

- It is likely that in a liquid material like animal slurry part of the organic matter already is in soluble form. Therefore the model gives the possibility to define the part FRCA(fn) per fraction FR(fn), which contains soluble material of fraction fn. Because the solubilization step is the rate limiting factor in decomposition in the model, the presence of already soluble material means an initial acceleration in decomposition.
- It was not possible to reach a result of 50% mineraliza-

tion in the first year, even with  $a = 0.25$ . It is, however, not clear on which experiments this 'practice' value of 50% is based. A value of  $a = 0.25$  for the assimilation factor was thought realistic, because the conditions will not always be optimal.

The results for the other materials are given in table 6.5. Some remarks on these fittings:

- In these runs of HISTOR the values of
  - $a_h = 0.02 \text{ j}^{-1}$
  - $a_s = 30.0 \text{ j}^{-1}$
  - $a = 0.25$as used for animal slurry, were also taken
- For these materials the nitrogen content of the fractions cannot be determined with the help of mineralization data. Therefore it seems suitable to divide the total nitrogen content of those materials inversely proportional to their decomposition rates. The total nitrogen contents of the different materials should be given in the input data.
- Only for peat the constraint  $a_n \geq 0.1 \text{ j}^{-1}$  was not taken into account; it was assumed that this material already contains a fraction of humus-like material.
- For crop residues & grass and for straw it was not possible to choose the parameters in such a way that after 7 years less than 16% of the amount added initially, was left.

To get an idea of the soil organic matter build-up on the long term, we made a run with HISTOR of 400 years, simulating yearly fall additions of 300 t pig slurry, under the same conditions as in the lysimeter experiment. The main results are given in table 6.6.

The build-up of organic material in layer 2 is totally caused by transport of soluble organic material. Comparing to the amount in layer 1 it looks a little small as compared to the results reported by McGrath (1981).

Table 6.4. Inputs and results of parameter fittings for decomposition of animal slurry with the model HISTOR (Simulation of measurements given by Kolenbrander (1969)).

Parameter values:

FR(1) = 0.1	FRCA(1) = 0.1	a1 = 1.0	nifr(1) = 0.07
FR(2) = 0.7	FRCA(2) = 0.05	a2 = 0.6	nifr(2) = 0.05
FR(3) = 0.2	FRCA(3) = 0.0	a3 = 0.1	nifr(3) = 0.01
	ah = 0.02		
a = 0.25	as = 30.0		

\* not used because this fraction is completely in solution; dummy value

Moisture fractions of the layers:

Layer nr.	Moisture fraction
1	0.17
2	0.18
3	0.19
4	0.21
5	0.24

Precipitation surplus: 0.330 m j-1

#### A. Simulation of slurry decomposition curve

Year	Remaining organic matter (%)	
	Corrected observations	Simulated values
1	57.7	63.5
2	45.7	49.4
3	43.4	40.6
4	39.7	34.8
5	32.2	31.0

Percentage mineralization in first year = 40

#### B. Simulation of lysimeter experiments (Steenvoorden, 1983)

Additional input data:

Amount of slurry added: 300 t ha-1 each time

Composition of the slurry: pig slurry with average dry matter content of 9.93% and probable organic matter content of 7.8%, resulting in an addition of 23400 kg ha-1 organic matter each time

Times of addition: spring 1977, falls of 1977 through 1979

Comparison of measured and calculated TOC-profiles (kg C m-3) in layers of 20 cm, using data of column nr. 4.

Layer nr.	Profile spring 1978		Profile spring 1980	
	Measured	Simulated	Measured	Simulated
1	0.234	0.310	0.339	0.412
2	0.194	0.377	0.403	0.442
3	0.243	0.205	0.217	0.241
4	0.221	0.114	0.252	0.134
5	0.138	0.060	0.150	0.071

Table 6.5. Simulation results for the other materials of figure 6.1.

	Drop residues and grass	Straw	Foliage	Pine needles	Peat	Sawdust
Parameter values:						
FR(1)	0.05	0.0	0.05	0.05	0.0	0.0
FR(2)	0.70	0.70	0.35	0.40	0.40	0.80
FR(3)	0.25	0.30	0.60	0.55	0.60	0.20
FRCA(1)	0.05	0.0	0.05	0.05	0.0	0.0
FRCA(2)	0.0	0.0	0.0	0.0	0.0	0.0
FRCA(3)	0.0	0.0	0.0	0.0	0.0	0.0
a1	1.0*	1.0*	1.0*	1.0*	1.0*	1.0*
a2	2.0	1.00	0.60	0.70	0.40	0.23
a3	1.7	3.50	0.50	0.30	0.045	0.33

\* = dummy value

Fitting results: residue after						
0.5 year	.616	.650				
1 year	.281	.352	.624	.666	.866	.814
2 years	.192	.226	.438	.499	.772	.671
3 years	.177	.185	.331	.396	.704	.562
4 years	.172	.170	.269	.329	.653	.477
5 years	.168	.165	.232	.285	.613	.411
6 years	.164	.161	.210	.253	.580	.360

Table 6.6. Results of a run of 400 years of addition of 300 t ha<sup>-1</sup> pig slurry with the model HISTOR.

Layer 1:	fresh organic material:	6.27 *10 <sup>4</sup> kg ha <sup>-1</sup>
	soil organic material :	2.11 *10 <sup>5</sup> kg ha <sup>-1</sup>
	total :	2.74 *10 <sup>5</sup> kg ha <sup>-1</sup>
		or ca. 8.9% of dry matter
	C/N quotient :	13.6
Layer 2:	soil organic material :	3.33 *10 <sup>4</sup> kg ha <sup>-1</sup>

## 6.2. Root development

In par. 5.1.3 it has been made clear that a difference should be made between effective rooting depth  $L_{re}$  and "standard" rooting depth development in time,  $L_r(t)$ . Because in the future the model ANIMO will be applied to the southern Peel region, where the ICW carries out a project "Optimization of regional water use", in table 6.7 effective rooting depths, used in the regional water quantity model FEMSAT-P (Querner and van Bakel, 1984), for different types of land use and for different soil physical units present in the southern Peel area are given. In practice, for every subregion to which the model is applied, the maximum possible rooting depth has to be determined. Table 6.8 gives root development data for different crops, derived from different literature sources; these data can be used as "standard" development data; sometimes data from different authors were averaged; sometimes interpolation has been done between the data given by an author; sometimes extrapolation was necessary to get a complete data-set. Data on root length and -mass data are given as a function of the daynumber in a year and not as a function of the time after sowing, because it is assumed that when the sowing is done later than usual, the development can be faster, because of higher temperatures. Average values for time of sowing and time of harvesting are given. Some sowing data had to be estimated from vague indications. Data on root mass were not always available in the desired form ( $\text{kg ha}^{-1}$ ). When they were given as  $\text{kg m}^{-2}$ , they were transformed as follows: By dividing the known root mass at the time of harvest (see table 6.15) by the corresponding root amount in  $\text{kg m}^{-2}$  at harvest, a transformation factor was calculated, which was subsequently applied to the other root amount data. The presented data should not be taken too absolute, because they were mostly derived from single experiments on one type of soil and under unknown weather-, fertilizer- and watermanagement conditions. For crops like lettuce, which can be sown during most months of the growing season, the data should be taken as relative to the sowing date. The list of crops for which the data are given, is not complete, although it contains the main crops grown in the Netherlands.

Table 6.7. Effective rooting depths (m) used in the model Femsat-P (Querner and van Bakel, 1984).

	Soil physical unit					
	1	2	3	4	5	6
Soil use						
Horticulture	0.25	0.25	0.30	0.40	0.25	0.40
Potatoes	0.25	0.25	0.30	0.60	0.25	0.60
Cereals	0.30	0.25	0.40	0.80	0.30	0.80
Maize	0.30	0.25	0.40	0.80	0.30	0.80
Grass	0.25	0.20	0.30	0.50	0.25	0.60
Natural areas	0.25	0.20	0.30	0.50	0.25	0.60
Forest	1.00	1.00	1.00	1.00	1.00	1.00

Table 6.8. Root development data for different crops  
Between parentheses the sources are given; see the list at the end of the table. If a source is given for one number of a column only, it applies to the whole column, until another number appears. Sources named in the time-column only apply to the sowing and harvesting dates.

Kind of crop	Time (day nr)	Rooting depth (m)	Dry root mass (kg ha-1)
Maize			
sowing time	115(2)	-	-
	130	0.05(3,7)	80(7)
	151	0.20	120
	166	0.35	400
	181	0.57	1880
	196	0.75	3200
	212	0.85	4400
	232	0.90	4800
harvest time	258(5)	0.90	4600
Early potatoes			
planting time	90(8)	-	-
	130	0.30(7)	697(7,8)*
	140	0.35	880
	153	0.60	977
	174	0.65	1200
	181	0.62	1500
	196	0.60	3200
	212	0.60	4600
	243	0.60	7400
	263	0.60	7700
Late potatoes = consumption?			
planting time	113(3)	-	-
	130	0.04(3)	697(7,8)*
	140	0.05	880
	153	0.07	977
	174	0.34	1200
	181	0.45	1500
	196	0.59	3200
	212	0.60	4600
	243	0.60	7400
	263	0.60	7700

\* = roots and tubers; at harvest, 80% of the material is tubers

# Winter cereals

sowing time	281(6)	-	-
	0	0.30(6)	38(10)
	31	0.40	50
	59	0.55	69
	90	0.80	100(6)
	120	1.05	350
	151	1.07	1050
	171	1.09	1300
	212	1.12	1600(8)
harvest	227(5)	1.13	1600

# Summer cereals

sowing time	64(1)	-	-
	91	0.10(3)	20(10)
	110	0.20	100(9)*
	115	0.25	200
	121	0.30	300
	127	0.40	400
	135	0.50	620
	145	0.60	850
	156	0.70	1050
	182	0.85(9)	1370
	195	1.00	1580
	237(5)	1.00	1250 (10)**

\* = data for summer wheat

\*\* = average of: 1400 (8) for summer wheat  
1000 (8) for summer barley  
1400 (8) for oats  
1200 (8) for rye

# Sugar beet

sowing time	91(1)	-	-
	120	0.13(6)	300(10)
	151	0.50	600
	181	0.75	700(1)*
	212	1.10	4800
	243	1.15	7900
	273	1.20	9700
	288(5)	1.20	10000

\* = derived from total root mass assuming dry matter = 20%

# Cauliflower

sowing time	99(4)	-	-
	129	0.11(4)	0.26(4)*
	151	0.50	26.9
	174	0.80	278
	194	>=0.80	592
harvest	212	>=0.80	1000(8)

\* = calculated with transformation factor =  $1000/11.9 = 84$   
kg ha<sup>-1</sup>/(km m<sup>-2</sup>)

# Pea

sowing time	90(7)	-	-
	135	0.45(7)	571(7)
	158	0.75	738
	170	0.75	971
	193	0.70	665
	214	0.60	534
harvest	181(1)	?	?

Lettuce				
sowing time	100(4)	—	—	
	133	0.08(4)	?	
	158	0.50	?	
	174	0.60	?	

- 1 = Akkerbouwpraktijk (1980)
- 2 = Becker (1976)
- 3 = Feddes (1985)
- 4 = Greenwood e.a. (1982)
- 5 = Van Heemst e.a. (1978)
- 6 = Jonker (1958)
- 7 = Van Lieshout (1956)
- 8 = PAGV-handboek (1961)
- 9 = Schuurman and Knot (1970)
- 10 = own interpretation

### 6.3. Nitrogen-crop data

In this chapter the results of literature research on nitrogen uptake by and nitrogen contents of crops are presented. The information presented is not complete; for simulation of some crops additional data will have to be found or calculated from additional literature data.

#### 6.3.1. Nitrogen fertilization

When animal slurry is added as fertilizer, the amount given depends on

- the fertilizing element on which the dosage is based
- additional anorganic nitrogen given
- possible overdose

In the southern Peel study, standard N-fertilizer amounts per technology (= kind of crop or group of crops) are used in all (also economical) calculations; table 6.9. (Reinds, 1985) gives these data. For waterquantity calculations, it may be necessary to distinguish between different crops per technology, due to differences in fertilization and rooting depth. For instance, large scale outdoor horticulture includes spinach with shallow rooting depth and fertilization of 200 kg N ha<sup>-1</sup> as well as garden peas with rooting depth ca. 0.75 m and no N fertilization. Fertilization data per crop can be found in Kwantitatieve informatie (1985).

#### 6.3.2. Maximal N uptake

For the nitrogen uptake model described in par. 5.4, it is necessary to know the value of N<sub>max</sub>, the total maximal N-uptake per crop, if necessary for two distinguished periods during the growing season.

Aslyng and Hansen (1982) give percentages of N in the plant at which N-uptake ceases. These percentages change during the growing season; generally, the curve has a shape as given in fig. 6.3.

Corresponding data for some crops are given in table 6.10. To determine N<sub>max</sub> values from these data, they have to be related to maximal productions. Van Heemst e.a. (1978) give maximal yields for different crops under dutch weather conditions and optimal nitrogen and moisture supplies. These are the yields at  $t = t_3$ . Following the calculation scheme of Van Heemst e.a. (1978), we can also determine a maximal yield at  $t = t_1$ . This calculation scheme consists of: Maximal dry matter production per month = potential production of the "standard crop" during that month (see table 6.11), reduced for a possible period with incomplete soil cover. Table 6.12 gives the calculations leading to the maximal dry matter productions at  $t_1$  and  $t_3$ .

Table 6.9. Nitrogen fertilization as used in the Southern Peel study (Reinds, 1985).

Technology	N fertilization (kg N ha <sup>-1</sup> y <sup>-1</sup> )	
	total	inorganic
Horticulture		
under glass	1000*	800
outdoor small scale	250	150
outdoor large scale	200	100
remaining	150	75
Cereals		
100% N-level	66	52
75% N-level	50	46
50% N-level	33	33
Row crops		
100% N-level	162	66
75% N-level	121	52
50% N-level	81	50
Silage maize		
level I	250	50
level II	450	50
level III	850	50
Grassland with		
Dairy cattle level I	600	360
Dairy cattle level II	470	270
Rearing cattle	300	180

\* = For horticulture under glass the N fertilization often largely exceeds the N-need (ca. 500 kg ha<sup>-1</sup>). Also, the fertilization widely differs from case to case, so that specification per crop is not really necessary.

The dry matter yields at t3 are either calculated as

$\text{yield} = \text{grain yield} * (1 - \text{moisture fraction}) / \text{harvest index}$   
 (summer cereals and winter cereals), or as

$\text{yield} = \text{D.m. harvest (Aslyng)} * \text{Epot (dutch)} / \text{Epot(Aslyng)}$   
 $+ \text{harvest residue (Aslyng)}$

(s. rape and f. beet)

If we divide the growing period in the periods t0 to t1 and t1 to t3, we can calculate the corresponding Nmax1 and Nmax2 for these periods as is done in table 6.13, using the maximal yields and the values of c1 and c2 of table 6.10.

The concentration with which at potential evapotranspiration Epot (m3 ha-1), Nmax (kg ha-1) is reached, can now be calculated as:

$\text{Copt1} = \text{Nmax1} / \text{Epot}(t0-t1)$   
 $\text{Copt2} = \text{Nmax2} / \text{Epot}(t1-t3)$

Potential evapotranspiration values and resulting Copt values for the different crops are calculated in table 6.14. The effect of this way of period division is that if at t1 Nmax1 is reached and the uptake after t1 is also maximal (with the lower Copt2), the % N in the plant will indeed slowly decrease in the direction of c2. If at t1 Nmax1 is not realized, the model gives the possibility of uptake of higher concentrations than Copt2, even after t1, until the maximal possible uptake (calculated for each timestep) is reached.

If no information of the kind presented in table 6.10 is available, Nmax (total) can be estimated from known harvested N-amounts by optimally fertilized crops, by adding an amount present in roots and multiplying by a factor  $\text{Epot}(\text{average dutch or in a warm year}) / \text{Erealized}$ .

Figure 6.3. Percentage N in the plant at which the N-uptake stops (from Aslyng and Hansen, 1982).

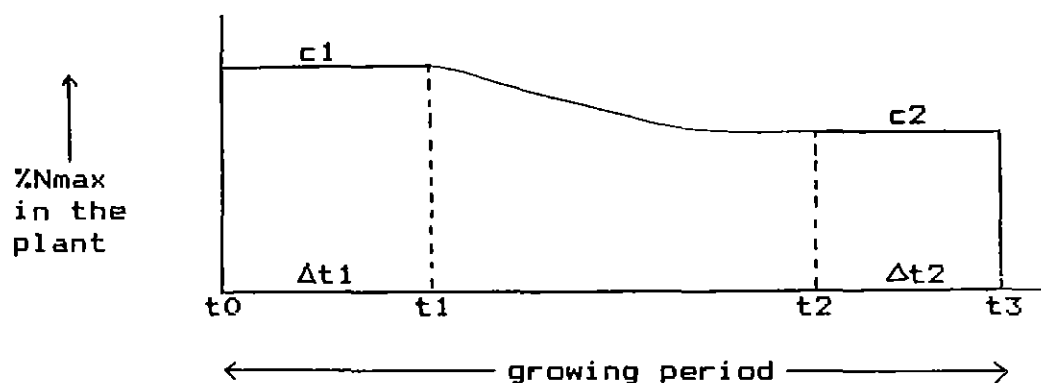


Table 6.10. Maximal percentages of N in different crops (from Aslyng and Hansen, 1982).

Crop	At onset of growth		At end of growth	
	$\Delta t1$ days	c1 %N	$\Delta t2$ days	c2 %N
Winter wheat	15	4.3	20	1.6
Summer barley	15	4.3	20	1.6
S.? rape	15	4.3	20	2.0
Fodder beet	20	4.3	50	2.0

Table 6.11 . Potential dry matter production of the "standard" crop in kg ha<sup>-1</sup> (from Van Heemst e.a., 1978).

April	5500	August	6400
May	7100	September	4700
June	7600	October	3200
July	7300	Total	41800

Table 6.12. Maximal dry matter productions at t1 and t3 for different crops. Data used from van Heemst e.a. (1978)

	Crop			
	Winter cereals	summer cereals	s. rape*	f.beet*
t1	15/4-30/4	1/5-15/5	10/5-25/5	1/6-20/6
%soil cover during t1	25	25	12.5	20
D.m. yield at t1 (kg ha <sup>-1</sup> )	687.5	887.5	444.0	1013
t3	15/8	25/8	25/8	31/10
Grain yield (kg ha <sup>-1</sup> ) at t3	10400	9700	-	-
Harvest index	0.4	0.4		
% Moisture in grain	15	15		
Max. d.m. harvest** (kg ha <sup>-1</sup> )			16600	23400
Epot(t0-t3)** (mm)			284	284
Epot(t0-t3) average dutch (see table 6.14)			255	328
Crop residue (kg ha <sup>-1</sup> ) **			2000	1000
Max. dry mat. yield at t3 (kg ha <sup>-1</sup> ) whole plant	22100	20600	16900	28000

\* = data of sugar beet used

\*\* = data given by Aslyng and Hansen (1982)

Table 6.13. Calculation of Nmax1 and Nmax2

Crop	Max. d.m. prod. (kg ha <sup>-1</sup> )			%Nmax		Nmax (kg ha <sup>-1</sup> )	
	t0 - t1	t0 - t3	t1 - t3	c1	c2	Nmax1	Nmax2
w.wheat	688	22100	21400	4.3	1.6	29.6	343
s.barley	888	20600	19700	4.3	1.6	38.2	315
s.rape	444	16900	16500	4.3	2.0	19.1	330
f.beet	1013	28000	27000	4.3	2.0	43.6	540

Table 6.14. Calculation of Copt1 and Copt2 (data adapted from van Heemst e.a., 1978)

		Epot (m3 ha-1) at full soil cover	Fraction soil cover	Epot (m3 ha-1) for this crop period cum	Copt (kg m-3)
winter cereals					
Period					
april	16-30	185	0.25	46.25	0.640=Copt1
may	1-15	495	0.5	247.5	
may	16-31	495	1.0	495.0	
june		1160	1.0	1160.0	
july		1120	1.0	1120.0	0.106=Copt2
august	1-15	450	0.50	225.0	
summer cereals					
may	1-15	495	0.25	123.75	0.309=Copt1
may	16-31	495	0.50	247.5	
june		1160	1.00	1160.0	
july		1120	1.00	1120.0	
august	1-10	300	1.0	300.0	0.103=Copt2
august	11-25	450	0.5	225.0	
s.rape					
may	11-25	479.0	0.125	59.9	0.319=Copt1
may	26-31	159.7	0.25	39.9	
june	1-10	386.7	0.25	96.7	
june	11-25	580.0	0.50	290.0	
june	26-30	193.3	1.00	193.3	0.129=Copt2
july		1120	1.0	1120.0	
august	1-25	750	1.0	750.0	
f.beet					
june	1-15	580	0.25	145.0	0.180=Copt1
june	16-20	193.3	0.50	96.7	
june	21-30	386.7	0.50	193.3	
july		1120	1.00	1120.0	
august		930	1.00	930.0	0.165=Copt2
september		560	1.0	560.0	
october		230	1.0	230.0	

### 6.3.3. Nitrogen contents of crop residues

In the model ANIMO crop yields are not calculated. Important is the amount of crop residues, coming available for decomposition at the harvest, and their nitrogen content. Whereas crop yields are strongly dependent of weather and nitrogen conditions, for root yields this is less the case. Table 6.15, adapted from PAGV handboek (1981) gives the amounts of crop residues staying behind at the harvest.

Nitrogen contents of these materials are influenced by fertilization. Therefore in table 6.16, presenting nitrogen percentages of crop residues, fertilization data are given, if mentioned by the authors. This table is also far from complete.

Table 6.15. Crop residues (from: PAGV-handboek, 1981)

Crop	Residues at harvest (kg d.m. ha <sup>-1</sup> )		Total*
	Belowground	Aboveground	
Winter wheat	1600	3600	
Summer wheat	1400	3800	
Winter barley	1400	3600	
Summer barley	1000	3200	
Oats	1400	3600	
Rye	1200	3600	
Sweet maize	2000	5000	
Silage maize	1500	500	
Potatoes			4000
Sugar beet			1500
S.beet incl. heads + leaves			6000
Cabbage	1000	4000	
Sprouts	1000	500	
Pea	400	100	
Pea inclusive foliage	400	1600	

\* = tuber crop residues, brought to the topsoil at harvest

Table 6.16. N contents of crop residues at harvest

Crop	part	%N in dry matter	N-ferti- lization kg ha <sup>-1</sup> y <sup>-1</sup>	source
Barley	abovegr.	0.94	0	3
	abovegr.	1.00	60	3
	abovegr.	1.07	120	3
	root	0.60		3
	stubble	0.74	0	3
	stubble	0.78	60	3
	stubble	0.88	120	3
Beet	leave	3.5-5.0		?
Butter bean	foliage	0.18*		2
Broad bean	foliage	0.27*		2
Carrots	foliage	0.41*		2
Cauliflower	abovegr.	0.48*		2
Celeriac	foliage	0.25*		2
Curled kale	abovegr.	0.51*		2
Endive	abovegr.	0.27*		2
Leek	foliage	0.34*		2
Pea	whole pl.	1.5-2.3		***
Pea	foliage+Pods	0.48*		2
Potatoes	root	0.79	0	3
	root	0.93	180	3
	root	0.83	360	3
	foliage	1.59	0	3
	foliage	2.02	180	3
	foliage	2.07	360	3
	tuber	1.4		1
	top	0.17		1
Red beet	foliage	0.20*		2
Red cabbage	foliage	0.51*		2
Rye	abovegr.	0.58*		2
Savoy cabb.	foliage	0.55*		2

Spinach	leave	4.0-6.0		?
Sugar beet	fol.+heads	0.32*		2
Swedish turnip	fol.+heads	0.31*		2
Sweet maize	whole pl.	1.9	0	****
	whole pl.	2.2	224	?
Tomatoes	leave	3.0-6		?
White cabb.	foliage	0.32*		2
Wint. wheat	abovegr.	1.25	0	3
	abovegr.	1.33	60	3
	abovegr.	1.42	120	3
	root	0.80		3
	stubble	1.02	0	3
	stubble	1.06	60	3
	stubble	1.17	120	3
	straw	0.51*		2

\* = on fresh weight basis  
\*\* = dependent of species  
\*\*\* = at 80% silk stage

Sources:

1. Greenwood e.a., 1985
2. de la Lande Cremer & van der Veen, 1982
3. Verveda, 1984

## 7. CONCLUSIONS AND RECOMMENDATIONS

### 7.1. Conclusions

About the modelling of nitrogen behaviour:

1. To predict the extent of nitrate leaching to groundwater and surface water it is necessary to model the whole nitrogen cycle and the transport behaviour of the different forms of nitrogen in soil.
2. The fate of nitrogen is closely related to that of carbon, especially when mineralization/immobilization and denitrification are considered. Therefore also part of the carbon cycle was modelled in ANIMO.
3. Especially for long-term prediction purposes, it is necessary to include the transport of organic material in solution in the model, and this has been done in ANIMO. In other models, it has not been done often before because of lack of knowledge. McGill e.a. (1981) included it in their model, but give no experimental data to compare the results with. For ANIMO, we tried to derive the necessary parameters on some scarce measurements; the model has to be considered as tentative in this aspect.
4. Denitrification is a process which is qualitatively understood; quantification is difficult because of the dependence of short-time weather conditions. Still it is a very essential part of the nitrogen cycle, especially where contamination of groundwater is concerned. In ANIMO, we tried to model the occurrence of partial anaerobiosis; partial in space as well as in time; here, too, the modelling is tentative.

About the possibilities of the model:

1. The model ANIMO can be used for predicting the nitrogen load on surface- and groundwater and the development of organic matter properties of soil profiles as influenced by land use, water management and environmental factors.
2. The model can be used on field scale; extension to regional use is being worked out.
3. Because no complete test results are available yet, it is not possible to draw conclusions about the working of the model; results of a test object, simulating N-behaviour in a silage maize field at Cranendonk, will be given in a following report.

### 7.2. Recommendations

1. The model in its present form is operational for arable land; the modelling of grassland and of natural areas with a permanent vegetation should be included. Some ideas about this extension are given in Appendix E.
2. More information about the quantitative aspects of denitrification would be useful. A laboratory incubation experiment investigating the decomposition of low-C soil with added known C-components and the disappearance of nitrate influenced by high, low, intermediate or controlled alternate moisture content, high and low nitrate

supply could answer questions like:

- Is the decomposition rate of organic matter under water saturated, nitrate-rich conditions the same as under aerated conditions with no lack of mineral N? (this is assumed to be so in the model). If not, how can differences be modelled?
  - Is the assimilation factor the same in those cases or how does it change?
  - Is denitrification under intermediate moisture conditions comparable to denitrification under alternate high and low moisture conditions? (Is partial anaerobiosis in space comparable to that in time?)
3. Much more information should become available concerning organic material in solution (OMS). Production- and decomposition rate of OMS could be studied for instance in incubation experiments of slurry with soil, by separating solution from dry matter at different points in time (sacrificing a soil sample each time), analysing a subsample of the solution, and adding the solution to a slurry-free soil sample to determine the decomposition rate of the formed OMS. In field trials the investigation of OMS is much more difficult, because of the uncontrolled environmental conditions and transport processes occurring.
  4. For N-balance studies of field trials or testing data for a nitrogen model it is necessary to have available measurements of amounts of nitrogen fixed in roots, not only for checking the amount of N taken up by plants, but also for checking the amount of N denitrified, which is often taken as the saldo item of the other processes. It is known that root research involves its own complications; maybe it is possible to develop a simple rough routine method of determining the N content of roots when the recovery of that method is determined in advance by a single experiment comparing the rough and a precise method.
  5. More quantitative data should be collected about the processes of volatilization and exudate production- and decomposition.

## LITERATURE

Akkerbouwpraktijk. 1980. Onder red. van L. van Deveren.  
Doetinchem, Misset.

Aslyng, H.C., and S. Hansen. 1982. Water balance and crop  
simulation model WATCROS for local and regional application.  
Copenhagen, Royal Veterinary and Agricultural University.

Bakker, J.W. 1965. Luchthuishouding van bodem en plantewor-  
tels; een literatuurstudie. Wageningen, Instituut voor Cul-  
tuurtechniek en waterhuishouding.  
ICW-nota 302.

Becker, W.R. 1976. Mais; een handleiding voor de teelt van  
korrel- en snijmais. Lelystad, Proefstation voor de akker-  
bouw.  
Publicatie nr. 21.

Berguijs-van Dijk, J.T. van. 1985. WATBAL; a simple water  
balance model for a unsaturated/saturated soil profile.  
Wageningen, Institute for Land and Water Management Re-  
search.  
ICW-nota 1670.

Brogan, J.C. (ed.). 1981. Nitrogen losses and surface runoff  
from landspreading of manures; proceedings of a workshop in  
the EEC programme ... The Hague etc., Martinus Nijhoff.  
Developments in Plant and Soil science, vol. 2.

Dijk, T.A. van, and H. Sturm. 1983. Fertilizer value of  
animal manures on the continent.  
London, Fertilizer society  
Proceedings. no. 220.

Dirven, J.G.P., and K. Wind. 1982. De invloed van bemesting  
op de beworteling van verschillende grassoorten en -rassen.  
Wageningen, Landbouwhogeschool, Vakgroep Landbouwplanten-  
teelt en Graslandkunde.  
Mededeling no. 61.

Feddes, R.A. 1985. Personal communication.

Frissel, M.J., and J.A. van Veen (eds.). 1981. Simulation of  
nitrogen behaviour of soil-plant systems; papers on a  
workshop Models for the behaviour of nitrogen in soil and  
uptake by plant; comparison between different approaches.  
Wageningen, January 28 - February 1, 1980. Wageningen,  
PUDOC.

Goedewaagen, M.A.J., and J.J. Schuurman. 1950. Wortelproduc-  
tie van bouw- en grasland als bron van organische stof in de  
grond. Landbouwkundig tijdschrift 62: 469-482.

Greenwood, D.J., A. Gerwitz, D.A. Stone e.a. 1982. Root  
development of vegetable crops. Plant and soil 68: 75-96.

Greenwood, D.J., J.J. Neeteson and A. Draycott. 1985. Res-  
ponse of potatoes to N fertilizer; quantitative relations  
for components of growth. Plant and soil 85:163-183.

Handboek voor de rundveehouderij. 1980. 3e dr. Onder red. van L. Pelser. Lelystad, Proefstation voor de Rundveehouderij.

Heemst, H.D.J. van, H. van Keulen and H. Stolwijk. 1978. Potentiële produktie, bruto- en nettoproduktie van de Nederlandse landbouw. Wageningen, PUDOC.  
Verslagen van Landbouwkundige onderzoekingen, 879.

Hoeks, J. 1972. Effect of leaking natural gas on soil and vegetation in urban areas. Wageningen, PUDOC.  
Dissertatie Landbouwhogeschool Wageningen.

Huet, H. van. 1982. Simulaties van temperatuurvariaties in de bodem (Proefveld Ruurlo, 1980). Wageningen, Instituut voor Cultuurtechniek en Waterhuishouding.  
ICW-nota 1389.  
Projectgroep Zuidelijk Peelgebied, 12.

Huet, H. van. 1983. Kwantificering en modellering van de stikstofhuishouding in bodem en grondwater na bemesting. Wageningen, Instituut voor Cultuurtechniek en Waterhuishouding.  
ICW-nota 1426.  
Projectgroep Zuidelijk Peelgebied, 26.

Janssen, B.H. A simple method for calculating decomposition and accumulation of 'young' soil organic matter. Plant and Soil 76: 297-304.

Johnen, B.G. 1974. Bildung, Menge und Umsetzung von Pflanzenwurzeln im Boden. Bonn, s.n.

Jonker, J.J. 1958. Bewortelingsonderzoek en ondergrondbewerking in de Noordoostpolder. Zwolle, Tjeenk Willink.  
Van Zee tot land, nr. 25.

Kolenbrander, G.J. 1969. De bepaling van de waarde van verschillende soorten organische stof ten aanzien van hun effect op het humusgehalte bij bouwland. Haren, Instituut voor Bodemvruchtbaarheid.  
C6988.

Kortleven, J. 1963. Kwantitatieve aspecten van humusopbouw en humusafbraak. Wageningen, PUDOC. Dissertatie Landbouwhogeschool Wageningen.  
Verslagen van Landbouwkundige onderzoekingen, 69.1.

Kwantitatieve informatie 1985-1986 voor de Akkerbouw en de Groenteteelt in de Vollegrond, 1985. Ed. by W.P. Noordham and M. van der Ham. Lelystad, Consultantschap in algemene dienst voor de Akkerbouw en de Groenteteelt in de Vollegrond etc.  
Publication nr. 29.

Lammers, H.W. 1983. Gevolgen van het gebruik van organische mest op bouwland. Wageningen, Consultantschap voor bodemaangelegenheden in de landbouw.

Lande Cremer, L.C.N. de la, and L. van der Veen. 1982. Chemische samenstelling van groentegewassen en de benutting van groente-afval als organische bemesting. Haren, Instituut voor Bodemvruchtbaarheid. IB-nota 103.

Lieshout, J.W. van. 1956. De beworteling van een aantal landbouwgewassen. 's-Gravenhage, Staatsuitgeverij. Verslagen van landbouwkundige onderzoekingen, 62.16.

McGill, W.B., H.W. Hunt, R.G. Woodmansee e.a. 1981. Formulation, process controls, parameters and performance of PHOENIX: a model of carbon and nitrogen dynamics in grassland soils. In: Frissel and van Veen (1981).

McGrath, D. 1981. Accumulation of organic carbon and nitrogen in soil as a consequence of pig slurry application to grassland. In: Brogan (ed), 1981.

Merckx, R., A. den Hartog and J.A. van Veen. 1985. Turnover of root-derived material and related microbial biomass formation in soils of different texture. Soil Biol. Biochem. 17: 565-569.

Oorzaken, wezen en gevolgen van waterverontreiniging; onderzoek van water. 1974. Wageningen, Landbouwhogeschool, Vakgroep Waterzuivering.

Oosterom, H.P., and J.H.A.M. Steenvoorden. 1980. Chemische samenstelling van oppervlakkig afstromend water (Proefveld onderzoek te Achterveld). Wageningen, Instituut voor Cultuurtechniek en Waterhuishouding. ICW-nota 1237.

PAGV-handboek. 1981. Onder red. van P. de Jonge. Lelystad, Proefstation voor de akkerbouw en de groenteteelt in de vollegrond. Publicatie nr. 16.

Querner, E.P., and P.T.J. van Bakel. 1984. Description of second level water quantity model, including results. Wageningen, Institute for Land and Water Management Research. ICW-nota 1586. Projectgroup Southern Peel region, report no. 37.

Reinds, G.H. 1985. The technologies in the Southern Peel region. Wageningen, Institute for Land and Watermanagement Research. ICW-nota 1653. Projectgroup Southern Peel region, report no. 43.

Russel, R.S. 1977. Plant root systems. London, McGraw-Hill.

Schuurman, J.J. 1973. Overzicht van de resultaten van het bewortelingsonderzoek bij grassen en op grasland aan het Instituut voor Bodemvruchtbaarheid. Haren, Instituut voor Bodemvruchtbaarheid. IB-rapport 10-1973.

Schuurman, J.J., and L. Knot. 1970. Vergelijking van de wortelontwikkeling van drie grassoorten en zomertarwe. Wageningen, PUDOC. Verslagen van landbouwkundige onderzoekingen, 745.

Shamoot, S., L. McDonald and W.V. Bartholomew. 1968. Rhizodeposition of organic debris in soil. Soil Sci. Soc. Am. Proc. 32: 817-820.

- Stanford, G., and S.J. Smith. 1972. Nitrogen mineralization potentials of soils. Soil Sci. Soc. Am. Proc. 36: 465-472.
- Steenvoorden, J.H.A.M., 1983. Nitraatbelasting van het grondwater in zandgebieden; denitrificatie in de ondergrond. Wageningen, Instituut voor Cultuurtechniek en Waterhuishouding.  
ICW-nota 1435.
- Troughton, A. 1981. Length of life of grass roots. Grass and forage science 36: 117-120.
- Troughton, A. 1957. The underground organs of herbage grasses. Hurley, Berkshire, Commonwealth bureau of pastures and field crops.  
Bulletin no. 44.
- Verveda, H.W. 1984. Opbouw en afbraak van jonge organische stof in de grond en de stikstofhuishouding onder een vierjarige vruchtwisseling met grasgroenbemester. Wageningen, Landbouwhogeschool, Vakgroep Bodemkunde en plantevoeding.  
Interne mededeling 58.
- Wijk, W.R. van. 1963. Physics of plant environment. Amsterdam, North Holland Publishing Company.

## APPENDIX A

### Format of input files

The model ANIMO uses a number of input files:

GEN.DAT	contains general data for a run of ANIMO
GENAR.DAT	contains general data of the subregion
INI.DAT	contains initial data of the subregion
CROP.DAT	contains crop and fertilization data for the subregion

and one of the following files:

FEMSAT.DAT	contains moisture data calculated by the model FEMSAT-P. This file is needed when the model ANIMO is used on regional scale
WATBAL.DAT	contains moisture data calculated by the model WATBAL. This file is needed when the model ANIMO is used on field scale.

The parameter values needed in the input files and their order is given below. The files FEMSAT.DAT and WATBAL.DAT are automatically formed when running the models FEMSAT-P or WATBAL.

There is no prescription for the format of parameters, except that their type should be right (real or integer); also, a free choice can be made concerning the number of data on one line, except when a '\*' before the parameter name, in the first column of the following table, is given, indicating that the value of this parameter should be the first on a new line.

Input data on amounts of materials (root mass, fertilizer, etc.) should be given on dry matter basis.  
Input data on amounts of NO<sub>3</sub> and NH<sub>4</sub> should be given in amounts of N.

If the model is used on regional scale with more than one subregion, there should be one file GEN.DAT, and as much files of the type "GENAR.DAT" and "INI.DAT" as there are subregions. Of course these files have different names; a procedure still has to be worked out through which they get the name GENAR.DAT or INI.DAT at the moment they are needed for input.

The input file GEN.DAT:

This file is read once in a run.

New line in ANIMO used	Parameter name in this report	Type	Dimension	Description and remarks
	IWA	-	I	-
				Indicator for type of waterquantity model used IWA = 1 FEMSAT-P IWA = 2 WATBAL
	NA	-	I	-
				Number of areas (subregions) (max. 40)
	NF	nf	I	-
				Number of fractions in fresh and soluble organic material (max. 10)
	NM	nm	I	-
				Number of materials defined (max. 5)
	FRNI(MN=1-NM)	-	R	-
				Fraction of nitrate-N in the materials 1 to NM
	FRNH(MN=1-NM)	-	R	-
				Fraction of ammonium-N in the materials 1 to NM
	FROR(MN=1-NM)	-	R	-
				Fraction of organic material in materials 1 to NM
	ST	t	R	d
				Length of timestep
	TIME	-	R	d
				Time of the year when simulation starts
	YRMA	-	I	-
				Yearnumber when simulation ends
	YRMI	-	I	-
				Yearnumber when simulation starts
	for MN=1 to NM			
*	FR(MN, FN=1-NF)	FR(mn, fn)	R	-
	for MN=1 to NM			
*	FRCA(MN, FN=1-NF)	-	R	-
				Fraction of fraction numbers 1 to NF present in organic part of material MN Part of organic fractions 1 to nf of material MN which is in solution Example: FR(1,3) = 0.3 and FRCA(1,3) = 0.05 means that 0.3 - 0.05 = 0.25 of the organic material consists of solid fraction 3, and 0.05 of the organic material consists of soluble fraction 3
	For KC=1 to 5			In each run 5 crops must be defined (if lesss are needed, dummies or duplicate crops can be introduced)
*	NUANRO(KC)	-	I	-
				Number of data on root amount given for crop KC
	NULNRO(KC)	-	I	-
				Number of data on root length given for crop KC
	for N=1 to NULNRO			
*	AMROTI(KC,N)	-	R	kg ha-1
				Value nr. N of root mass for crop KC
	LNROTI(KC,N)	-	R	m
				Value nr. N of length of roots of crop KC
	TIAMRO(KC,N)	-	R	d
				Value nr. N of time for which value of rootlength for crop KC is given
	TI LNRO(KC,N)	-	R	d
				Value nr. N of time for which root mass is given N.B. The data must include zero root length and mass at TIHA
	TISO(KC)	t0	R	d
				Time of sowing of crop KC
	TIHA(KC)	t3	R	d
				Time of harvesting of crop KC
	TUTO	-	R	kg ha-1
				Amount of tubers harvested
	UPNIMA1(KC)	Nmax1	R	kg ha-1
				Maximal uptake of N by crop KC in first period
	UPNIMA2(KC)	Nmax2	R	kg ha-1
				Maximal uptake of N by crop KC in second period
	SUEVMA1(KC)	Epot(t0-t1)R	m	
				Sum of maximal evapotranspiration in first period for crop KC
	SUEVMA2(KC)	Epot(t1-t3)R	m	
				Sum of maximal evapotranspiration in second period for crop KC
	TIUP1(KC)	t1	R	d
				Time after sowing when maximal uptake rate of N by crop KC alters
*	FRVD	-	R	-
				Fraction of added NH4-N that volatilizes
	COPRNH	-	R	kg m-3
				Ammonium-N concentration in precipitation
	COPRNI	-	R	kg m-3
				Nitrate-N concentration in precipitation
*	NIFREX	nifrex	R	-
				Nitrogen fraction in exudates
	NIFRHU	nifrhu	R	-
				Nitrogen fraction in soil organic material (humus)
	NIFR(1-NF)	nifr(fn)	R	-
				Nitrogen fraction in fractions 1 to NF of organic material
	For the following rate constants, positive values must be given.			
	RECFEXAV	-	R	y-1
				Decomposition rate constant for exudates; average year-value
	RECFHUAV	-	R	y-1
				Decomposition rate constant for soil organic material; average year-value
	RECFAV(1-NF)	-	R	y-1
				Decomposition rate constant for fractions 1 to NF; average year-values

RECFAAV	-	R	y <sup>-1</sup>	Decomposition rate constant for organic material in solution; average year-value
RECNTAV	-	R	y <sup>-1</sup>	Nitrification rate constant; average year-value
DFCFOXWA(1-5)	-	R	m <sup>2</sup> d <sup>-1</sup>	Values 1 to 5 of diffusion coefficient of oxygen in water
DFCFOXWATE(1-5)	-	R	°C	Values 1 to 5 of temperature for which diffusion coefficients of oxygen in water are given

The input file GENAR.DAT:

This file is read again for every simulated year of a run.

ASFA	a	R	-	Assimilation factor
NL	-	I	-	Number of layers (max. 100)
APTE	A0	R	C	Amplitude of yearly temperature wave in sinus model
AVTE	Ta	R	C	Average yearly temperature
DRADNH(1)	Rd	R	-	Distribution ratio for ammonium in rootzone
DRADNH(NL)	Rd	R	-	Distribution ratio for ammonium in the subsoil
FQTE	w	R	rad d-1	Frequency of yearly temperature wave
HE(1-NL)	L	R	m	Height of the layers 1 to NL
DG	-	R	m-1	Density of drains of third order (trenches, ditches, field drains) N.B. For interflow it is possible to define a "model" trench (not really existing), but only if this has also been done in the water quantity model
DS	-	R	m-1	Density of drains of second order (ditches, drains)
DK	-	R	m-1	Density of drains of first order (canals)
AR(AN)	-	R	m2	Acreage of subarea nr. AN
TESMCF	a	R	m2 d-1	Thermal diffusivity
* PMDF1	p1	R	-	Parameter in calculation of diffusion coefficient for oxygen in airfilled part of soil (see par. 5.3, page 53)
PMDF2	p2	R	-	Parameter in calculation of diffusion coefficient for oxygen in airfilled part of soil (see par. 5.3, page 53)
AIENSCPF	Y	R	cm	Air entry value of pF curve of the rootzone
MOFRPF1(1-10)	-	R	-	Moisture fractions 1 to 10 of pF curve of the rootzone (from low to high)
SCPF1(1-10)	-	R	cm	Suction values 1 to 10 of the pF curve of the rootzone
MOFRPF2(1-10)	-	R	-	Moisture fractions 1 to 10 of pF curve below the rootzone (from low to high)
SCPF2(1-10)	-	R	cm	Suction values 1 to 10 of the pF curve below the rootzone
MOFRWIUN	-	R	-	Moisture fraction at wilting point below the rootzone
MOFRSARO	-	R	-	Moisture fraction at saturation in the rootzone
MOFRSAUN	-	R	-	Moisture fraction at saturation below the rootzone
CDSA	-	R	m d-1	Hydraulic conductivity of the rootzone
LR	-	I	-	Layer number from which a reduction in soil organic matter decomposition occurs
RDFADCHU	-	R	-	Reduction factor for soil organic matter decomposition for the layers LR and deeper

The file INI.DAT:

This file is closed after reading. At the end of the simulated year it is opened again and new initial data for the next year are stored.

MOFRD(NL=1-NL)	0	R	-	Moisture fraction of the layers 1 to NL
EX(NL=1-NL)	Ex	R	kg m <sup>-2</sup>	Exudate content of the layers 1 to NL
HUEX(NL=1-NL)	He	R	kg m <sup>-2</sup>	Soil organic material content of the layers 1 to NL
CONH(NL=1-NL)	cnh	R	kg m <sup>-3</sup>	Concentration of ammonium-N in the layers 1 to NL
CONI(NL=1-NL)	-	R	kg m <sup>-3</sup>	Concentration of nitrate-N in the layers 1 to NL
for LN=1 to NL				
* OS(LN,FN=1-NF)	Os	R	kg m <sup>-2</sup>	Amount of fresh organic material in the fractions 1 to NF present in layer LN
for LN=1 to NL				
* HUOS(LN,FN=1-NF)	Hs	R	kg m <sup>-2</sup>	Amount of soil organic material from fresh organic material fractions 1 to NF present in layer LN
for LN=1 to NL				
* COCA(LN,FN=1-NF)	s(fn)	R	kg m <sup>-3</sup>	Concentration of soluble organic material fractions 1 to NF in layer LN

N.B. For MOFRD zero's can be given. The first initial values are calculated from the waterquantity model data (see input files WATBAL.DAT or FEMSAT.DAT).

Values for OS and HUOS can be derived from previous runs with HISTOR (see appendix C), making sure that the sum over the fractions fn of HUOS(LN,FN) plus OS(LN,FN) equals measurements of total organic matter in layer LN at the starting time of simulation with ANIMO. If the cropping history is unknown, but if measurements of organic C and N are available, and the N-mineralization during the previous year can be estimated from the N-uptake by an unfertilized crop, it is also possible to take all the organic matter present as one OS-fraction (divided in amounts per layer) with one N-content and one decomposition rate, in accordance with these measurements. This method is much easier, perhaps less accurate, but for calculation of long-term effects on manured fields it might work.

For COCA zero's can be given, because the amounts of soluble organic material are usually negligible compared to the other forms of organic material.

The file CROP.DAT:

This file is opened once, and contains data for one subarea for all years; each simulated year part of it is read.

for each year of the run:				
KICR	-	I	-	Kind of crop grown
RM	-	I	-	Number of the material defined as root material
				Because at harvest, root residues are automatically added to the profile)
				N.B. This material should have FRDR = 1, because the root mass AMROTI is expressed as dry matter.
				FRNI and FRNH of this material should be zero.
LNMRD	-	I	-	Number of layers in the effective rootzone
TINEAD	-	R	d	Time of next addition (first addition of the year)
HVTE	-	I	-	Indicator for kind of temperature model to be used:
				HVTE = 1 means temperatures are known and given in the input; use Fourier model for this year
				HVTE ≠ 1 means no temperatures given; use sinus model for this year
Only if HVTE = 1:				
* TIMJAITE	-	R	d	Daynumber of first temperature measurement
AITE(1-52)	T(0,i)	R	C	Weekly measured air temperatures
For each planned time of				
addition (addition, fertilization, ploughing)				
* NUAD	-	I	-	Number of additions (actions) (max. 3 at the same time)
for each addition				
* MTNU	mn	I	-	Material number
QUMT	-	R	kg ha-1	Amount of material added
WYAD	-	I	-	Way of addition = number of layers over which the addition is distributed.
				WYAD = 0: addition on top of layer 1 = addition to layer 1 + volatilization
				WYAD = 1: addition to layer 1 (no volatilization)
				WYAD = 2: addition to layers 1 and 2, etc.
PL	-	I	-	Number of layers to be ploughed
* TINEAD	-	R	d	Time of next addition

The file MATBAL.DAT or FEMSAT.DAT;  
Each simulated year part of this file is read.

Initial values for the first year, first timestep:

MOCORD	$V_r(0)$	R	m	Moisture volume of rootzone
WALE	$h(0)$	R	m	Groundwater level
MODEUN	-	R	m	Moisture deficit below rootzone

Per timestep:

* TINA	-	R	d	Time in waterquantity model (not used)
EVMA	-	R	m d-1	Maximal evapotranspiration flux
PR	$P_r$	R	m d-1	Precipitation flux
EV	$E_r$	R	m d-1	Evapotranspiration flux
FG	$f_g$	R	m d-1	Flux to trenches (3rd order drainage system)
FS	$f_s$	R	m d-1	Flux to drains/ditches (2nd order drainage system)
FK	$f_k$	R	m d-1	Flux to canals (1st order drainage system)
PE	-	R	m d-1	Percolation flux from rootzone (not used)
LEAK	$f_l$	R	m d-1	Discharge flux to aquifer
MOCOROT	$V_r(t)$	R	m	Moisture volume of rootzone at end of timestep
WALET	$h(t)$	R	m	Depth of groundwater table at end of timestep

N.B. Dummy values can be given for TINA, EVMA and PE; they are not used in ANIMO presently.

## APPENDIX B

### Description of the computer program

In this appendix the actions performed by the main program and the subprograms of ANIMO are explained. To follow these explanations, a copy of the main programs and subprograms is necessary, as well as a copy of the vocabulary ANIMO.MEM. Calculations described comprehensively in the main text of this report are not lingered on.

Before the description of the different parts of the computer program a summary of the main variables used for moisture, organic material and  $\text{NH}_4\text{-N}$  and  $\text{NO}_3\text{-N}$  contents per layer will be given, to get a better insight in the terminology of the program.

Description	Name of variable used for value at		
	Beginning of timestep	Average	End of timestep
Moisture fraction	MOFRO(LN)	MOFR(LN)	MOFRT(LN)
Fresh organic material per fraction	OS(LN, FN)	—	RSOS(LN, FN)
Total fresh organic matter	TOOS(LN)	—	SUOS
Organic material in solution (OMS) per fraction	COCA(LN, FN)	AVCOCA(LN, FN)	RSCOCA(LN, FN)
Total OMS	COCATO(LN)	AVCOCATO(LN)	RSCOCATO(LN)
Humus from OMS per fraction	HUOS(LN, FN)	—	RSHUOS(LN, FN)
Humus from exudates	HUEX(LN)	—	RSHUEX(LN)
Total humus	TOHU(LN)	—	SUHU(LN)
Exudates	EX(LN)	—	RSEX(LN)
$\text{NH}_4\text{-N}$ concentration	CONH(LN)	AVCONH(LN)	RSCONH(LN)
$\text{NH}_4\text{-N}$ at complex	CXNH(LN)	—	RSCXNH(LN)
$\text{NO}_3\text{-N}$ concentration	CONI(LN)	AVCONI(LN)	RSCONI(LN)
Soluble species in general (subroutine TRANSPORT)	COTO(LN)	AVCO(LN)	CO(LN)

The order of treatment of the program parts is:

1. Main program ANIMO
2. Subroutine INIMO
3. Subroutine BALANCE
4. Subroutine ROOT
5. Subroutine ADDIT
6. Subroutine TEMPER
7. Subroutine MINER\_1
8. Subroutine TRANSPORT
9. Subroutine MINER\_2
10. Subroutine PLANT
11. Subroutine DENITR
12. Subroutine MASSBALANCE
13. Subroutine CONCDRAIN
14. Subroutine OUTPUT

#### 1. Main program ANIMO

Specification statements:

The file COMMON.FOR contains a declaration of all variables used in the main program as well as in the subprograms. It also contains statements declaring most of these variables (except for those transferred to subprograms by arguments) as COMMON.

General input data per run from file GEN.DAT:  
Described in appendix A.

Number of timesteps per year:

Note that a possible rest of the division  $365/ST$  will not be used.

Maximal nitrate concentration for uptake per crop:

This is the calculation of Copt1 and Copt2 as described in par. 6.3.2, from the input values for Nmax1, Nmax2, Epot(t0-t1) and Epot(t1-t3).

Converting year-data to day-data:

Most rate constants are known as year-rates and can be given in the input as such; here they are transformed into the units used in the model.

Combination with waterquantity model:

If IWA = 1 results from a file FEMSAT.DAT are used,  
if IWA = 2 results from WATBAL.DAT

Year loop and area loop: see flow scheme in par. 3.1.

General data subarea AN from inputfile GENAR.DAT:

See appendix A.

This file is opened and closed each year of the simulation.  
Each year the same data are read in.

Initial data of the subarea from the file INI.DAT;

See appendix A.

This is a file from which the initial data are read in. At the end of a simulation year, the new initial data for the next year are written into it, and the old values disappear.

Crop and fertilizer data of the subarea for this year from the file CROP.DAT:  
See appendix A.  
This file is opened once in a run; each simulation year new values are read from it.

General calculations subarea AN:

Geometry of profile:

Because only the heights of all the layers was input, here the depth of the bottom of each layer from soil surface, BO, and that of the middle of the layer, DP, are calculated.

Max. moisture deficit fraction under root zone; moisture fraction at saturation:  
Speaks for itself.

Initial moisture data calculation:

When, in the first year of simulation, calculations for a subarea start, the initial moisture distribution over the layers is calculated from a few extra moisture input data (see subroutine INIMO).

Distribution of ammonium:

The ratio for all the layers in the rootzone is made equal to that of the first layer; the ratio for all the other layers is made equal to that of the last layer. In this way only two numbers have to be given in the input.

Parameters for temperature models:

Damping depth DMDF: see par. 5.5.

Fourier coefficients: these are only calculated (according to par. 5.5) if input temperature values for the year under consideration are given. They are calculated assuming that the measurements have all been made in one calendar year, so the transformation DANU(1) = 7 etc. means that later on in the program, when temperatures are calculated for a time of the year TI, in the Fourier formula the term TI - TIMIAITE - 7 has to be used.

Totals of organic matter per layer:

These are the variables interesting for output, and used in mass balances.

Calculation of average distance between drains:

The distance between drainage systems is calculated as  $\text{distance} = 1/\text{density}$ ; for trenches (3rd order drainage systems) it is assumed that the canals and drains/ditches (first and 2nd order drainage systems) also have a dewatering function of a trench (3rd order drainage system); for drains/ditches (2nd order drainage systems) it is assumed that a canal (1st order drainage system) also has the dewatering function of a drain/ditch (2nd order drainage system).

Calculation of drain lengths:

$\text{Drainlength} = \text{acreage of subarea} * \text{density of drains}$ .

Plant parameters:

KC is used in indices instead of KICR.

SUUPNI, SUUPNIMA and RD are put at zero to avoid the use of

values stemming from another subarea.

Calculate situation subarea AN after one year:

Here the time-loop starts. The number of timesteps NST in a year is calculated before. Formulated like this, calculations for the subarea are always performed for a whole year, irrespective of the starting time TIMI. The variable TI gets values from TIMI to  $TIMI + NST * ST$ , and can become greater than 365 if TIMI is not equal to the beginning of a calendar year; the variable TIYR represents the daynumber of the current year, and cannot become greater than 365.

Moisture contents and fluxes:

Depending on the type of waterquantity model, moisture data are either read from FEMSATP.QUA or from WATBAL.DAT.

N.B. The values TIWA, EVMA and PE are not used in ANIMO presently; dummy values can be given in the input (see appendix A).

The subroutine BALANCE calculates from these data the moisture contents of all layers and the fluxes between the layers and in and out of the soil system from each layer.

Root production and exudate production:

See par. 5.1.3..

Fertilization, harvest, ploughing:

All these actions are described in the subroutine ADDIT; they are only performed when the time for the next "addition", TINEAD, has been reached; specification of which actions are performed at each TINEAD, is given in the input file CROP.DAT (see appendix A).

Temperature:

Temperature of all the layers is calculated using either the Fourier-analysis- or the sinus model.

Production rate of organic material in solution:

The rate constants  $k_0(DMS)$  per fraction are needed for the next part:

Transport, production and decomposition of org. mat. in sol.:

The subroutine TRANSPORT, applying the transport- and conservation equation to the layers in the profile, is called separately for each fraction of organic material, because each fraction has its own nitrogen content, so that the net released  $NH_4$  can be evaluated for each fraction later on. After each call the results are stored in the appropriate variables for DMS (RSCOCA and others).

Formation and decomposition of humus; decomposition of fresh organic material; production rate of  $NH_4$ :

The following lines of the program until "Carbon and nitrogen balance" correspond with the calculation scheme given in figure 5.4.

Carbon and nitrogen balances:

This is a check on the correctness of calculations performed on C and mineral N.

Concentration in drainage water from different layers:  
The carbon- and nitrogen loads on the drainage systems are calculated according to par. 4.5.

Here the timestep-loop ends (go to next timestep)

Write final data subarea AN year YR to file INI.DAT:  
The file INI.DAT is opened again and filled with the results of the calculation of the year, which are initial data for the next year.

Then the subarea-loop ends (go to next subarea)

The calculations of the average concentration in the deep drainage water and in the deep aquifer have not been worked out yet, because they are only used when the model is applied on regional scale.

The results of these calculations can be used in the next simulated year for those subregions where upward seepage takes place. This is the reason why calculations for all subareas are made in each year of simulation, and not calculations for all the years per subarea.

After these calculations the year-loop ends (go to next year)

When all the years have passed, the simulation ends.

## 2. Subroutine INIMO

From the 3 initial moisture data MOCORO, WALE and MODEUN (see appendix A) which this subroutine reads from WATBAL.DAT or FEMSAT.DAT the initial moisture distribution is calculated using the same procedure as in subroutine BALANCE.

## 3. Subroutine BALANCE

In this subroutine the moisture deficits per layer, the thickness of the layers discharging to the drainage systems, and the fluxes per layer, are calculated.

Calculation of moisture deficits:

The moisture deficit in the rootzone is determined from moisture content at saturation and actual moisture content at the end of the timestep. The moisture deficit of the soil below the rootzone is calculated from the water balance. If the phreatic level is in the rootzone this moisture deficit is zero.

Calculation of moisture fractions per layer:

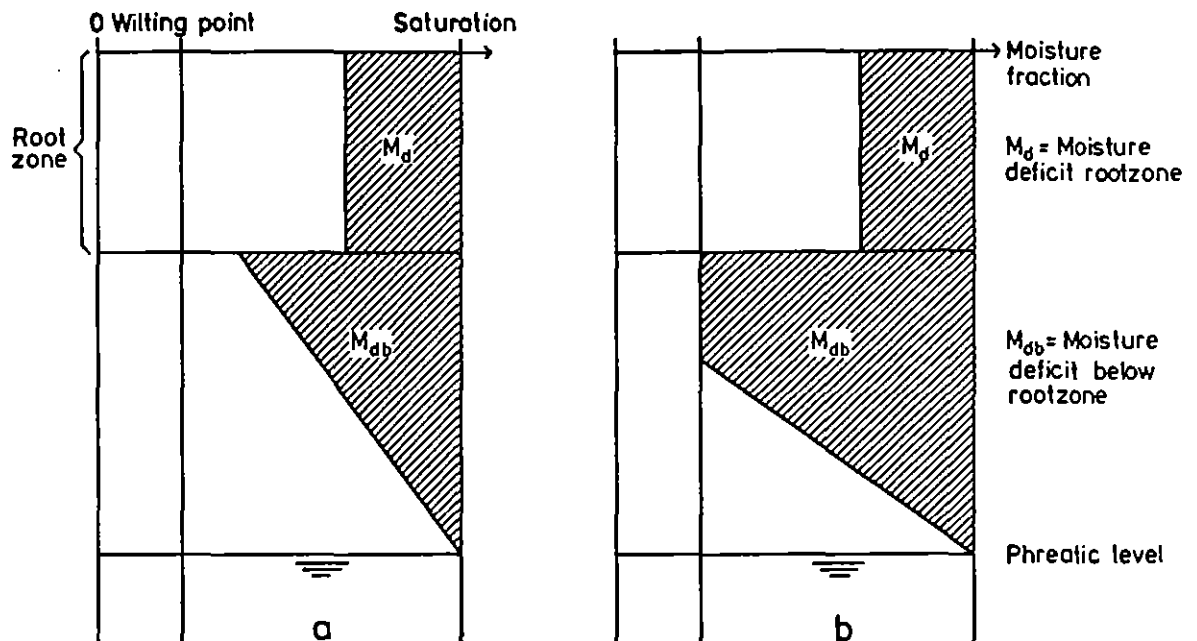
Rootzone:

If the phreatic level is below the rootzone the moisture fraction is considered constant with depth in the rootzone. If the phreatic level is in the rootzone the moisture frac-

Figure A.1. Schematic relationship of moisture fraction with depth.

Case a: Linear relation below rootzone

Case b: Non-linear relation below rootzone.



calculation the saturated part of the rootzone is multiplied by the factor KF. The equivalent flux density FEKMD follows then as the ratio of FMK and LEMK. Using this flux density below the rootzone and the product of KF and FEKMD in the rootzone the 1st, 2nd and 3rd order discharge layers can be identified. Subsequently the lower boundary of the 2nd order and 3rd order discharge layers are determined as the minimum of the boundary calculated on the basis of the equivalent flux density FEKMD and  $(1/4 * A + HD)$ . In subroutine FLUX that is called 3 times the discharge fluxes to the 3rd order drains FLG(LN), 2nd order drains FLS(LN) and 1st order drains FLK(LN) are calculated for each layer. In FLUX dummy names are used for some of the variables in the argument:

FM	for the discharge rate FG, FS or FK
B	for the upper boundary of the discharge layer HGB, HSB or HKB
U	for the lower boundary of the discharge layer HGO, HSO, HKO
F(LN)	for the discharge flux per layer FLG(LN), FLS(LN), FLK(LN)

#### Calculation of evapotranspiration fluxes:

For each layer the evapotranspiration flux FLEV(LN) is calculated. Below the rootzone (LNMARO layers) FLEV(LN) equals zero.

#### Calculation of fluxes per layer:

For each layer the vertical incoming flux from above FLAB(LN) is evaluated and using the water balance of each layer the vertical outgoing flux FLBE(LN) is calculated. These quantities are considered positive when downward.

tion is constant with depth for layers that are completely above the phreatic level. For layers completely below the phreatic level the moisture fraction equals saturation. For the layer with the waterlevel the weighted average of the unsaturated part and the saturated part is calculated.

Below the rootzone (see also fig. A.1):

Below the rootzone a linear relationship of the moisture fraction with depth is considered. This relationship is such that at the phreatic level the moisture fraction equals saturation and the total moisture content in this zone fits the water balance under the restriction that the moisture fraction should never be less than wilting point. If the latter is the case for the upper part of the zone below the rootzone the moisture fraction is considered to be at wilting point for part of this zone (constant with depth) and below this part a linear relation of moisture fraction with depth is assumed. The calculations below the rootzone proceed as follows:

Calculate the uppermost point of the assumed linear relationship of moisture fraction with depth MOFRBORO. If this moisture fraction is above wilting point calculate the slope of the moisture fraction-depth relation and calculate the moisture fraction of each layer based on the position of the phreatic level.

If MOFRBORO is less than wilting point the height of the bend-point in the moisture fraction-depth relation HEDR is calculated. Above HEDR the moisture fraction equals wilting point and below HEDR the linear relationship is valid. Based on the position of HEDR and the phreatic level the moisture fraction of each layer is calculated.

Thickness of layers discharging to drainage systems:

Because a canal (1st order drainage system) has also the dewatering function of a drain (2nd order drainage system) and also receives surface runoff and interflow (3rd order drainage system) LG is increased with the length of drains (2nd order) and canals (1st order). The total length of drains LS is increased with the length of canals, LK. Taking the total length of canals LK as a reference the discharge rate to drains (2nd order) with a length of LK can be calculated: FMKS. The discharge rate for surface runoff and interflow (3rd order) is evaluated in a similar way: FMG. The total discharge rate to a canal system with length LK follows then:

$$FMK = FK + FMS + FMG$$

At the location of such a canal this discharge rate FMK has to be discharged from the saturated soil system. If the waterlevel is in the rootzone a correction for the flux in this saturated part for the (higher) permeability is made with the parameter KF (ratio of hydraulic conductivity of rootzone and that of the subsoil).

First the lower boundary HKO of the canal discharge layer (1st order) is evaluated as the minimum of the lower boundary of the model scale BO(NL) and  $(1/4 * AK + HDK)$  where AK is the average distance between canals and HDK is the bottom level of the canals. Based on the phreatic level and the value of KF the equivalent thickness LEMK of the saturated soil system discharging to a canal is calculated. In this

Starting point of the calculations is the incoming flux of the first layer (precipitation PR) and endpoint is the outgoing flux of the last layer (= leakage LEAK). Next the fluxes as required for the transport and conservation equation are calculated:

FLID(LN) incoming flux from below (zero when downward, positive when upward)  
FLIB(LN) incoming flux from above (zero when upward, positive when downward)  
FLID(LN) incoming flux from the drainage system (zero when drainage takes place; positive when infiltration takes place)  
FLOU(LN) total flux leaving the soil layer to the drainage systems or to layers above or below.

#### 4. Subroutine ROOT

Amount and length of roots:

Only calculated during the growing season. The amount of roots is an interpolation between the "standard" data given in par. 6.2.; the function RINT, described below, is used for the interpolation. The same applies to the calculation of the length of the roots, except that the length can be limited when the effective rooting depth + 10 cm is smaller than the interpolated value (see par. 5.1.3.):

LNRO = MIN(BO(LNMARD) + 0.10, RINT(...))

Distribution of roots over the layers (see par. 5.1.3):

First the root increase compared to the last timestep, is calculated. Then the amount of roots in the layer RO(LN) is displaced by the new value.

The way of calculation for the last layer containing roots, NURD, is a bit different, due to the fact that only a part of the layer contains roots.

Exudate production:

See par. 5.1.3.

The subroutine RINT interpolates linearly between Y-values corresponding with X-values, both given as arrays of N numbers, using a X1 which must be within the range X(1) - X(N). At attempted extrapolation the program execution stops. The argument K stands for 'kind of crop': each crop has its own X- and Y-arrays.

#### 5. Subroutine ADDIT

This subroutine is used whenever a special action takes place: harvest, ploughing, addition of fertilizer, or addition of crop residues or other organic materials. See also par. 5.7.

Harvest:

At harvest time the root mass AMRO of the crop comes available for decomposition, and is automatically 'added' as fresh

organic material to the soil; division over the layers follows from the root mass distribution  $RO(LN)$ , except when a tuber crop is concerned. In that case, a 'standard' harvest of tubers  $TUTO$  is subtracted from the total root mass  $AMRO$ , and the rest of the material,  $AMORMT$ , is incorporated in the first (few) layer(s) of the soil  $NURO$ , calculated in this case as the number of layers for which the middle of the layer is less than 10 cm from soil surface. For other crops,  $AMORMT$  is calculated as the amount of organic material per root-containing layer, which amount is subsequently divided in its organic fractions. The composition of the root material should be given in the input data of the run.  $RM$  is the number of the material representing the root material,  $FR(RM, FN)$  gives the distribution of organic material of the roots over a number of fractions,  $FRCA(RM, FN)$  gives the distribution of the material over soluble fractions. The root material is thought to consist of organic material only; therefore no fractions  $NO_3-N$  or  $NH_4-N$  are calculated.

Read the data concerning additions:

Addition data are given in the input file `CROP.DAT` (see appendix A). Action is taken when the last `TINEAD` (time of next addition(s) is reached (or just passed; the addition data do not have to coincide with timestep boundaries). A maximum of 3 additions per timestep can be performed. It should be stressed here too, that crop residues, other than root mass, should be given in the input file, because they can vary in amount.

After reading the data for all the additions, each addition is separately carried out; ploughing can be done after each separate addition.

Divide the material in its anorganic and organic parts:

The fractions  $AMOR(FN)$  in the total organic material  $AMORMT$  are determined. These fractions will be divided over one or more layers.

Then the way of addition is considered; addition 'on top of layer 1' ( $WYAD = 0$ ) means addition to the contents of layer 1 and volatilization of a part  $FRVO$  of the ammonium added, if present; addition to one or more layers ( $WYAD \geq 1$ ) means equal distribution to  $WYAD$  layers. The only difference between  $WYAD = 1$  and  $WYAD = 0$  is the volatilization.

Addition on top of layer 1:

The fraction nitrate-N  $FRNI$  is contributed to solution; the fraction  $FRNH$  ammonium-N is divided between solution and soil complex.

The fractions of (soluble) organic matter are added to the amounts already present.

Addition to one or more layers:

The material is equally distributed over the  $WYAD$  layers, proportional to their heights  $HE$ ; the partition factor for each layer  $LN$  for addition number  $I$  is  $HE(LN)/BO(WYAD(I))$ .

Ploughing:

First the materials present in the layers to be ploughed  $PL$  are accumulated, resulting in the values for the  $SU$ -variables. Then they are equally distributed again, proportional to the

heights of the layers HE, except for nitrate; all layers get the same concentration SUNI/SUMO. The NH<sub>4</sub> is distributed over solution and complex.

#### 6. Subroutine TEMPER

The temperature at average time of the year AVTI, that is in the middle of the timestep, and for the middle of the layers DP(LN) is calculated. For years with known air temperatures (HVTE = 1) the Fourier analysis model is used. For other years the sinus model is used. See par. 5.5. In the Fourier model, AVTI - TIMIAITE + 7 has to be used instead of AVTI itself, because of the phase shift applied in calculating the Fourier coefficients.

#### 7. Subroutine MINER\_1

The calculations about mineralization are divided over two subroutines; this is done because the subroutine TRANSPORT has to be used for organic material before calculations about mineralization of ammonium can be made; also, the aeration of the profile should be determined by the subroutine DENITR before anything can be said about the rate of formation and decomposition of nitrate. The calculations performed in the following sections (7 through 11) are those schematically depicted in figure 5.4., and explained in the paragraphs 5.1 through 5.6.

First the influence of temperature (par. 5.5), expressed in a factor RDFATE per layer, by which several rate constants will be multiplied, is calculated. For temperatures below zero RDFATE is put at 1.E-5.

Then the reduction factors for suboptimal moisture are calculated, according to par. 5.6. The suction per layer is calculated with the interpolation-function MINT (which works the same as the function RINT used in the subroutine ROOT, except that no specification per crop has to be given). The calculation of RDFAMO itself is also an interpolation, only here extrapolation is allowed, as long as RDFAMO >= 0.

Calculate reduced rate constants for all layers:  
The appropriate rate constants for transformation processes are multiplied by one or more of the factors calculated above.

Calculate zero-order reaction rate of OMS:  
See par. 5.1.2.

## 8. Subroutine TRANSPORT

Because subroutine TRANSPORT is called several times a number of variables receive dummy names through the argument. Based on the flow direction of water the sequence of calculations is determined (see chapter 4.4). The calculation of concentrations for each layer takes place in subroutine TRANSSUB. In TRANSSUB the parameters HV (change of moisture fraction with time), HV1 (= A in chapter 4.4) and HV2 (= B in chapter 4.4) are calculated. The functions FCONIT and FAVCO are used to calculate the concentrations. FCONIT calculates the end concentrations (see chapter 4.4); FAVCO calculates the average concentrations during the timestep (see chapter 4.4). In both functions are REAL\*8 calculations are used to avoid inaccuracies in the results.

## 9. Subroutine MINER\_2

When the concentrations of OMS at the end of the timestep and the totals of OMS influx and outflux are calculated with TRANSPORT, the results for organic material dissociation per layer can be assessed.

The remaining amounts of soil organic matter, fresh organic material and exudates are calculated, according to the theory in par. 5.1.4., 5.1.1. and 5.1.3., respectively.

Total dissociation of organic material; total mineralization of nitrogen; production rate of NH<sub>4</sub>; see par. 5.2.

With the production rate for NH<sub>4</sub> and the nitrification rate under aerobic conditions, only influenced by temperature and suction, TRANSPORT can be applied to NH<sub>4</sub>; when the resulting NH<sub>4</sub>-concentrations have been calculated, the oxygen demand for nitrification can be determined.

## 10. Subroutine PLANT

The selectivity constant for uptake by plants of a soluble species has a value other than 1 when:

- there is no crop present
- organic matter is concerned. This is not accomplished in this subroutine, but simply by putting RD = 0 in the argument when TRANSPORT is called for organic matter. The RD for NH<sub>4</sub> and NO<sub>3</sub> is calculated after this call, so the new value can be used when TRANSPORT is called for these species.

Maximal sum of uptake for this timestep;  
See par. 5.4.

## 10. Subroutine DENITR

The calculations performed by this subroutine are described in par. 5.3. mainly; some parts of 5.2. and 5.5. are used (indicated in the following text).

Oxygen demand for complete aeration:

This is the oxygen demand resulting from oxydation of organic material and from nitrification.

OXPDRA is the 'production' rate of oxygen, expressed in kg per m<sup>3</sup> soil system per day which will be negative; this parameter is used in the calculation of oxygen distribution in saturated soil around a gasfilled pore; OXDDRA is the oxygen demand rate, expressed in m<sup>3</sup> per m<sup>3</sup> soil system per day, which will be positive; it is used in the calculation of the vertical oxygen distribution in the soil gasfilled pore system.

Diffusion coefficients for oxygen per layer in pore air and soil water:

The formula for the temperature-dependence of the diffusion coefficient in air is given in par. 5.5.; that for the influence of the gasfilled fraction in combination with parameters for soil type is given in par. 5.3.; these two formulas are combined in the calculation of DFCFOXAI.

For the diffusion coefficient in water the value at saturation is calculated, because it is used for determining the horizontal oxygen distribution in saturated soil around an airfilled pore.

Vertical oxygen distribution in pore air:

The definitive oxygen profile is determined after a number of iterations including the next sections (until 'extra denitrification ...'). The iteration scheme is given in figure 5.3. At the first iteration the reduced oxygen demands RDOXDDRA and production rates RDOXPORA are still equal to their maxima OXDDRA and OXPORA. Per iteration with new RDOXDDRA-values the vertical profile is calculated in this section, according to the scheme given in figure 5.2. The last calculated oxygen profile OXCO2 is stored in OXCO1, because iteration (over the sections mentioned) is stopped when the difference between these two is small enough (sum of squares of differences SUSQDI < 1.E-6, see end of this section).

Water-saturated layers are assumed to be completely anaerobic.

Reduced oxygen demand per layer as a result of partial anaerobiosis:

Calculations according to the formulas given in par. 5.3. The calculation of the equilibrium concentration CV of oxygen in water at the air/water boundary is described in par. 5.5.

The starting value for the calculation of the aerated radius per soil pore RIAE with Newton-Raphson iteration, is a value interpolated between RIAE-results obtained with extreme values of OXDDRA/(2\*DFCFOXSD) and CV, in calculations performed beforehand; in the interpolation (three-dimensional linear) the actual values of RDOXPORA/(2\*DFCFOXSD) and CV are used.

The extreme values (FAA, FB, O1 and O2) and results (R1 through RB) are given at the beginning of the subroutine in a DATA statement.

FUN is the function for which the zero has to be found, DIFU is its derivative.

With the new values for RDOXDDRA another vertical oxygen profile in pore air can be calculated. No more than 3 iterations between vertical and horizontal oxygen-distribution are allowed, because these calculations are rather time-consuming; for each vertical oxygen profile 10 iterations are allowed, for the calculation of RIAE for each layer in each iteration also a maximum of 10 iterations can be used.

Extra denitrification in rootzone related to precipitation surplus:

TIAN is calculated for each layer in the rootzone according to the theory given at the end of par. 5.3.

Reaction coefficients for NH<sub>4</sub> and NO<sub>3</sub>:

When, at last, the aerobic and anaerobic parts of layers are determined, the decomposition rate for NH<sub>4</sub>-N, REKINH, and the zero-order rate constant for production (if negative: consumption), REKONI, can be calculated for each layer, according to par. 5.2., taking into account the extra anaerobic time TIAN, as calculated at the end of 5.3.

## 12. Subroutine MASSBALANCE

This subroutine performs the calculations described in par. 5.9. Sometimes the formulation is not exactly the same as in this paragraph, because totals of fresh and soluble organic matter are used which do not occur in this text, and the model uses moisture fraction\*layer thickness instead of moisture volume.

At the end of this subroutine the values for moisture, organic matter and N at the end of the timestep are transformed into the values at the beginning of the next timestep.

## 13. Subroutine CONCDRAIN

In this subroutine the concentration of the drainage water of the three drainage systems and of the leakage water are calculated according to par. 4.5.

## 14. Subroutine OUTPUT

At the end of each subroutine mentioned before, OUTPUT is called. The argument NUPA causes a jump to a certain part of the subroutine, where the output of the calling subroutine is given, after which a return to that calling subroutine follows.

## APPENDIX C

### Using the model HISTOR

The model HISTOR uses a input file HISTOR.IN, in which the following data should be present in the order given here:

Parameter	Type	Units	Description
ASFA	R	-	Assimilation factor
NL	I	-	Number of layers (always 5)
NF	I	-	Number of fractions (always 3)
FR(1-3)	R	-	Fractions in the organic material
FROR	R	-	Fraction of added material that is organic
FRCA(1-3)	R	-	Fractions of soluble organic material in the added mat.
HE	R	m	Height of the layers
MOFR(1-5)	R	-	Moisture fractions of the layers
NIFR(1-3)	R	-	Nitrogen fractions in the organic material fractions
NIFRHU	R	-	Nitrogen fraction in soil org.mat
NIFREX	R	-	Nitrogen fraction in exudates
PRSU	R	m	Yearly precipitation surplus
QUMT	R	kg ha-1	Yearly amount of material added (dry matter)
RECFEXAV	R	y-1	Average yearly rate constant for decomposition of exudates
RECFHUAV	R	y-1	Average yearly rate constant for decomposition of soil organic matter
RECFAV(1-3)	R	y-1	Average yearly rate constant for decomposition of fresh org. mat. fractions
RECFCAAV	R	y-1	Average yearly rate constant for decomposition of OMS
RO	R	kg ha-1	Yearly amount of roots at harvest
ST	R	d	Length of timestep (always 183)
NY	I	-	Number of years to simulate
NUADS	I	-	Number of additions in spring
NUADW	I	-	Number of additions in fall
If yearly additions are wished for the whole simulation period, NUADS and/or NUADW = NY			
PE	I	-	Period to start simulation PE = 1 summer period PE = 2 winter period

The output file has the name HISTOR.OUT. It produces per timestep of half a year the values:

NS	I	y	Number of summer periods passed
NW	I	y	Number of winter periods passed
TOOM	R	kg m-2	Total organic matter layer 1 (OS-fractions + TDHU)
OS(2)	R	kg m-2	Fresh organic matter fraction 2 in layer 1 (only layer 1 contains OS)
OS(3)	R	kg m-2	Fresh organic matter fraction 3

TOHU(2)	R	kg m <sup>-2</sup>	in layer 1
COTCTO(1-4)	R	kg m <sup>-3</sup>	Amount of soil org. mat. layer 2 Concentration of organic carbon in solution N.B. COTCTO ≠ COCATO Here, COTCTO = 0.58*COCATO
TOMNNI(1-4)	R	kg m <sup>-2</sup>	Total mineralization of N in the layers 1 thru 4

but other output values like TOHU(3-5) can easily be obtained by changing the output statements at the end of the summer period and at the end of the winter period.

Separate runs should be made per type and amount of addition and per type of crop with different rooting depth and root mass.

Example:

The effect of 30 years of history of the following field should be simulated:

- 20 years of grassland with yearly spring additions of manure M1
- 5 years of grassland with yearly spring additions M1 and fall additions of manure M2
- 5 years of maize with its own spring addition of manure M3

The following runs should be done:

1. Effect of spring additions to grassland

QUMT = M1  
NUADS = 25  
NUADW = 0  
PE = 1  
NY = 30 (no additions of this kind for the last 5 years)  
RO = 0.  
HE = 0.2 (example of depth of incorporation of manure)  
FR(1-3), FRCA(1-3), and A(1-3) : values for manure (table 6.4)

2. Effect of fall additions on grassland

QUMT = M2  
NUADS = 0  
NUADW = 5  
PE = 2  
NY = 10 (5 years with additions M2, 5 years with no additions M2 during maize)  
RO = 0.  
HE = 0.2  
FR(1-3), FRCA(1-3), and A(1-3) : values for manure (table 6.4)

3. Effect of grass roots and -exudates

QUMT = 2\*average root mass (see appendix E)  
NUADS = 0  
NUADW = 25 (roots considered to become available in fall in this model for grass roots too; in ANIMO this must be modelled in a different way (see appendix E)  
PE = 1  
NY = 30  
RO = 2\*average amount of roots (see appendix E)  
(used for exudate production calculations)  
HE = 0.3  
FR(1-3), FRCA(1-3), and A(1-3) : values for root material;  
this is not determined in table 6.5; an average curve can be

taken in between that of crop residues and that of straw.

#### 4. Effects of spring additions to maize

QUMT = M3  
NUADS = 5  
NUADW = 0  
PE = 1  
NY = 5  
RO = 0.  
HE = 0.2  
FR(1-3), FRCA(1-3), and A(1-3) : values for manure (table 6.4)

#### 5. Effect of maize roots

QUMT = amount of roots formed by maize (added to profile  
in fall)  
NUADS = 0  
NUADW = 5  
PE = 1  
NY = 5  
RO = amount of roots formed by maize (used for exudate  
production calculations)  
HE = rooting depth of maize  
FR(1-3), FRCA(1-3), and A(1-3) : values for root material;  
this is not determined in table 6.5; an average curve can be  
taken in between that of crop residues and that of straw.

The results of these runs should be combined to give the situation at the start of simulation of ANIMO. In this combination of results attention should be paid to:

1. Output data of HISTOR have to be transformed into ANIMO input data taking into account differences in layer thicknesses used in animo and in the separate runs of HISTOR.
2. HISTOR always works with one kind of material at a time; for ANIMO more materials and more fractions can be used. Per kind of material 2 or 3 fractions are needed; the fraction numbers can be defined as follows for the example above:

HISTOR	ANIMO
fractions 1-3 for manure	fractions 1-3
fractions 1-3 for root material	fractions 4-6
3. HISTOR stops when NS = NY and NW = NY. Dependent on the value of PE and the time of year the ANIMO-run should start, not always the last output line of HISTOR is the line to be used.

APPENDIX D  
List of symbols used

N.B. Layer indices  $n$  or  $k$  are not always used in the text  
N.B. Some symbols are used for different purposes. In that case, behind the description of the less frequent used one, a paragraph number is written.

Symbol	units	description
A	-	Parameter used in par. 4.4 (no physical meaning)
a	-	assimilation factor
a	$\text{cm}^2 \text{ s}^{-1}$ $\text{m}^2 \text{ d}^{-1}$	thermal conductivity (par. 5.5)
a, a'	$\text{kg m}^{-3} \text{ d}^{-1}$	oxygen production rate (par.5.3.)
A(n)	-	coefficient in Fourier analysis
a(n)	-	coefficient in Fourier analysis
A0	C	amplitude of yearly temperature wave
AE	-	aerated fraction of soil layer
ae	$\text{d}^{-1}$	first-order rate constant for root exudates
ae	$\text{m}^2$	aerated area per pore (par. 5.3.)
Ag	m	average distance between trenches (3rd order drainage systems)
ah	$\text{d}^{-1}$	first-order rate constant for soil organic material
Ak	m	average distance between canals (1st order drainage systems)
an	$\text{d}^{-1}$	first-order rate constant for fraction $f_n$ of fresh organic material
As	m	average distance between drains/ditches (2nd order drainage systems)
as	$\text{d}^{-1}$	first-order decomposition rate constant for soluble organic material
Ar	$\text{kg m}^{-2}$	amount of roots present in profile
B	-	constant used in par. 4.4. (no physical meaning)
b, b'	$\text{m}^3 \text{ m}^{-3} \text{ d}^{-1}$	oxygen consumption rate
b(n)	-	coefficient in Fourier analysis
c	$\text{cal cm}^{-3} \text{ }^{\circ}\text{C}^{-1}$	specific heat (par. 5.5)
c(n,t)	$\text{kg m}^{-3}$	concentration of a species in layer $n$ at time $t$
$\bar{c}(n)$	$\text{kg m}^{-3}$	average concentration of a species in layer $n$ during the timestep
c1	%	maximal N-content of a plant in the first growing period
c2	%	maximal N-content of a plant in the second growing period
ca	$\text{m}^3 \text{ m}^{-3}$	oxygen concentration in atmosphere
ce	$\text{kg m}^{-3}$	concentration in evapotranspiration flux
cg	$\text{kg m}^{-3}$	concentration in trench (3rd order drainage) discharge water
ci	$\text{kg m}^{-3}$	concentration in incoming flux
cid	$\text{kg m}^{-3}$	concentration in infiltration water
ck	$\text{kg m}^{-3}$	concentration in canal (1st order) discharge water
cnh	$\text{kg m}^{-3}$	ammonium-N concentration
$\bar{c}_{nh}$	$\text{kg m}^{-3}$	average ammonium-N concentration during timestep
cni	$\text{kg m}^{-3}$	nitrate-N concentration

$\bar{c}_{ni}$	kg m <sup>-3</sup>	average nitrate-N concentration during timestep
$c_o$	kg m <sup>-3</sup>	concentration in outgoing flux
$C_{opt}$	kg m <sup>-3</sup>	optimal mineral N concentration for uptake by plant roots
$c_p$	m <sup>3</sup> m <sup>-3</sup>	oxygen concentration in pore air
$c_s$	kg m <sup>-3</sup>	concentration in drain/ditch (2nd order drainage) discharge water
$c_w$	kg m <sup>-3</sup>	oxygen concentration in soil water
$c_{we}$	kg m <sup>-3</sup>	equilibrium oxygen concentration in solution at water/air boundary
$D$	m <sup>2</sup> d <sup>-1</sup>	diffusion coefficient of oxygen in airfilled pore system of soil
$D_0$	m <sup>2</sup> d <sup>-1</sup>	diffusion coefficient for oxygen in atmosphere
$D_a$	cm <sup>2</sup> s <sup>-1</sup>	diffusion coefficient for oxygen in air
$D_g$	m	thickness of the layer discharging to the 3rd order drainage system
$D_k$	m	thickness of the layer discharging to the 1st order drainage system
$D_m$	m	damping depth
$D_n$	kg m <sup>-3</sup> d <sup>-1</sup>	nitrate-N demand for denitrification
$dp(n)$	m	depth of middle of layer n from soil surface
$Dr$	m	thickness of rootzone
$D_s$	m	thickness of the layer discharging to the 2nd order drainage system
$E(t)$	kg m <sup>-2</sup>	amount of exudates in a layer
$E_{pot}$	m	potential evapotranspiration
$E_r$	m d <sup>-1</sup>	evapotranspiration flux
$f$	m d <sup>-1</sup>	steady state percolation flux
$f_a$	m d <sup>-1</sup>	discharge flux from the previous layer
$f_b$	m d <sup>-1</sup>	discharge flux to the next layer
$f_e$	m d <sup>-1</sup>	evapotranspiration flux
$f_g$	m d <sup>-1</sup>	total discharge flux to trench (3rd order drainage system)
$f_g(n)$	m d <sup>-1</sup>	discharge flux to trench (3rd order drainage system) from layer n
$f_i$	m d <sup>-1</sup>	total incoming flux
$f_{ib}$	m d <sup>-1</sup>	downward flux from layer n-1 to layer n
$f_{id}$	m d <sup>-1</sup>	infiltration flux from the drainage systems
$f_{io}$	m d <sup>-1</sup>	upward flow from layer n+1 to layer n
$f_{in}$	m d <sup>-1</sup>	incoming flux in the unsaturated zone
$f_k$	m d <sup>-1</sup>	total flux to canals (1st order drainage systems)
$f_k(n)$	m d <sup>-1</sup>	flux to canals (1st order drainage systems) from layer n
$f_l$	m d <sup>-1</sup>	discharge flux to or from the aquifer
$f_n$	-	fraction number
$f_o$	m d <sup>-1</sup>	outgoing flux
$f_{ou}$	m d <sup>-1</sup>	outgoing flux of the unsaturated zone
$FR$	-	name of a matrix used in fraction division of fresh organic matter
$f_s$	m d <sup>-1</sup>	discharge flux for ditch/drain (2nd order) discharges
$f_s(n)$	m d <sup>-1</sup>	discharge flux for ditch/drain (2nd order) discharges from layer n
$f_{ub}$	m d <sup>-1</sup>	upward flux to the previous layer (n-1)
$f_{uo}$	m d <sup>-1</sup>	downward flux to the next layer (n+1)

fz	m d-1	discharge flux to the drainage systems from a layer
H	kg m-2	amount of soil organic material (humus)
H(t)	kg m-2	amount of soil organic material
h	m	height of a water column (par. 5.3)
h(t)	m	depth of the water table at the end of a timestep
He(t)	kg m-2	amount of soil organic material originating from exudates
Hs(fn,t)	kg m-2	amount of soil organic material originating from soluble organic matter
HV	d-1	change rate of moisture fraction
Is	kg m-2	amount transported into the layer during the timestep
k	-	layer number (par. 5.3)
k	g d-1	production rate of OMS (par. 6.1)
k0	kg m-3 d-1	zero-order rate constant for a soluble species
k1	d-1	first-order rate constant for a soluble species
ke	kg m-2 d-1	zero-order rate constant for production of exudates
knh	d-1	first-order rate constant for nitrification
kr	kg m-2 d-1	production rate of dead grass root mass
ks(1)	m d-1	saturated conductivity of layer 1
L(n)	m	height of a layer
Lr	m	rooting depth
Lre	m	effective rooting depth
m	-	number of moles
Mn	kg m-2	ammonification rate
mn	-	material number
N	-	number of airfilled pores
n	-	layer number
n	-	number of Fourier coefficient (par. 5.5)
na	-	number of aerated layers
nf	-	number of fractions
nifr(fn)	-	nitrogen fraction in organic material fraction fn
nifrex	-	nitrogen fraction in exudates
nifrhu	-	nitrogen fraction in soil organic material (humus)
n1	-	number of layers
Nm	kg m-2	maximal cumulative N uptake of N by the crop for the timestep
nm	-	number of materials
Nmax	kg m-2	maximal uptake of N by the crop during a favourable growing season
nr	-	number of layers with roots
Nre	kg m-2	realized cumulative N uptake by the crop
OMS	-	organic material in solution
Os(fn,t)	kg m-2	amount of a fresh organic material fraction fn
p	atm	gas pressure
p1	-	parameter for soil type in determining D
p2	-	parameter for soil type in determining D
Pr	m d-1	precipitation rate
Ps	m	precipitation surplus
Q	kg m-3	amount of NH4-N adsorbed per unit of soil system

q	-	part of a layer discharging to a certain drainage system
qnh	kg m <sup>-2</sup>	amount of NH <sub>4</sub> -N adsorbed in a layer
R(t)	kg m <sup>-2</sup>	amount of roots in a layer
R	m	radius of aeration of a gasfilled soil pore
r	m	radial distance from centre of gasfilled pore
r	different	rate of a process (par. 5.5)
Rd	-	distribution ratio for ammonium
Rg	l atm C <sup>-1</sup> mole <sup>-1</sup>	gas constant
rv	m	radius of gasfilled pore
S	-	selectivity constant for uptake of solutes by the plant
s(fn,t)	kg m <sup>-3</sup>	concentration of a fraction of soluble organic material
g(fn)	kg m <sup>-3</sup>	average concentration of a fraction of soluble organic material
T	C	temperature
t	d	time, timestep
t	-	fraction of timestep for temporary anaerobiosis
Ta	C	average yearly temperature
Us	kg m <sup>-2</sup>	amount transported out of a layer during a timestep
V(n)	m	average moisture content of a layer n
V(n,t)	m	moisture content of a layer n at time t
v	l	gas volume
Vb	m	moisture volume below rootzone
Vr	m	moisture volume of rootzone
Z	different	constant in law of Arrhenius (par. 5.5)
Z(k)	m	depth of the bottom of layer k from soil surface
z	m	depth
λ	-	labyrinth factor
λ	cal cm <sup>-1</sup> s <sup>-1</sup> C <sup>-1</sup>	thermal conductivity (par. 5.5.)
φ	rad	phase shift
φ(n)	rad	Fourier coefficient (par. 5.5)
θ	-	moisture fraction
θ <sub>0</sub>	-	moisture fraction at the beginning of the timestep
θ <sub>+</sub>	-	increase of moisture fraction from θ <sub>av</sub> to air entry value
θ <sub>av</sub>	-	average moisture fraction during timestep
θ <sub>g</sub>	-	gasfilled fraction
θ <sub>sat</sub>	-	saturated moisture fraction
Y	cm	moisture suction
w	rad d <sup>-1</sup>	frequency of temperature wave

## APPENDIX E

### Modelling concept for grassland

The amount of roots in grassland can vary between extremes of 2300 to 30000 kg dry matter per ha in the layer 0-20 cm. On comparable natural grasslands the root mass is generally higher than on culture grasslands. The amount is influenced by: profile properties, botanical composition, age, cutting regime, time of the year, fertilization and watermanagement (Dirven and Wind, 1982). It will be clear that precise modelling of this amount is too complicated in this stage. When new grass is sown, the amount of roots will generally increase during the first 6 to 8 years, after which a certain stabilization takes place (Schuurman, 1973). When fertilization takes place, the equilibrium can be reached sooner (Schuurman and Knot, 1970). During one year, however, there is also a general trend in root mass fluctuation. This is illustrated in fig. F.1. (Schuurman, 1973). When the growth is not interrupted, maxima occur in may and september. When the grass is cut more often, the first maximum becomes smaller and the second disappears (Schuurman, 1973). Therefore it seems possible to model the amount of roots in culture grassland as a sine function of the time of year, with a maximum on the 15th of may, a minimum on the 15th of november, and amplitude of 15%:

$$Ar = Ar(av) + 0.15 \cdot Ar(av) \cdot \sin\left(\frac{2\pi}{365} \cdot (\text{daynr.} - 46)\right)$$

The average amount  $Ar(av)$  can be determined by measurements. Measurements of root mass amounts mean measurements of the net result of formation and decomposition rates; they do not give information about these rates separately. Troughton (1981) measured the length of life of grass roots. This was about one year at uninterrupted growth, and about 0.5 year at frequent cutting for Lolium Perenne. For culture grasslands this means that the root mass is renewed twice a year; the production of dead roots is twice the average amount. When root exudates are also considered (see par. 5.1.3. and 6.1.), it means that an amount of  $0.41 \cdot 2 = 0.81$  times the average root mass comes available per year as exudates. These total amounts come available at average rates (kg m<sup>-2</sup> d<sup>-1</sup>) of

$$kr = \frac{2 \cdot Ar(av)}{365} \quad (\text{root mass}) \quad \text{and} \quad ke(\text{grass}) = \frac{0.81 \cdot Ar(av)}{365} \quad (\text{exudates}).$$

in which:

$$kr = \text{production rate of dead grass root mass} \\ (\text{kg m}^{-2} \text{ d}^{-1})$$

The fluctuation of the root mass during spring and summer is generally explained by assuming the growth rate is initially higher than the death rate, and later on the situation gets reversed (Goedewaagen and Schuurman, 1950; Troughton, 1957). This means that the death rate in summer is highest. Therefore it is possible to relate the rate  $kr$  to the temperature in the same way as the rate constants for organic matter transformations (see par. 5.5).

The easiest way to describe dead grass root mass production

in the model ANIMO is by considering the amount formed during a timestep as an "addition" at the beginning of that timestep. In this case the behaviour of this material can be described by that of a stepwise added, fresh organic material (Os), although the "addition" really is a continuous process.

Beside the temperature dependence of dead root mass production, for timesteps when the grass is cut a relatively greater dead root mass production could be taken as compared to other timesteps (with relatively lower dead root mass production)

Figure F.1. Variation in root mass during a year dependent on frequency of cutting (Schuurman, 1973)

