Simulation of Nitrogen Dynamics in the Soil-Plant System
Using the Danish Simulation Model DAISY

S. HANSEN, H.E. JENSEN, N.E. NIELSEN & H. SVENDSEN
The Royal Veterinary and Agricultural University,
Department of Agricultural Sciences, Section of
Soil and Water and Plant Nutrition,
Thorvaldsensvej 40, DK-1871 Frederiksberg C,
Denmark

ABSTRACT A dynamic simulation model for the soil
plant system is described. The model includes a
number of main modules viz. a water model, a soil
temperature model, a soil nitrogen model including
a submodel for soil organic matter dynamics, and
a crop model including a submodel for nitrogen
uptake. The soil part of the model has a one
dimensional vertical structure. The soil profile
is divided into layers on the basis of physical
and chemical soil characteristics. The model was
used to simulate soil nitrogen dynamics and
biomass production at five locations for crops
grown at various levels of nitrogen fertilization.
The simulated results were compared to experimen­
tal data on nitrogen accumulated in the shoot part
of the crop and nitrogen leaching from the root
zone. Based on this validation it is concluded
that the overall performance of the model is
satisfactory although some minor adjustments of
the model may prove to be necessary.

INTRODUCTION

Due to the fact that losses of nitrogen from arable agricul­
tural land to the aquatic environment have increased in many
areas, in particular during the last four decades, great
concern has arisen as to how an economically and environmen­
tally sustained agricultural crop production system can be
developed. This includes sustained crop yield and crop
quality, sustained natural resources for crop production,
high resource use efficiency in crop production and limita­
tion of the impact of crop production on environmental
quality.

The present Danish simulation model Daisy, which is
described in detail elsewhere (Hansen et al., 1990) was
developed to enable simulation of crop production, soil
water dynamics and nitrogen dynamics in crop production for
various agricultural management practices and strategies.
Thus a model has been developed to facilitate its use as a management tool at the field level, as well as at higher level, e.g. regionally, as part of a model system for administrative purposes.

MODEL DESCRIPTION

The model comprises a number of main modules viz. a water model including a submodel for soil water dynamics, a soil temperature model, a soil nitrogen model including a submodel for soil organic matter dynamics, and a crop model including a submodel for nitrogen uptake. The soil part of the model has a one dimensional vertical structure. The soil profile is divided into layers on the basis of physical and chemical soil characteristics.

The water model

The hydrological processes considered in the model include snow accumulation and melting, interception of precipitation by the crop canopy, evaporation from crop and soil surfaces, infiltration, water uptake by plant roots, transpiration, and vertical movement of water in the soil profile. In the model snow melting is influenced by incident radiation, and soil and air temperatures. Interception is determined by precipitation and by the crop canopy. The soil water dynamics is modelled by Richards equation (Richards, 1931):

\[
C_w \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z} \left( K_w \frac{\partial \psi}{\partial z} - K_w \right) - S
\]  

(1)

where \( C_w \) is the specific water capacity, \( \psi \) is the soil water pressure potential, \( K_w \) is the hydraulic conductivity, \( S \) represents water uptake by plant roots, \( t \) is time, and \( z \) is soil depth. The vertical flow rate \( q \) is given by the Darcy equation:

\[
q = -K_w \frac{\partial \psi}{\partial z} + K_w
\]  

(2)

Modelling of water uptake by plant roots is based on steady-state radial flow to the root surfaces:

\[
S = \frac{\theta_s \theta_r}{\theta_s^{-1/2} \ln (r^2/\pi L)}
\]  

(3)
where \( L \) is the root density, \( \theta \) is the soil water content at the root surface, \( \theta_s \) is the soil water content at saturation, \( \psi \) and \( \psi_s \) are the soil water pressure potentials of the bulk soil and at the root surface, respectively; and \( r \) is the root radius.

Potential evapotranspiration constitutes the upper limit for the considered evaporation and transpiration processes.

### The soil temperature model

Soil temperature is modelled by solving an extended heat flow equation which includes the effect of frost and thaw processes:

\[
\frac{\partial}{\partial t} \left( C_h T \right) - L_f \rho_i \frac{\partial x_i}{\partial t} = \frac{\partial}{\partial z} \left( k_h \frac{\partial T}{\partial z} \right) - \rho_w c_w \frac{\partial (T q)}{\partial z} \tag{4}
\]

where \( C_h \) is the volumetric heat capacity of soil, \( T \) is soil temperature, \( L_f \) is the latent heat of freezing, \( \rho_i \) is density of ice, \( x_i \) is volumetric fraction of ice, \( k_i \) is the thermal conductivity calculated according to de Vries (1963), \( \rho_w \) is the density of water, and \( c_w \) is the specific heat capacity of water. The freezing process induces water flow in the soil as ice formation is assumed to take place in the large soil pores; this process extracts water from small pores resulting in water flow towards the freezing zone (Miller, 1980).

### The soil nitrogen model

The transformation and transport processes considered in the model include net mineralization of nitrogen, nitrification, denitrification, nitrogen uptake by plants, and nitrogen leaching from the root zone. It appears that before mineralization can take place, soil organic matter has to be degraded and dissolved in the soil solution. This process may be considered as the rate-limiting step determining the turnover rate of soil organic matter (Nielsen et al., 1988). Net mineralization is thus governed by the turnover rate of organic matter in the soil. Soil organic matter is conceptually divided into three main pools, viz. dead native soil organic matter (SOM), microbial biomass (BOM), and added organic matter (AOM). Each main pool of organic matter is subdivided into two or three subpools characterized by a particular carbon nitrogen ratio and by a particular turnover time (Fig. 1). Thus, dead native soil organic matter (SOM) is subdivided into three subpools designated SOM 0, SOM 1, and SOM 2, respectively. The subpool SOM 0 can be neglected as it consists of almost inert organic matter. The rates of decomposition of SOM 1 and SOM 2 are simulated by first-order reaction kinetics. The subpool SOM 1 is assumed to consist of chemically stabilized organic matter, i.e. compounds with a chemical structure that implies resistance
to biological attack, while the subpool SOM is assumed to
consist of organic matter part of which is physically
stabilized, i.e. compounds which are protected against
biological attack because of adsorption to soil colloids or
entrapment within soil aggregates (Jenkinson & Rayner, 1977;
vvan Veen et al., 1985).
The microbial biomass in the soil is subdivided into two
subpools designated BOM and BOM, respectively, in order to
obtain a relatively stable as well as a more dynamic part of
the microbial biomass (van Veen et al., 1985). The subpool
BOM is considered to be relatively stable while subpool
BOM is assumed to be the more dynamic part of the microbial
biomass. Simulation of biomass turnover is based on growth
efficiency, maintenance respiration, and death rate coeffi­
cients.
The added organic matter (AOM) is made up of organic
fertilizers such as farmyard manure, slurry, green crop
manure, or crop residues left in the field after harvest.
The added organic matter is allocated to the subpools AOM,

![Diagram of organic matter turnover](image)

FIG. 1 The structure of the DAISY submodel of organic
matter turnover. Pools and subpools of organic matter and
related partition coefficients (f). AOM: Added organic
matter; BOM: Biomass; SOM: Soil organic matter.
AOM and SOM. The subpool AOM is assumed to consist mainly of cell wall material, while AOM is assumed to consist primarily of water-extractable cell material. The organic matter allocated to the soil subpool SOM is assumed to consist mainly of lignin and other resistant compounds (van Veen & Paul, 1981). The subpool AOM is a substrate for both BOM and BOM, and decomposes slowly, while the more easily decomposed AOM is a substrate for BOM only. The rates of decomposition of AOM and AOM are simulated by first-order reaction kinetics. The considered abiotic factors influencing carbon turnover are soil temperature and soil water status, and in the case of subpools SOM, SOM, BOM, also clay content.

Referring to Fig. 1, a carbon balance for each pool of organic matter can be established resulting in an expression for the rate of change of carbon \( \frac{dC}{dt} \) in each particular pool. Since each pool of organic matter is characterized by a particular carbon nitrogen ratio \([C/N]\), an overall organic nitrogen balance can be established resulting in an equation for the net mineralization rate \( \xi_m \) for nitrogen:

\[
\xi_m = -\sum_{i} \left( \frac{C/N_i}{dC_i/dt} \right)
\]

If net mineralization is negative, i.e. net immobilization occurs, it is assumed that NH\(_{4}\)-N is utilized in preference to NO\(_3\)-N by the microbial biomass.

In well aerated arable soils at relative high water content (1.5 < pF < 2.5), pH in the range 5-8, and soil temperature higher than 5°C, microbial activity is usually limited by the availability of organic carbon; most NH\(_{4}\)-N is then biologically oxidized to NO\(_3\)-N as rapidly as it is formed by the process of mineralization. Under such conditions nitrification can be expressed by first-order reaction kinetics. The considered abiotic factors influencing the nitrification process are soil temperature and soil water status.

Denitrification is modelled by defining a potential denitrification rate, i.e. the denitrification rate under complete anaerobic conditions. The potential denitrification rate \( \xi^*_d \) is assumed to be proportional to the CO\(_2\) evolution rate (Lind, 1980) as follows:

\[
\xi^*_d = \alpha_d \xi_{CO_2}
\]

where \( \alpha_d \) is an empirical constant and \( \xi_{CO_2} \) is the CO\(_2\) evolution rate. Under partially anaerobic conditions the potential denitrification rate is reduced according to the oxygen status of the soil expressed as a function of soil water content (Rolston et al., 1984). The actual denitrification rate is either determined as the reduced potential
denitrification rate or as the rate at which nitrate in soil is available for denitrification.

The nitrogen uptake model is based on the concept of a potential nitrogen demand simulated by the crop model, and the availability of nitrogen in the soil for plant uptake, i.e. the rate at which nitrogen can be made available at the root surfaces. The transport of nitrogen from the bulk soil to the root surfaces is based on a number of assumptions. Each root exploits an average effective volume of soil which is assumed to form a cylinder around each root. The radius of this cylinder is assumed to correspond to the average half-distance between the roots. It is assumed that nitrogen is transferred to the root surface by mass flow and diffusion that the concentration-distance profile develops in time in a stepwise manner, and that at each timestep the profile can be approximated by a steady-state distribution (Baldwin et al., 1973). The present model assumes that nitrogen uptake equals the nitrogen flux toward the root surface. Based on these assumptions the flux $I$, of nitrogen towards the root surface is calculated:

$$ I = \begin{cases} \frac{2\pi D b (\bar{C} - C_r)}{q} \left[ \frac{\beta^2 \ln \beta - \gamma_C}{\beta^2 - 1} \right]^{-1} & \alpha = 0 \\ \frac{(\beta^2 - 1)\bar{C} - C_r \ln \frac{\beta^2}{2}}{q} & \alpha = 2 \\ \frac{(\beta^2 - 1)(1 - \frac{\gamma_C}{2}\alpha) - (\beta^2 - \alpha - 1) C_r}{q} & \text{else} \end{cases} $$

where $D$ is the diffusion coefficient, $\bar{C}$ is the average concentration in solution, $C_r$ is the concentration at the root surface, and $b$ is the buffer power of soil. If uptake is limited by the availability of nitrogen then $C_r$ is equal to zero, in which case the root acts as a zero sink. Total uptake of nitrogen is then calculated by integrating $I$ over the entire root system. In the case of ample nitrogen supply the total nitrogen uptake is determined by the potential nitrogen demand. Total uptake is then distributed over the entire root zone by assuming a common value of $C_r$ to exist along the root surfaces of the entire root system. Soil layers in which $C < C_r$ are assumed not to contribute to nitrogen uptake. The calculations are performed for both ammonium and nitrate. Ammonium is assumed to be taken up by plant roots in preference to nitrate.

The vertical movement of nitrogen is modelled by solving the convection-dispersion equation:

$$ \frac{\partial (A + \theta C)}{\partial t} = \frac{\partial}{\partial z} \left[ \theta D + \frac{\partial C}{\partial z} - qC \right] + \Phi $$

(8)
where $A$ is adsorbed nitrogen, $D^*$ is the dispersion coefficient, $C$ is the bulk concentration of nitrogen in solution, and $\Phi$ is a sink/source term. The convection dispersion equation is solved for ammonium as well as for nitrate. In the case of ammonium the relation between adsorbed and dissolved ammonium is described by an adsorption-desorption isotherm derived from Schouwenberg and Schuffelen (1963), while adsorption for nitrate is considered insignificant. The source/sink terms for ammonium ($\Phi_{NH_4}^+$) and nitrate ($\Phi_{NO_3}^-$) in the convection-dispersion equation integrate the transformation and transfer processes of ammonium and nitrate, respectively:

$$
\begin{align*}
\Phi_{NH_4}^+ &= \xi_m + \xi_{f,NH_4} - \xi_{u,NH_4} - \xi_n \\
\Phi_{NO_3}^- &= \xi_n + \xi_{f,NO_3} - \xi_{u,NO_3} - \xi_d
\end{align*}
$$

where $\xi_m$, $\xi_n$, and $\xi_d$ are the net mineralization, nitrification, and denitrification, respectively, while $\xi_{f,NH_4}^+$, $\xi_{f,NO_3}^-$, and $\xi_{u,NH_4}^+$, $\xi_{u,NO_3}^-$ are the fertilizer input and root uptake of $NH_4^+$ and $NO_3^-$, respectively. Note that $C$ in equation (7) corresponds to $C$ in equation (8).

The crop model

In the present model a crop is considered to consist of two parts viz. shoot and root. The shoot is characterized by its dry matter content and leaf area index, while the root system is characterized by its dry matter content, rooting depth and root density. The crop model is based on the thermal unit concept which implies that crop development from emergence to harvest can be described in terms of temperature sum. Leaf area index is simulated as a function of both temperature sum and accumulated amount of shoot dry matter. Simulation of crop dry matter production is based on calculation of daily gross canopy photosynthesis, partitioning of assimilates between shoot and root, and respiration of shoot and root, respectively. The gross canopy photosynthesis may be limited due to water or nitrogen deficiency. Growth-limiting effects other than those caused by water or nitrogen deficiencies are not taken into account. Root penetration is assumed to take place if a daily net root dry matter production occurs, the soil temperature is above 4°C, and the actual rooting depth is less than the maximum rooting depth allowed for the particular soil considered. The root density distribution in the soil profile is described in accordance with Gerwitz and Page (1974). The daily potential nitrogen demand is calculated on the basis of crop nitrogen concentrations which are assumed to be function of temperature sum.
Driving variables

The driving variables required to run the model are daily values of global radiation, air temperature and precipitation. In the case of shallow ground water, the height of the ground water table is required as a driving variable in order to correctly simulate the soil water and soil nitrogen dynamics.

MODEL VALIDATION

The experimental data used for initialization and validation of the model were obtained from field experiments comprising spring barley grown on a coarse sandy soil in Jyndevad, Denmark, spring barley on a sandy loam in Askov, Denmark, winter wheat on a sandy loam in de Eest and PAGV, The Netherlands, and grass on a sandy loam in Ruurlo, The Netherlands. The field experiments are described by Lind et al. (1990) and Djurhuus (1990), Groot & Verberme (1990), and Jansen (1989a, 1989b), respectively. The field experiments involve various fertilizer treatments including unfertilized plots, mineral nitrogen fertilized plots, and pig and cattle slurry fertilized plots.

Validation emphasis is put on nitrogen uptake by the crop and leaching from the root zone. N-uptake is important from an agricultural point of view, whereas leaching is important from an environmental protection point of view. The scatter diagrams in Fig. 2 show simulated values of nitrogen content in the harvested above-ground biomass plotted versus the corresponding experimental values (left), and simulated values of nitrogen leaching from the root zone plotted versus the experimental values (right). It is noted that no experimental data on annual nitrogen leaching exists in the

FIG. 2 Scatter diagrams. Relation between experimental and simulated values of annual nitrogen uptake in harvested above ground biomass (left) and nitrogen leaching (right). O spring barley in Askov or Jyndevad, ◊ winter wheat in de Eest or PAGV, and □ grass in Ruurlo.
TABLE 1 Model performance statistics.

<table>
<thead>
<tr>
<th>Statistic</th>
<th>Range</th>
<th>Optimal Uptake</th>
<th>Leaching Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of Residual Mass</td>
<td>≤ 1</td>
<td>0</td>
<td>0.08</td>
</tr>
<tr>
<td>Maximum Error</td>
<td>≥ 0</td>
<td>0</td>
<td>45 kg N ha⁻¹</td>
</tr>
<tr>
<td>Root Mean Square Error</td>
<td>≥ 0</td>
<td>0</td>
<td>27 %</td>
</tr>
<tr>
<td>Coefficient of Determination</td>
<td>≥ 0</td>
<td>1</td>
<td>0.92</td>
</tr>
<tr>
<td>Modeling Efficiency</td>
<td>≤ 1</td>
<td>1</td>
<td>0.97</td>
</tr>
</tbody>
</table>

case of winter wheat at de Eest and PAGV. A visual inspection of the scatter diagrams shows that the data are distributed evenly relatively close around the 1:1 line in both cases. An evaluation of model performance in terms of statistical criteria is shown in Table 1. The considered criteria, including coefficient of residual mass, maximum error, root mean square error, coefficient of determination, and modelling efficiency, were proposed by Loague et al. (1988). Ranges and optimal values for these statistical parameters are also indicated in Table 1.

The coefficient of residual mass indicates slight tendencies towards over-prediction for nitrogen uptake and under-prediction for nitrogen leaching. However, it should be noted that the model does not consider any detrimental effects on crop growth other than those caused by soil water and/or nitrogen deficiency. If other detrimental effects were present, or if the fertilizer were distributed unevenly in the field, over-prediction of nitrogen uptake and under-prediction of nitrogen leaching would be expected. Regarding maximum error it is noted that the relatively large values for nitrogen uptake and for nitrogen leaching originated from the grass simulations conducted for the Ruurlo location. The coefficient of determination as well as the modelling efficiency are relatively close to their optimal value of 1. Thus it is concluded that the overall performance of the model is satisfactory although some minor adjustments may prove to be necessary.

REFERENCES


Danish Research Service for Plant and Soil Sciences, 1990.


