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Development and critical evaluation of a generic 2-D agro-hydrological model (SMCR_N) for the responses of crop yield and nitrogen composition to nitrogen fertilizer

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Abstract

Models play an important role in optimizing fertilizer use in agriculture to maintain sustainable crop production and to minimize the risk to the environment. In this study, we present a new Simulation Model for Crop Response to Nitrogen fertilizer (SMCR_N). The SMCR_N model, based on the recently developed model EU-Rotate_N for the N-economies of a wide range of crops and cropping systems, includes new modules for the estimation of N in the roots and an associated treatment of the recovery of soil mineral N by crops, for the reduction of growth rates by excessive fertilizer-N, and for the N mineralization from soil organic matter. The validity of the model was tested against the results from 32 multi-level fertilizer experiments on 16 different crop species. For this exercise none of the coefficients or parameters in the model was adjusted to improve the agreement between measurement and simulation. Over the practical range of fertilizer-N levels model predictions were, with few exceptions, in good agreement with measurements of crop dry weight (excluding fibrous roots) and its %N. The model considered that the entire reduction of soil inorganic N during growth was due to the sum of nitrate leaching, retention of N in fibrous roots and N uptake by the rest of the plant. The good agreement between the measured and simulated uptakes suggests that in this arable soil, losses of N from other soil processes were small. At high levels of fertilizer-N yields were dominated by the negative osmotic effect of fertilizer-N and model predictions for some crops were poor. However, the predictions were significantly improved by using a different value for the coefficient defining the osmotic effect for saline sensitive crops. The developed model SMCR_N uses generally readily
available inputs, and is more mechanistic than most agronomic models and thus has
the potential to be used as a tool for optimizing fertilizer practice.

**Abbreviations:**

- %N - percentage of N in $W$, %N$_{\text{crit}}$ - critical %N in $W$, i.e. the
  minimum %N at which growth is not restricted, %N$_{\text{max}}$ - maximum percentage of N in $W$,
- %N$_{p_{\text{pot}}}$ - potential percentage of N in $W_r$, %N$_{r}$ - percentage of N in $W_r$, $\Delta W$ -
  maximum possible increment in growth on the day (t ha$^{-1}$), $\alpha$, $\beta$ - parameters which
  relate critical %N to crop dry weight, $\alpha_{\text{osmo}}$ - species specific correction factor for the
  osmotic effect of growth, $\theta_{\text{osmo}}$ - average soil volumetric water content in the depth of $Z_{\text{osmo}}$, $\rho_s$ - soil bulk density (g cm$^{-3}$), $a_x$, $a_z$ - shape parameters controlling root
  distribution in $x$ and $z$ directions, $ET_0$ - daily reference evapotranspiration (mm), $ET_c$ -
  daily crop evapotranspiration under standard conditions (mm), $f$ - soil fraction not
  covered by plants and exposed to evaporation, $f_{\text{Nmin}}$ - response function for soil
  temperature, $k$ - coefficient for the rate of organic matter oxidation (yr$^{-1}$), $K_1$ - value of
  $W$ at which the rate of increase is half the maximum (t ha$^{-1}$), $K_2$ - growth rate
  coefficient (t ha$^{-1}$ d$^{-1}$), $K_c$ - crop coefficient for calculating evapotranspiration from
  $ET_c$, $K_{c0}$ - basal crop coefficient for transpiration, $K_{c_{\text{max}}}$ - maximum evapotranspiration
  coefficient, $K_e$ - evaporation coefficient, $K_{ri}$ - root growth rate in the corresponding
  direction (m day$^{-1}$ $^\circ\text{C}^{-1}$) ($i = x, z$), $L_0$ - total root length (m m$^{-3}$), $m_C$ - soil organic C
  content (%), $M_{\text{N_{osmo}}}$ - mineral N in the depth of $Z_{\text{osmo}}$ (kg ha$^{-1}$), $N_{\text{min}}$ - daily N
  mineralization rate from soil organic matter (kg ha$^{-1}$), $Q_{10}$ - a factor for correcting
  rates of soil organic matter breakdown for differences in temperature, $R_{CN}$ - C:N ratio
  of the soil organic matter, $R_r$ - rooting width and depth (m) ($i = x, z$), $R_{\text{start}}$ - starting
  rooting width and depth (m) ($i = x, z$), $R_{\text{lax}}$ - coefficient of crop luxury N consumption,
  $R_N$ - reduction coefficient of increment in $W$ due to N deficiency in crop, $R_{\text{osmo}}$ -
reduction coefficient of increment in \( W \) caused by the osmotic pressure, \( t \) - time (d), \( T \) - daily mean air temperature (°C), \( T_{gmax} \) - temperature above which plant growth is the maximum (°C), \( T_{gb} \) - base temperature below which plant does not grow (°C), \( T_{0.5} \) - a half life of soil organic matter (\( y \)), \( T_{lag} \) - threshold of cumulative day degree for root growth (°C d), \( T_s \) - base temperature at which \( f_{Nmin}(t) \) equals 1 (°C), \( T_{soil} \) - daily mean soil temperature (°C), \( U_N \) - potential N uptake (kg ha\(^{-1}\)), \( U_{Nr} \) - potential N demand by fibrous roots (kg ha\(^{-1}\)), \( W \) - dry weight of the entire plant excluding fibrous roots (t ha\(^{-1}\)), \( W_r \) - dry weight of fibrous roots (t ha\(^{-1}\)), \( Z_{osmo} \) - soil depth used in the calculation of mean osmotic pressure (cm), \( Z_{smin} \) - depth of soil below which no N mineralization is assumed to take place (cm), \( \Delta W_r \) - root dry weight increment (t ha\(^{-1}\)).

Key words: simulation, agronomic model, crop response, nitrogen fertilizer, crop growth, SMCR_N

1. Introduction

It is a common feature that agro-ecosystems, like many other ecosystems, receive excessive applications of nitrogen (Schlesinger et al., 2006). This has caused nitrate pollution to surface water (Schlesinger et al., 2006), to groundwater via leaching through soils (Neeteson and Carlton, 2001), and contributed to the rise in N\(_2\)O emissions (Jungkunst et al., 2006). Imbalance in N supply relative to crop demand can also compromise growth and quality of produce. Therefore, it is important to develop effective systems to optimize fertilizer-N application in agricultural systems to maintain sustainable crop production and to minimize the risk to the environment.
The optimum levels of fertilizer-N are controlled by various dynamic factors such as the weather, soil conditions and the N demand for plant growth. It is generally impossible to obtain reliable estimates of optimum N levels by conventional statistical interpretation of a programme of field trials. Attempts have been made to use the knowledge of fundamental processes governing availability and acquisition of nutrient-N in the soil-plant system to devise mechanistic models for various crop species (Bergstrom et al., 1991; Hutson and Wagenet, 1991; Williams et al., 1993; Diekkruger et al., 1995; Jarvis, 1995; Hoogenboom et al., 1999; Brisson et al., 2003; Keating et al., 2003; Jones et al., 2003; Stöckle et al., 2003; van Ittersum et al., 2003; Liang et al., 2007; Rahil and Antonopoulos, 2007). The most prominent individual nutrient response models that cover a range of crops are the EPIC models (Williams et al., 1993; Sharpley and Williams, 1990a, b) and the DSSAT models (Hoogenboom et al., 1999; Jones et al., 2003). EPIC uses a single group of algorithms for simulating more than 20 crops, with each crop having its own unique parameter values. Versions of the model have been used widely to simulate soil-N dynamics on a large scale by many researchers (Huffman et al., 2001). The DSSAT group of models, on the other hand, focussed more on the physiological development of crops, dealing specifically with potential yields and their dependence on the environment. The models used different routines for the various crop types. This group of models includes CERES (Jones and Kiniry, 1986; Wu et al., 1989) for cereals, CROPGRO (Boote et al., 1998) for grain legumes, and SUBSTOR (Ritchie et al., 1995) for root and tuber crops. In all, they cover more than 16 different crops and most have been successfully evaluated in different climatic zones (Huffman et al., 2001). The EPIC and DSSAT models have been used in both basic and applied research to study the effects of climate and management on growth and yield. However, these models are generally species
dependent, and therefore different models are required for different crops to study N response on yield, causing difficulties in the application of model to devise environmentally friendly and sustainable fertilization strategies. Moreover, the required inputs of these models are generally difficult to obtain and the models can be difficult to run due to their complexity.

In order to overcome these problems, a new agronomic model named EU-Rotate_N has been developed for N response of vegetable and arable crops (Rahn et al., 2007). The model inherits some routines used in the N_ABLE (Greenwood et al., 1985; Greenwood and Draycott, 1989a, b; Greenwood et al., 1996) which has been independently tested in different countries (Riley and Guttormsen, 1993; Goodlass et al., 1997; Yang et al., 1999; Huffman et al., 2001; Yang et al., 2002) and served as a key component in the integrated model for N, P and K fertilizers (Zhang et al., 2007), but is much more advanced and more mechanistic in dealing with many soil and plant processes. Compared with other agronomic models, EU-Rotate_N has the advantages of generality, 2-D which is able to simulate N dynamics in the soil domain in the horizontal and vertical directions, utilisation of readily available data, and the ability to simulate crop rotations. The generality of the model was made possible due to the discoveries that both crop critical %N for maximum growth and crop dry matter increments during growth could be described by unified equations (Greenwood et al., 1985). These discoveries have been used in the previous crop N models such as various versions of the N_ABLE (Greenwood, 2001). By setting a pre-defined set of values for each crop, the model used the same algorithm to simulate N responses for different crops. The 2-D nature of the model makes it more accurate in simulating N-economy for row crops. However, although the EU-Rotate_N model is one of the
most innovative models of its kind, it does not properly account for N allocated in
fibrous roots during growth, and is unable to consider the depressive osmotic effect
due to excessive application of fertilizer-N on crop growth and therefore cannot
reproduce some data collected from crop N response experiments (Zhang et al., 2007).
Furthermore, the parametrization of the complex N mineralization routine for release
of soil mineral N could be problematic. To address these problems, a new Simulation
Model for Crop Response to Nitrogen fertilizer (SMCR_N) based on the EU-
Rotate_N is developed in the study.

Agronomic models concern many processes in the crop-soil systems such as plant
growth, N turnover, water and N transfers etc., and therefore systematic validation of
models is difficult due to the lack of appropriate data, especially for the models like
SMCR_N which covers a wide range of crops. Ideally the developed model SMCR_N
requires to be tested against data from field experiments in different climates and soils,
and over a range of crops, which is unfortunately not possible in the study due to the
lack of data. However, we were able to test many features of the new model with a
dataset from field experiments on 16 vegetable crops grown under different fertilizer-
N treatments carried out at Wellesbourne UK (Greenwood et al., 1980). The
advantage of using such a dataset is that the dataset was comprehensive and the
measurements were systematic. The fertilizer-N treatments for each crop spanned
over a wide range from zero fertilizer-N, ensuring the responses of yield and N
composition to fertilizer-N.

The objectives of this study are therefore: 1) to present the SMCR_N model which
rectifies the above-mentioned faults in the EU-Rotate_N model by incorporating
newly developed modules to take account of N-partition into the roots and the osmotic
effect of mineral N in the soil on crop growth, and to devise a simplified algorithm for
calculating N mineralization based on soil organic C content and its C:N ratio and the
half-lives of organic matter in different soils, 2) to rigorously test and validate the
model against a comprehensive dataset collected from 192 sets of measurements
obtained in 32 fertilizer-N field experiments on 16 different vegetable species.

2. Model description

2.1. Model structure

SMCR_N is a comprehensive, dynamic, process-based mechanistic model for the
responses of crop yield and nitrogen composition to fertilizer-N. Here we present a
full description of the new model, which contains some modules from EU-Rotate_N
and the inclusion of improvements. The model comprises various modules simulating
processes in plant, soil and at the plant-soil and plant-atmosphere interfaces. Figure 1
illustrates the diagram of the system showing the flows of material and information
between different modules and the interactions between variables and modules. The
implementation of algorithms in the modules is realized using the programming
language FORTRAN. The soil profile is represented by 5 cm thick layers down to 2 m.
For row crops, the number of horizontal segments in each layer depends on row width,
but there is only a single horizontal segment for crops with row widths below 15 cm.
Soil properties can be assigned in each segment, allowing the change of soil down the
profile. During the simulation all the processes are recalculated for each day. The
algorithms in the major modules are formulated in the following sections.
2.2. Plant growth

Plant growth module consists of two parts, i.e. growth in plant excluding fibrous roots and root growth. This module is inherited from the EU-Rotate_N.

Potential maximum daily increments in dry weight $W$ excluding fibrous roots are calculated by the main growth equation. It defines the growth rate until harvest and was derived from the notion that the interception of radiation increased asymptotically with increase in plant mass per unit area (Greenwood et al., 1977; 1985; Greenwood, 2001). The equation is:

$$\Delta W_t = \frac{K_2 W}{K_1 + W}$$

where $\Delta W$ (t ha$^{-1}$) is the maximum possible increment in growth on the day, $W$ (t ha$^{-1}$) is the dry weight of the entire plant excluding fibrous roots, $t$ (d) is the time, $K_2$ (t ha$^{-1}$ d$^{-1}$) is a growth rate coefficient, and $K_1$ is the semi-maximum $W$ for growth rate. $K_2/K_1$ and $K_2$ approximate to the specific growth rate when $W\rightarrow0$ and to the absolute growth rate when $W\gg0$, respectively. Eq. (1) thus mimics initial exponential followed by near constant growth as $W$ increases. By assuming plant growth is driven by air temperature, integrating Eq. (1) gives:

$$K_2 = \frac{K_1 \ln W_{\text{max}} + W_{\text{max}} - W_0}{\Sigma \text{max}[\min(T, T_{g_{\text{max}}}) - T_{gb}, 0]}$$

(2)
where $W_0$ and $W_{\text{max}}$ are the plant dry weight at planting and at harvest, respectively. $T$ ($^\circ$C) is the daily mean air temperature, $T_{\text{gmax}}$ ($^\circ$C) is the temperature above which the growth rate is at its maximum, and $T_{\text{gb}}$ ($^\circ$C) is the base temperature below which no growth occurs. Eq. (1) with $K_f = 1 \text{ t ha}^{-1}$ gave a good description of sequential measurements of $W$ during growth, under near-optimum conditions, of 18 C3 species during the main growing season in the UK (Greenwood et al., 1977).

The reduction coefficient of increment in plant weight due to N deficiency in crop, $R_N$, is calculated from:

$$R_N = 1 - \min \left( \frac{\%N}{\%N_{\text{crit}}}, 1 \right)$$

(3)

where $\%N$ is the percentage of N in $W$, $\%N_{\text{crit}}$ is the critical $\%N$, i.e. the minimum $\%N$ at which growth proceeds at the maximum rate.

$\%N_{\text{crit}}$ is defined by (Greenwood et al., 1985):

$$\%N_{\text{crit}} = \alpha(1 + \beta e^{-0.26W})$$

(4)

where $\alpha$ and $\beta$ are crop specific parameters that relate critical $\%N$ to crop dry weight.

Some crops are able, when there is much soil mineral N, to take up more N than necessary for maximum growth. In these circumstances, the maximum crop $\%N$ is calculated as follows:
\[
\%N_{\text{max}} = R_{\text{lux}} \%N_{\text{crit}}
\]  
(5)

where \(R_{\text{lux}}\) is the coefficient of crop luxury N consumption.

Root growth simulation is in accordance with that proposed by Pedersen et al. (2007).

The rooting depth and width are calculated based on the cumulative mean day temperature according to:

\[
R_i = \min \{ R_{\text{start}} + \max [0, (\sum T - T_{\text{lag}})K_{ri}], R_{i\text{max}} \} 
\]  
(6)

where \(i = x, z\) stands for the coordinates in the horizontal and vertical directions, \(R_i\) (m) is the rooting width and depth, \(R_{\text{start}}\) (m) is the starting rooting width and depth, \(\sum T\) (°C d) is the cumulative day degree, \(T_{\text{lag}}\) (°C d) is the threshold of cumulative day degree for root growth, \(K_{ri}\) (m day\(^{-1}\) °C\(^{-1}\)) is the root growth rate in the corresponding direction. \(R_{i\text{max}}\) (m) is the maximum rooting depth and width restricted by physical barriers or the effective rooting width (= a half row width) for row crops. Eq. (6), given a proper parameterisation, gives a good description of root penetration of crops observed in a number of studies (Thorup-Kristensen, 1998, 2001, 2006; Thorup-Kristensen & Van den Boogaard, 1998, 1999; Kage et al., 2000; Kristensen & Thorup-Kristensen, 2004).
Crop total root length is calculated as a product of root dry weight and a fixed specific root length. The increment in root dry weight $\Delta W_r$ is a function of the increment in crop dry weight $\Delta W$, crop dry weight $W$, and a parameter defining root class:

$$\Delta W_r = \Delta W \times R_{root}$$

(7)

where $R_{root}$ is the ratio of $\Delta W_r$ to $\Delta W$, which declines with $W$ and varies with the root class parameter as shown in Fig. 2.

The root length declines logarithmically from the soil surface downwards, as originally proposed by Gerwitz and Page (1974), and also logarithmically laterally from the crop row to the inter-row soil. However, different from Gerwitz and Page’s (1974) the module extends the rooting depth by 30% from the calculated penetrating depth where the root density declines from a calculated value at the penetrating depth to zero, i.e.:

$$L(x, z) = \begin{cases} 
L_0 e^{-(a_z a_x z)} & z < R_z \\
L_0 e^{-(a_z a_x z)} (1 - \frac{z - R_z}{0.3R_z}) & R_z \leq z \leq 1.3R_z 
\end{cases}$$

(8)

where $L_0$ (m m$^{-3}$) is the total root length, $a_x$ and $a_z$ are the shape parameters controlling root distribution in $x$ (horizontal) and $z$ (vertical) directions, respectively.

2.3 N and water requirement
In the EU-Rotate_\text{N} there is only one N compartment in crops, and the N partition to the roots is ignored. This fault has been rectified in the SMCR_\text{N}. SMCR_\text{N} assumes that there are two N compartments in crops, a top N compartment and a root N compartment. The top N compartment contains N of the entire plant excluding N in fibrous roots, whereas the root N compartment stores N allocated in fibrous roots. The potential N requirement in the top compartment is calculated from its dry weight, N concentration, the maximum possible concentration for a plant of the same mass and its potential maximum increment in weight, i.e.:

\[
U_N = 10[(W + \Delta W) \times \%N_{\text{max}} - W \times \%N]
\]

where \(U_N\) (kg ha\(^{-1}\)) is the potential N uptake of the entire plant excluding fibrous roots.

The demand of N in the root compartment can be expressed as:

\[
U_{N_r} = 10[(W_r + \Delta W_r) \times \%N_{\text{pot}} - W_r \times \%N_r]
\]

where \(U_{N_r}\) (kg ha\(^{-1}\)) is the potential N demand by fibrous roots, \(W_r\) and \(\Delta W_r\) are the root dry weight on the previous day and the potential root dry weight increment on the day, respectively, \(\%N_r\) is the actual percentage of N in \(W_r\), and \(\%N_{\text{pot}}\) is the root potential \%N, which is calculated from:

\[
\%N_{\text{pot}} = 1 + \beta e^{-0.26W}
\]
Eq. (11) was derived by assuming that the potential %N in the roots decreased with increase in crop dry weight, and the decrease rate followed the same pattern as the critical %N in \( W \). The ratio of critical %N in \( W \) to that in \( W_r \) is \( \alpha \), a parameter in calculating critical %N in \( W \) (Eq. 4) and always greater than 1.0. For crops with large yields, \( \%N_{pot} \) approaches 1% at maturity. The derivation was based on the observations of %N in roots over a number of field crops made by Osaki et al., (1997) that root %N decreased during growth and the %N at maturity ranged from 0.5% to 2.0% with wheat and maize having the value of about 1%.

The potential water demand is the crop evapotranspiration, which is calculated using a FAO 56 crop coefficient method (Allen et al., 1998):

\[
ET_c = K_c ET_0
\]  

(12)

where \( ET_c \) (mm) is the daily crop evapotranspiration under standard conditions, \( K_c \) is the crop coefficient and \( ET_0 \) (mm) is the reference evapotranspiration.

The crop coefficient method partitions the \( K_c \) factor into two separate coefficients:

\[
K_c = K_{cb} + K_e
\]  

(13)

where \( K_{cb} \), dependent on crop species and its development stage, is the basal crop coefficient for transpiration, and \( K_e \) is the soil evaporation coefficient, which is defined as:
\[ K_c = \min(K_{c_{\text{max}}} - K_{c_{\text{cb}}}, fK_{c_{\text{max}}}) \]  

where \( K_{c_{\text{max}}} \) is the maximum evapotranspiration coefficient, and \( f \) is the soil fraction not covered by plants and exposed to evaporation, i.e. the fraction of soil surface from which most evaporation occurs. The parameter values of \( ET_0, K_{c_{\text{cb}}, K_{c_{\text{max}}} \text{ and } f} \) can be determined according to Allen et al. (1998).

2.4. \textit{N} mineralization from soil organic matter

In the EU-Rotate_N, N release from soil organic matter, added crop residues and organic fertilizers to the soil is calculated based on the N mineralization routines in the DAISY model (Hansen et al., 1990). The latter is a sophisticated module for C dynamics in the soil that includes separate equations for the metabolism of different pools of soil organic matter, soil microbial dry weight and added organic matter. Unfortunately, not all this information was measured in the field experimental data to test the validity of the module. In the SMCR_N model an alternative simplified algorithm was therefore devised for calculating N mineralization rates. It required inputs of the average yearly half-life of soil organic matter, the organic C content and C:N ratio.

Assume the organic matter breakdown rate is in first-order, i.e.:

\[ \frac{dm_c}{dt} = -km_c \]
where $m_C$ (g g$^{-1}$) is the organic C content, and $k$ (yr$^{-1}$) is a coefficient for the rate of organic matter oxidation.

From Eq. (15) the relationship between a half life and the breakdown rate $k$ is:

$$kT_{0.5} = -\ln(0.5) \quad (16)$$

where $T_{0.5}$ (yr) is the average half life over an entire year.

Both soil temperature and soil water content influence N mineralization from soil organic matter (Johnsson et al., 1987). However compared to the soil moisture, soil temperature has a dominant effect on N mineralization in many soils cropped with field vegetables and arable crops as these are usually irrigated as required. In this study we considered that soil N mineralization was controlled solely by soil temperature.

A $Q_{10}$ relationship is used to express the effect of temperature (Bunnell et al., 1977; Johnsson et al., 1987):

$$f_{N_{min}}(t) = Q_{10}^{\frac{\text{T}_{\text{soil}(z)} - T_s}{10}} \quad (17)$$

where $f_{N_{min}}(t)$ is the response function for soil temperature, $T_{\text{soil}(z)}$ is the soil temperature at the soil depth $z$, $T_s$ ($^\circ$C) is the base temperature at which $f_{N_{min}}(t)$ equals 1, and $Q_{10}$ is the factor change in rate with a 10 degree change in temperature.
Thus, provided the half life of organic matter breakdown is known, the daily N
mineralization from soil organic matter can be calculated:

\[
N_{s\min} = \frac{k}{365} \sum f_{N\min}(t) \rho_s Z_{s\min} m_{s} \times 10^5
\]  

(18)

where \(N_{s\min}\) (kg ha\(^{-1}\)) is the daily N mineralization rate from soil organic matter, \(\rho_s\) (g cm\(^{-3}\)) is the soil bulk density, \(Z_{s\min}\) (cm) is the soil depth where N mineralization takes
place, and \(R_{CN}\) is the C:N ratio of the soil organic matter.

2.5. Effect of osmotic pressure on crop growth

To consider the negative osmotic effect caused by mineral N in the soil on crop
growth, a growth reduction coefficient \(R_{osmo}\) is introduced by modifying Zhang et al.
(2007):

\[
R_{osmo} = 1 - \alpha_{osmo}K_r
\]  

(19)

where \(\alpha_{osmo}\) is the species specific correction factor for the osmotic effect of growth, 
\(\alpha_{osmo}K_r\) is the reduction in the daily increment caused by the osmotic pressure, which
is defined by the following equation:

\[
K_r = \frac{1}{6.73} \times 1.5 \times 273 \times 8.27 \times \frac{M_{N_{osmo}}}{\theta_{osmo}Z_{osmo}} = 1.6 \times 10^{-3} \frac{M_{N_{osmo}}}{\theta_{osmo}Z_{osmo}}
\]  

(20)
in which $Z_{\text{osmo}}$ (cm) is the soil depth where the osmotic pressure induced by mineral N is considered, $M_{N_{\text{osmo}}}$ (kg ha$^{-1}$) is the mineral N in the depth of $Z_{\text{osmo}}$, $\theta_{\text{osmo}}$ is the average soil volumetric water content in the depth of $Z_{\text{osmo}}$ (30 cm). The equation was derived by considering that NH$_4$NO$_3$ was incorporated in the upper 30 cm from the surface and was immediately nitrified and converted into NO$_3^-$. As in standard theory each gram mole ion per litre of soil solution increased the osmotic pressure by 8.27 (kPa) × the absolute temperature, (273 K); no correction was made for differences in temperature. It was assumed that $K_r$ equalled the ratio of osmotic pressure in 6.73 kPa and that $K_r = 1$ when the ratio $\geq 1$ (Kramer, 1949; Mengel and Kirkby, 2001).

2.6. Root N and water uptake and evaporation

Root N uptake is calculated as a function of crop N demand, root length, the soil mineral N concentration, and the minimum soil mineral N concentration for uptake, as proposed by Pedersen et al. (2007). Root water uptake is simulated using the FAO approach (Allen et al., 1998). The uptake is at its potential rate when volumetric soil water in the rooting depth is above or equals a crop specific critical value. When soil water is below the critical value, the transpiration decreases linearly with decrease in soil water content until it ceases when the soil water content corresponds to a threshold value. Both the critical and the threshold values can be estimated by the FAO procedure (Allen et al., 1998). Evaporation from the top soil whose depth varied with soil type according to Allen et al. (1998) was computed using the approach proposed by Brisson and Perrier (1991) and Brisson et al. (1998; 2003).
2.7. Soil water and N movement

The simulations of soil water and N movement are the same as those in the EU-Rotate_N. Soil water movement and N transport were simulated with a cascade model, similar to that proposed by Ritchie (1998). Soil profiles were divided into layers. Infiltration, the difference between precipitation and potential evaporation, moved into the soil profile where it was routed through the soil layers. A drainage coefficient, which was calculated as the ratio of the difference between soil water content at saturation and field capacity to soil water content at saturation, was used to predict flow through each soil layer, with flow occurring when a layer exceeded field capacity. The proportion of nitrate transported from a soil layer was considered to be identical to the ratio of water drainage out of the layer to the total water in the layer. Diffusion terms for N transport in the soil were not included in the simulation.

2.8. Model inputs

The inputs for running the SMCR_N model include site characteristics, weather data, soil properties, and cropping parameters together with the initial conditions, i.e.

- Site properties: altitude and latitude of the site.
- Weather data: air temperature, radiation, rainfall, relative humidity and wind speed.
- Soil properties: bulk density, volumetric soil water content at saturation, field capacity and the permanent wilting point, soil organic C content, CN ratio, half-life of soil organic matter, and the depth from the soil surface of any
• Initial conditions: volumetric soil water content and mineral N concentration distributions in the soil profile and dates of measurement.
• Fertilization and irrigation: dates and amounts of fertilizer-N and irrigation applied.
• Crop data: species, spacings, sowing/planting and harvest dates, crop dry weight at planting, expected maximum crop dry weight excluding fibrous roots.

3. Experiments and parameter setting

3.1 Experimental set-up

The validity of the model SMCR_N was tested against a comprehensive dataset of the yield and N composition from historical field experiments on various crops at Wellesbourne, UK. Sixteen crops were grown in 32 fertilizer-N experiments during the period 1970-1975 on the same field: Big Ground of the National Vegetable Research Station, now Warwick-HRI (Greenwood et al., 1980). The soil was a sandy loam of the Wick series and is described in Whitfield (1974). The experiments followed the same general pattern. Six fertilizer-N treatments from N0 (the zero fertilizer-N) to N5 (the highest fertilizer-N) were tested in each crop. There were three plots in each fertilizer-N treatment, all with the expected optimum levels of P and K. In each plot there were three blocks or replicates. The plots were laid out systematically in order of fertilizer application. The direction of increase in fertilizer-N was chosen at random. The entire plant material excluding fibrous roots was
removed from each block and weighed at commercial maturity. All the plant material
from three plots with the same fertilizer-N treatment was bulked together and treated
as one sample. The dry weight and the N composition in the plant were then
determined. The dates of sowing and harvest and the levels of fertilizer-N for each of
the experiments are summarised in Table 1. Detailed description of the experiments
can be seen elsewhere (Greenwood et al., 1980).

3.2. Parameter setting

N-nutritional characteristics that are defined in terms of parameters $\alpha$, $\beta$ (Eq. 4) that
relate $\%N_{\text{crit}}$ to $W$ and $R_{\text{lux}}$ (Eq. 5) for each of the crops are given in Table 2. Also in
the table are the parameter values for calculating root development and estimating
potential evapotranspiration. It was assumed that the root distribution in the soil depth
is the same as that in the horizontal direction for row crops, thus $a_x$ and $a_z$ were set the
same value.

At the time of planting the estimated distributions of mineral N were 30 kg N ha$^{-1}$ in
the 0-30 cm layer, 15 kg N ha$^{-1}$ in 30-60 cm layer, and 5 kg N ha$^{-1}$ in the 60-90 cm
layer (Zhang et al., 2007). The soil bulk density was 1.4 g cm$^{-3}$, and the volumetric
water content at saturation, field capacity and the permanent wilting point were 0.45,
0.26 and 0.1 cm$^3$ cm$^{-3}$ (Zhang et al., 2007), respectively. As the soil moisture was not
measured at the time of planting, the soil water distribution in the profile at planting
was calculated by running the model from 1 January of the planting year when the soil
water deficit was assumed to be zero. For the exercise of model validation, the
maximum yield, obtained from the experiment on a crop grown at various fertilizer-N
on the same year, was taken to be the required input of maximum plant dry weight at harvest. However, if the model is used for prediction purposes, the maximum yield should be estimated independently based on previous experience or other measures. The minimum soil mineral N level below which plants were not able to take up N was set 0.0035 kg m\(^{-3}\), and the species specific correction factor for the osmotic effect of growth was set 1.0 for all crops. Broad bean and pea differed from other crops in that they were able to fix atmospheric-N in these experiments when N supply from the soil was limited, although it was recognised that this ability was dependent on the presence of suitable strains of Rhizobium in soil.

The organic matter breakdown rate \(k\) was calculated as 0.0185 yr\(^{-1}\) using Eq. (16) based on an estimated half life of 37.5 years, which is close to the turnover rate for resistant C of 0.02 yr\(^{-1}\) used in Fang et al. (2005), and similar with those used in other models (Mueller et al., 1996; Fu et al. 2000). Also used in the simulations are the measured organic C content of 0.9% (Costigan et al., 1983) and C:N ratio of 10 which is the approximate value for top soil of most arable soils (Nieder et al., 2003). A value of 3 was used for \(Q_{10}\) (Hansen et al., 1990). The base temperature, \(T_b\), at which the response function for soil temperature on N mineralization equals 1, was set 20 °C (Hansen et al., 1990). It was further assumed that soil N mineralization was restricted to the upper 30cm depth of soil.

4. Evaluation criteria

The evaluation criteria used in the study were similar with those described previously by Greenwood et al. (2001) and Zhang et al. (2007). If \(Y\) is the value predicted by the
model and \( y \) is the experimentally determined treatment mean then \( Y \) may be a good predictor either absolutely or after a both shift and scale change i.e. \( a + bY \).

The discrepancies in both cases are:

\[
D_1 = \frac{\sum(y - Y)^2}{K} \quad (21)
\]

\[
D_2 = \frac{\sum(y - a - bY)^2}{(K - 2)} \quad (22)
\]

where \( K \) is the number of comparisons, and

\[
a = \bar{y} - b\bar{Y}^2 \quad (23)
\]

\[
b = \frac{\sum y(Y - \bar{Y})}{\sum(Y - \bar{Y})^2} \quad (24)
\]

where \( \bar{y} \) and \( \bar{Y} \) are the average measurements and predictions.

These values were compared with the residual variance of \( y \) after removal of the block and treatment effects in an analysis of variance. The variance ratio test was applied. If the values were not significantly different at \( P < 0.05 \), the residual variance from \( D_1 \) and \( D_2 \) was attributed to experimental error.

5. Results

Simulated values of plant %N were almost proportional to the measured values for all 192 combinations of crops and fertilizer levels (Fig. 3). The model gave good
predictions of both $W$ and $\%N$ for some crops over the whole range of fertilizer levels as illustrated for turnip, summer cabbage, parsnip, potato, radish and spinach, in Fig. 4. Figure 5 compares the measured responses of plant $W$ to fertilizer-N for summer cabbage 70 and sugar beet 73 with the simulated values from the EU-Rotate_N and the SMCR_N models. A much better agreement was observed between measurement and simulation from the SMCR_N model for both cases, illustrating that the SMCR_N model performs better than the EU-Rotate_N model.

Statistical comparison was carried out between the measured and simulated $W$ and $\%N$ for 13 out 16 crops (Table 3). No attempt of statistical analysis was made for the other 3 crops due to lack of degree of freedom resulting from the crops grown only in a single year. The discrepancies between the simulated and measured $W$ at zero fertilizer-N which was crucial to test the model were less than 20% for 9 out of 13 crops (Table 3). If the ratio of $D_1$ or $D_2$ to the residual variance in Table 3 is not significant at $P < 0.05$ by the variance ratio test, all the discrepancies can be explained by experimental error (Greenwood et al., 2001; Zhang et al., 2007). Thus, it can be concluded that there was no significant difference between the measured and simulated values of $W$ for turnip and of $\%N$ for lettuce, as the ratio of $D_1$ to the residual variance was not significant at $P < 0.05$. The linear relationship between measured and simulated values of $\%N$ for winter cabbage accounted for the discrepancies between measurement and simulation, as the ratio of $D_2$ to the residual variance was not significant at $P < 0.05$.

Since the maximum dry weight yield was obtained from the experiment on a crop grown at various fertilizer-N, it is important to test the model’s ability to predict yield
reduction caused by either the lack of N supply to maintain the maximum growth or
the depressive effect of osmotic pressure on growth induced by excessive application
of fertilizer-N. All the crops were grown under a wide range of fertilizer-N treatments,
i.e. from zero fertilizer-N (N0) to the maximum fertilizer-N level (N5), to ensure that
crops grew under the conditions which varied from the deficit to the excessive N
supply. We grouped fertilizer-N treatments from N0 to N5 for all the crops for testing
the response of crop $W$ to fertilizer-N, although the grouping was somewhat arbitrary
since the fertilizer-N levels were not related to N requirement for optimal growth for a
given crop. Nevertheless, it could provide useful information for the assessment of the
model’s ability to simulate the response of crop $W$ to different fertilizer-N
management. Figure 6 compares the measured and simulated $W$ for each crop at
different fertilizer-N levels normalised by the maximum dry weight among all the
treatments. The correlations between the measured and simulated $W$ were fairly good
at the zero fertilizer-N level (N0) and relatively weak at a low fertilizer-N level (N1).
Also, at the N1 level the model appeared to over-predict yield. The simulated $W$ was
in good agreement with the measured values at the middle (sub-optimum) fertilizer-N
levels (N2 and N3). At the two highest fertilizer-N levels (N4 and N5), the measured
and simulated values spread over wider ranges and the correlations were weak.
However, better correlations were observed by excluding salt sensitive crops of carrot,
broad bean, pea and onion (McKenzie, 1988).

The simulated ratios of N contained in the plant excluding fibrous roots to that in the
whole plant including fibrous roots for different crops grown at sub-optimal N levels
crops are plotted in Fig. 7(a). The ratio, varying with crop species, ranged from 0.77
for crops with small yields to 0.93 for crops with big yields. The ratio calculated in
the study was correlated with a ‘recovery factor’ fairly well (Fig. 7b). The recovery
factor was obtained by plotting crop N uptake against fertilizer-N and determining the
gradient at near zero application for crops grown under conditions where there was no
leaching (Greenwood et al., 1989). The measured recovery factor includes effects of
loss of mineral by biological process such as denitrification which the simulated ratio
did not. When fertilizer-N was over applied, crop yields declined linearly with
increase in fertilizer-N (Fig. 8) as calculated using Eq. (19), and percentage reductions
in yield were greater for crops having a low than a high yield. For example, 300 kg-N
ha\(^{-1}\) depressed yield by 27% for radish but only about 16% for red beet, respectively.

Figure 9 shows how the osmotic correction factor \(\alpha_{osmo}\) affects carrot yield. Increasing
the correction factor value increases the depressive effect on crop yield. For the
default value set in the model, i.e. \(\alpha_{osmo} = 1\), an excessive application of 250 kg-N ha\(^{-1}\)
resulted in yield reduction by about 12%, whereas the reduction increased to 27% if
the correction factor was doubled. For carrots (Fig. 9a), \(\alpha_{osmo} = 2\) appeared more
appropriate than the default value of 1 in the model. Figure 9(b) shows the normalised
dry weight between the measured and simulated values for all the crops at two highest
fertilizer-N levels where the osmotic correction factor was set \(\alpha_{osmo} = 2\) for the salt
sensitive crops of carrot, pea and onion. This correction results in much better
agreement between the measured and simulated values of normalised \(W\) than was
obtained with the default value of \(\alpha_{osmo} = 1\) for all crops given in Fig. 6 (e)(f).

The simulated estimates of cumulative N mineralized from soil organic matter are
plotted against time in Fig. 10(a) for years 1973 and 1975; they were calculated
assuming that they were dominated either by measured mean daily soil or air
temperature. The differences between the simulated cumulative mineralization of N using each of the two types of temperature were always less than 7%. Inter-year differences were also small between 1973 and 1975. Figure 10(b) shows that there is a strong correlation between the measured temperature in top 30 cm soil and air temperature. The best regression lines for 1973 and 1975 are close to the 1:1 line.

6. Discussion

6.1. Model general performance and its comparison with EU-Rotate_N

The comparisons between the measured and simulated variables were made without any adjustment of parameter values to improve the degree of agreement. Nevertheless there was, with few exceptions, good agreement between the measured and simulated values of %N and of $W$ for each of the 16 crops over the practical range of fertilizer applications, which indicates that the model was properly constructed and calibrated and that the key modules worked well.

It can also be seen that the newly developed model SMCR_N performed much better in simulating the responses of crop $W$ to fertilizer-N than the EU-Rotate_N as illustrated in Fig. 5. It appears that both models produced approximately the same results for the positive effect of fertilizer-N on crop $W$. However, there is a fault in accounting for N in the soil-crop system in the EU-Rotate_N. The model does not account for N partitioned in the roots, and this means that crop requires less N for growth. If this factor had been accounted for properly, the performance of the EU-
Rotate\_N would have been less satisfactory even for the positive effect of fertilizer-N on crop $W$.

6.2. Mechanistic account of fractional recovery of fertilizer-N by crop

The routine for calculating the root N content is an important feature of the model. The ratio of the N content of the plant excluding fibrous roots to the N content of the plant including fibrous roots at sub-optimal levels of N for the different crops was strongly correlated with an independent measure of the recovery of fertilizer-N (Fig. 7b) (Greenwood et al., 1989). Moreover, the ratio was close to the recovery for crops with large yields, whereas it was generally lower than the recovery for small crops. The recovery was obtained by plotting N uptake at harvest against the fertilizer-N level and determining the gradient when the fertilizer level tended to zero. The discrepancies between the ratio and the recovery for small crops might be due to the fact that the lateral distribution of mineral N in the soil was not considered in determining recovery. For a small crop even grown under a low fertilizer-N, a significant amount of mineral N could be left at harvest due to failure of the crop to fully explore the inter row soil and extract mineral N from it. The recovery also assumed that there was no loss of mineral N through soil processes such as denitrification. The model assumes that the entire disappearance of fertilizer-N, excluding that lost by leaching, could be accounted for by uptake in the roots and in the remainder of the plant. Yet with this assumption the model gave good predictions of $W$, its %N content and the ratio in good agreement the recovery for crops with big yields. It therefore appears that N losses from low levels of fertilizer-N through soil processes such as denitrification, ammonia volatilization and ammonia fixation were
small. Though small, they may explain why the predicted values of $W$ for some crops are higher than the measured ones at level N1.

6.3. Mechanistic account of depressive osmotic effect on yield

Excessive application of fertilizer-N can cause negative osmotic effect on crop growth (Kramer, 1949; Mengel and Kirkby, 2001) and pollute the environment (Neeteson and Carlton, 2001). There are also limits for acceptable nitrate content for some crops such as lettuce and spinach set by EC legislation (EC, 2006). Although the effect can be qualitatively considered (Mengel and Kirkby, 2001), it is seldom included in most agronomic models, which makes the models unable to explain some measured results from crop N response experiments as shown in the study and in Zhang et al. (2007).

Good agreement between the simulated osmotic effect on yield for 12 out of 16 crops studied using the proposed approach and measurement indicates that soil mineral N in the top 30 cm, despite different rooting depths and root distributions resulting from different crops, exerts predominant effect on crop yield and the proposed approach to quantify the osmotic effect on growth with the value of the correction factor of 1 works well for most crops. The effect is linearly related to the excessive amount of fertilizer-N (Fig. 8). Nevertheless, salinity tolerance varies with crop species (McKenzie, 1988).

It is clear that the model with the osmotic correction factor of 1 did not work satisfactorily for the salt sensitive crops. The possibility of using the proposed approach with a different value for the correction factor for different crops to simulate
the osmotic effect was therefore explored. It appeared that a correction factor value of 2 for a low salt tolerant crop was more appropriate than 1 (Fig. 9). This underlines the possibility of improving the model by taking account of inter species differences in tolerance to salinity. Finally it should be pointed out that the osmotic effect on crop yield is a complex issue. The effect is not only dependent on crop species, but also on the soil since soil characteristics such as internal drainage play an important role in controlling soil salinity levels (Le Roux et al., 2007). Although the proposed approach of quantifying the osmotic effect on yield works reasonably well for the sandy loam soil used in the study, the adaptability of the devised equation and parameterisation for other soils such as the clay soil could be a subject of further investigation.

6.4. Evidence of satisfactory N mineralization routine for release of soil mineral N

Rigorous validation of the N mineralization routine was not possible in the study as the soil mineral N concentration was not directly measured in the experiments. However the indirect assessment of the performance of the routine can be carried out based on the following facts. Firstly the relationship between measured and simulated values of $W$ when fertilizer-N was withheld (Figs. 4 and 6) was near proportional. Secondly the measured %N (Figs. 3 and 4) was nearly 1:1 to the simulated values. This, together with the first point, indicates that prediction of crop N uptakes from the endogenous soil mineral N, was simulated correctly. Thirdly the model simulated that the unfertilized crops reduced soil inorganic N to around 10 kg N ha$^{-1}$ in the top 0.3 m of the soil, in agreement with the previous studies (Thorup-Kristensen and Sørensen, 1999; Thorup-Kristensen, 2006), suggesting that the minimum level of soil mineral N from which plant roots can extract mineral N was set correctly for most crops. Finally,
the simulated N leaching at 90 cm soil depth was small during crop growth, ranging from 0 to 2.5 kg-N ha$^{-1}$, which was supported by the previous study that N leaching mainly occurred from late autumn to early spring on the Western European soils, out of growing periods for most of crops (Neeteson and Carton, 2001). Based on these lines of evidence, it is clear that the mineral N input from soil organic matter into the crop-soil systems during growth was properly accounted for, and therefore it could be concluded that the proposed algorithm for N mineralization from soil organic matter worked reasonably well for this sandy loam arable soil.

It was found that when the soil temperature is not available, air temperature can be used instead without great loss of accuracy of estimating soil N mineralization (Fig. 10a) since the soil temperature in the top 30 cm depth is almost 1:1 related to the air temperature (Fig. 10b). This implies that in agronomic models the simulation of soil temperature might not be essential. Simulation of soil temperature concerns many complex processes such as heat transfer, moisture movement and water movement to the surface, and some of these processes are closely related to each other. Accurately modelling soil temperature has been proven extremely difficult (Akinyemi and Mendes, 2007).

7. Conclusions

A new generic model SMCR$_N$ for nitrogen response on yield and N composition for vegetable and arable crops has been developed. The model gave predictions of the responses of crop dry weight $W$ and its %N to fertilizer-N that with few exceptions were in close agreement with the measured values over the practical range of fertilizer
applications. This suggests that the model framework and the major modules
including newly developed ones for N allocation in roots, the depressive effect of
excessive fertilizer-N application on crop yield and the simplified N mineralization
algorithm for release of soil mineral N work reasonably well. Therefore, the
SMCR_N model can be used as a platform for optimizing fertilizer-N application in
crop production.

It was also found that to properly address the depressive effect of fertilizer-N on yield
the coefficient defining the osmotic component of fertilizer-N response varied with
the crop species. A coefficient of 2 worked well with salt sensitive species, whereas a
smaller value of 1 was appropriate for the other crops. For the different species grown
at a near optimum level of fertilizer-N, the ratio of N in the plant excluding fibrous
roots to that in the plant including fibrous roots was strongly correlated with previous
measurements of the N-recovery by the crop. As the model assumed that entire loss of
inorganic N resulted from incorporation of N into the whole plant including fibrous
roots, and there was good agreement between the measured and simulated N uptakes,
it follows that for this soil, losses of N from processes such as denitrification,
ammonia volatilization, and ammonia fixation in clay lattices were small.

The future work includes the further development of the EU-Rotate_N with the
obtained improvements in the study. Opportunities also exist to enhance the
performance of the SMCR_N model in predicting N leaching by replacing the current
cascade type algorithm for soil water movement with the one developed by Yang et al.
(2009) which, using an integration strategy on the basic flow equation, is simple and
highly accurate in hydrological simulations.
Acknowledgements

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References


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Table 1: Experimental details

<table>
<thead>
<tr>
<th>Crop</th>
<th>Sowing/planting date</th>
<th>Harvest date</th>
<th>Fertilizer rate (kg N ha(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Broad bean 72</td>
<td>26/04/72</td>
<td>10/08/72</td>
<td>0, 56, 140, 224, 308, 392</td>
</tr>
<tr>
<td>Broad bean 73</td>
<td>13/03/72</td>
<td>19/06/72</td>
<td>0, 56, 140, 224, 308, 392</td>
</tr>
<tr>
<td>Carrot 70</td>
<td>05/05/70</td>
<td>28/09/70</td>
<td>0, 56, 140, 224, 308, 392</td>
</tr>
<tr>
<td>Leek 70</td>
<td>29/04/70</td>
<td>09/11/70</td>
<td>0, 90, 224, 359, 493, 628</td>
</tr>
<tr>
<td>Leek 71</td>
<td>02/04/71</td>
<td>11/11/71</td>
<td>0, 90, 224, 359, 493, 628</td>
</tr>
<tr>
<td>Lettuce 70</td>
<td>15/06/70</td>
<td>07/08/70</td>
<td>0, 56, 140, 224, 308, 392</td>
</tr>
<tr>
<td>Lettuce 75</td>
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<td>20/08/75</td>
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<tr>
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<td>29/04/70</td>
<td>01/09/70</td>
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<td>Potato 73</td>
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<td>0, 67, 168, 269, 370, 471</td>
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</tr>
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<td>20/05/70</td>
<td>18/08/70</td>
<td>0, 90, 224, 359, 493, 628</td>
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<td>28/09/71</td>
<td>0, 90, 224, 359, 493, 628</td>
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<td>04/10/72</td>
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<td>26/09/73</td>
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<td>07/07/71</td>
<td>0, 90, 224, 359, 493, 628</td>
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<td>Turnip 72</td>
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<tr>
<td>Winter cabbage 72</td>
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</tr>
</tbody>
</table>

\(^a\) two digits in the crop names represent the year of experiment, for example 72 stands for year 1972.
Table 2: Crop parameter values used in the simulations

<table>
<thead>
<tr>
<th>Crop</th>
<th>N fixation</th>
<th>( \alpha )</th>
<th>( \beta )</th>
<th>( R_{lux} )</th>
<th>( T_{lag} )</th>
<th>( K_{rz} )</th>
<th>( a_z )</th>
<th>Root class</th>
<th>( K_{cb} )</th>
</tr>
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<tbody>
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<td></td>
<td></td>
<td>(day ( ^{\circ} )C)</td>
<td>(m day(^{-1}) ( ^{\circ} )C(^{-1}))</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Initial stage</td>
<td>Middle stage</td>
</tr>
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<td>Yes</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>100</td>
<td>0.0007</td>
<td>3</td>
<td>1</td>
<td>0.15</td>
</tr>
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<td>1.1</td>
<td>1</td>
<td>100</td>
<td>0.001</td>
<td>2</td>
<td>1</td>
<td>0.15</td>
</tr>
<tr>
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<td>1.1</td>
<td>1</td>
<td>100</td>
<td>0.001</td>
<td>1.5</td>
<td>2</td>
<td>0.15</td>
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<td>1.26</td>
<td>1.5</td>
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<td>0.0007</td>
<td>3</td>
<td>1</td>
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<tr>
<td>Leek</td>
<td>No</td>
<td>1.35</td>
<td>1.77</td>
<td>1.2</td>
<td>350</td>
<td>0.0003</td>
<td>8</td>
<td>2</td>
<td>0.15</td>
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<tr>
<td>Lettuce</td>
<td>No</td>
<td>1.35</td>
<td>1.35</td>
<td>1</td>
<td>100</td>
<td>0.001</td>
<td>3</td>
<td>1</td>
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<tr>
<td>Onion</td>
<td>No</td>
<td>1.35</td>
<td>2.42</td>
<td>1</td>
<td>250</td>
<td>0.0003</td>
<td>8</td>
<td>2</td>
<td>0.15</td>
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<td>Parsnip</td>
<td>No</td>
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<td>1.26</td>
<td>1</td>
<td>250</td>
<td>0.0007</td>
<td>3</td>
<td>1</td>
<td>0.15</td>
</tr>
<tr>
<td>Potato</td>
<td>No</td>
<td>1.35</td>
<td>3</td>
<td>1</td>
<td>100</td>
<td>0.0007</td>
<td>3</td>
<td>1</td>
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<td>Radish</td>
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<td>1.87</td>
<td>1.2</td>
<td>100</td>
<td>0.001</td>
<td>3</td>
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<td>Red beet</td>
<td>No</td>
<td>1.53</td>
<td>3</td>
<td>1.35</td>
<td>250</td>
<td>0.001</td>
<td>2</td>
<td>1</td>
<td>0.15</td>
</tr>
<tr>
<td>Spinach</td>
<td>No</td>
<td>1.35</td>
<td>3</td>
<td>1</td>
<td>100</td>
<td>0.001</td>
<td>3</td>
<td>1</td>
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<tr>
<td>Sugar beet</td>
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<td>1.11</td>
<td>1.38</td>
<td>1.65</td>
<td>250</td>
<td>0.001</td>
<td>2</td>
<td>1</td>
<td>0.15</td>
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<tr>
<td>Swede</td>
<td>No</td>
<td>1.35</td>
<td>3</td>
<td>2</td>
<td>100</td>
<td>0.001</td>
<td>1.5</td>
<td>1</td>
<td>0.15</td>
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<td>Turnip</td>
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<td>0.001</td>
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<tr>
<td>Peas</td>
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<td>100</td>
<td>0.001</td>
<td>3</td>
<td>1</td>
<td>0.15</td>
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</table>

\(^{2}\) \( \alpha \) and \( \beta \) are the parameters which relate critical \( \% \)N to crop dry weight.
\(^{3}\) \( R_{lux} \) is the luxury N consumption coefficient.
\(^{4}\) \( T_{lag} \) (\(^{\circ} \)C d) is the threshold of cumulative day degree for root growth.
\(^{5}\) \( K_{rz} \) is the vertical root growth rate.
\(^{6}\) \( a_z \) is the shape parameter controlling root distribution in the soil depth.
\(^{7}\) \( K_{cb} \) is the basal crop coefficient for transpiration.
Table 3: Statistical comparison between measured and simulated crop DW yield and %N

<table>
<thead>
<tr>
<th>Crop</th>
<th>Range</th>
<th>Simulated</th>
<th>Measured</th>
<th>$D_1^a$</th>
<th>$D_2^a$</th>
<th>$d.f.$ for $D_1$</th>
<th>Residual variance$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Broad bean</td>
<td>W (t ha$^{-1}$)</td>
<td>5.29 - 7.07</td>
<td>5.22 - 7.3</td>
<td>0.82</td>
<td>0.53</td>
<td>12</td>
<td>0.200</td>
</tr>
<tr>
<td></td>
<td>%N</td>
<td>2.59 - 3.5</td>
<td>2.62 - 3.58</td>
<td>0.23</td>
<td>0.11</td>
<td>12</td>
<td>0.013</td>
</tr>
<tr>
<td>Leek</td>
<td>W (t ha$^{-1}$)</td>
<td>5.13 - 16.6</td>
<td>9.62 - 16.82</td>
<td>5.63</td>
<td>3.90</td>
<td>12</td>
<td>0.711</td>
</tr>
<tr>
<td></td>
<td>%N</td>
<td>0.73 - 1.9</td>
<td>0.99 - 2.06</td>
<td>0.06</td>
<td>0.05</td>
<td>12</td>
<td>0.018</td>
</tr>
<tr>
<td>Lettuce</td>
<td>W (t ha$^{-1}$)</td>
<td>1.1 - 2.92</td>
<td>0.93 - 2.63</td>
<td>0.15</td>
<td>0.14</td>
<td>12</td>
<td>0.009</td>
</tr>
<tr>
<td></td>
<td>%N</td>
<td>1.59 - 2.72</td>
<td>1.72 - 2.81</td>
<td>0.01$^*$</td>
<td>0.01$^*$</td>
<td>12</td>
<td>0.026</td>
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<tr>
<td>Onion</td>
<td>%N</td>
<td>3.36 - 6.7</td>
<td>2.28 - 6.29</td>
<td>1.56</td>
<td>1.29</td>
<td>12</td>
<td>0.133</td>
</tr>
<tr>
<td>Parsnip</td>
<td>W (t ha$^{-1}$)</td>
<td>5.84 - 9.91</td>
<td>6.09 - 9.35</td>
<td>0.84</td>
<td>0.57</td>
<td>12</td>
<td>0.297</td>
</tr>
<tr>
<td></td>
<td>%N</td>
<td>1.04 - 1.72</td>
<td>0.96 - 2.3</td>
<td>0.09</td>
<td>0.09</td>
<td>12</td>
<td>0.036</td>
</tr>
<tr>
<td>Potato</td>
<td>W (t ha$^{-1}$)</td>
<td>3.55 - 12.7</td>
<td>3.46 - 13.21</td>
<td>3.47</td>
<td>3.38</td>
<td>12</td>
<td>0.174</td>
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<tr>
<td></td>
<td>%N</td>
<td>0.89 - 2.68</td>
<td>0.37 - 2.55</td>
<td>0.36</td>
<td>0.18</td>
<td>12</td>
<td>0.038</td>
</tr>
<tr>
<td>Radish</td>
<td>W (t ha$^{-1}$)</td>
<td>0.43 - 1.48</td>
<td>0.62 - 1.32</td>
<td>0.03</td>
<td>0.01</td>
<td>12</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>%N</td>
<td>1.99 - 4.33</td>
<td>2.75 - 4.42</td>
<td>0.19</td>
<td>0.13</td>
<td>12</td>
<td>0.043</td>
</tr>
<tr>
<td>Red beet</td>
<td>W (t ha$^{-1}$)</td>
<td>4.25 - 13.3</td>
<td>5.28 - 13.46</td>
<td>3.16</td>
<td>2.98</td>
<td>12</td>
<td>0.415</td>
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<tr>
<td></td>
<td>%N</td>
<td>1.09 - 2.71</td>
<td>1.25 - 2.7</td>
<td>0.05</td>
<td>0.05</td>
<td>12</td>
<td>0.007</td>
</tr>
<tr>
<td>Sugar beet</td>
<td>W (t ha$^{-1}$)</td>
<td>10.5 - 20.3</td>
<td>9.77 - 20.65</td>
<td>3.78</td>
<td>3.82</td>
<td>12</td>
<td>0.608</td>
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<tr>
<td></td>
<td>%N</td>
<td>0.62 - 1.92</td>
<td>0.81 - 1.82</td>
<td>0.19</td>
<td>0.06</td>
<td>12</td>
<td>0.011</td>
</tr>
<tr>
<td>Spinach</td>
<td>W (t ha$^{-1}$)</td>
<td>0.8 - 2.92</td>
<td>0.86 - 2.83</td>
<td>0.06</td>
<td>0.06</td>
<td>12</td>
<td>0.012</td>
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<tr>
<td></td>
<td>%N</td>
<td>1.8 - 4.64</td>
<td>2.14 - 4.7</td>
<td>0.47</td>
<td>0.26</td>
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<td>0.044</td>
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<tr>
<td>Swede</td>
<td>W (t ha$^{-1}$)</td>
<td>4.93 - 10.2</td>
<td>4.94 - 10.48</td>
<td>1.39</td>
<td>1.14</td>
<td>12</td>
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<tr>
<td></td>
<td>%N</td>
<td>1.06 - 3.83</td>
<td>1.23 - 3.96</td>
<td>0.54</td>
<td>0.54</td>
<td>18</td>
<td>0.099</td>
</tr>
<tr>
<td>Turnip</td>
<td>W (t ha$^{-1}$)</td>
<td>2.71 - 9.9</td>
<td>3.62 - 10.0</td>
<td>0.73$^*$</td>
<td>0.62$^*$</td>
<td>12</td>
<td>0.456</td>
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<tr>
<td></td>
<td>%N</td>
<td>0.97 - 4.19</td>
<td>1.23 - 3.97</td>
<td>0.21</td>
<td>0.09</td>
<td>12</td>
<td>0.009</td>
</tr>
<tr>
<td>Winter cabbage</td>
<td>W (t ha$^{-1}$)</td>
<td>3.29 - 6.36</td>
<td>1.73 - 5.9</td>
<td>1.23</td>
<td>1.21</td>
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</tr>
<tr>
<td></td>
<td>%N</td>
<td>1.64 - 3.65</td>
<td>2.18 - 3.85</td>
<td>0.16</td>
<td>0.12$^*$</td>
<td>12</td>
<td>0.055</td>
</tr>
</tbody>
</table>

$^a$ $D_1$ and $D_2$ are the mean square of the deviations calculated from the difference between the measured and simulated values on the absolute scale, and after both a shift in origin and a change of scale as described by Eqs. (21) and (22).

$^b$ $d.f.$ for residual variance ≥ 20.

$^c$ $W$ is the dry weight of the entire plant excluding fibrous roots.

$^d$ %N is the concentration of N expressed as a percentage of $W$.

$^*$ indicates not significantly different from the residual variance at $P < 0.05$. 

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Captions to figures:

**Fig. 1.** Schematic representation of the SMCR_N model.

**Fig. 2.** Variation of $R_{root}$ (i.e. $\Delta W_r / \Delta W$) with $W$ and the root class parameter.

**Fig. 3.** Overall comparison between measured and simulated crop %N of 16 crops grown under various N treatments during 1970-75. Some treatments were repeated in different years. In total there were 192 measurements of %N.

**Fig. 4.** Comparison of crop $W$ and %N between the measured and simulated results of turnip 72 and summer cabbage 70 (a) (d), of parsnip 70 and potato 71 (b) (e), and of radish 71 and spinach 71 (c) (f). Lines represent the simulations. Symbols □ and ◊ in (a) and (d) represent measurements for turnip 72 and summer cabbage 70, Δ and × in (b) and (e) represent measurements for parsnip 70 and potato 71, and * and + in (c) and (f) represent measurements for radish 71 and spinach 71, respectively.

**Fig. 5.** Comparison of responses of crop $W$ to fertilizer-N between the measured and simulated by the EU-Rotate_N model and the SMCR_N model for summer cabbage 70 (a) and sugar beet 73 (b).

**Fig. 6.** Comparison between the measured and simulated $W$ at different fertilizer-N levels normalised by $W_{max}$ from all fertilizer-N levels: N0 level (a) (0 fertilizer-N), N1 level (b), N2 level (c), N3 level (d), N4 level (e) and N5 level (f) (max. fertilizer-N).
Solid lines are the linear regressions for all crops, and dotted lines represent the linear
regressions for the crops excluding the low salt tolerant crops of broad bean, carrot,
pea and onion.

Fig. 7. Simulated ratios of N in the plant excluding fibrous roots to N in the entire
plant for all crops grown under sub-optimum N conditions (a), and the relationship
between the ratio and the ‘recovery’ value estimated by Greenwood et al. (1989) and
used in N_ABLE (b).

Fig. 8. Osmotic effect caused by excessive application of fertilizer-N on yield
reduction of radish and red beet. The data presented was calculated from the
experimental results of radish 71, 72 and red beet 70, 73.

Fig. 9. Effect of the correction factor of the osmotic effect caused by excessive
application of fertilizer-N on carrot yield normalised by the maximum dry weight
from different fertilizer-N levels (a), and overall comparison between the simulated
using $\alpha_{osmo}=2$ for carrot, pea and onion and measured $W$ at two highest fertilizer-N
levels normalised by $W_{max}$ from all fertilizer-N levels (b).

Fig. 10. Comparisons of cumulative soil N mineralization calculated using measured
air temperature and soil temperature (a), and measured mean air temperature and
measured mean soil temperature in top 30 cm depth for 1973 and 1975 (b).
START

W = W₀, T = 0

T = T + 1

**Plant growth module**, calculating:
- Potential increment in W, ∆W (Eq. 1);
- Growth reduction due to lack of N in W (Eq. 2), update ∆W;
- Root dry weight Wᵣ (Eq. 7);
- Rooting depth and width (Eq. 6);
- Root length distributions (Eq. 8).

**Osmotica module**, calculating:
- Growth reduction caused by osmotic effect due to soil mineral N (Eq. 19), update ∆W.

**N and water requirement module**, calculating:
- Potential reference evapotranspiration ETo;
- Potential soil evaporation and crop transpiration (Eqs. 12-14);
- Potential N requirement in the top N compartment (Eq. 9);
- Potential N requirement in the root N compartment (Eq. 10).

**N mineralization module**, calculating:
- N mineralization from soil organic matter (Eq. 18), update soil mineral N in top 30 cm.

**N and water uptake module**, calculating:
- N uptake by roots, and split into the top and root N compartments according to the demand, root length distribution and N availability;
- %N in W and Wᵣ;
- Water uptake according to the demand, root length distribution and water availability.

**N and water redistribution module**, calculating:
- Water movement in the soil, update soil water content in the soil domain;
- N transport in the soil, update mineral N content in the soil domain.

T = Tᵪ? YES

STOP

Fig. 1
Fig. 2
y = 0.9723x + 0.0852
$R^2 = 0.8083$

Fig. 3
Fig. 4
Fig. 5
Fig. 6
Fig. 7

(a) 

Species

<table>
<thead>
<tr>
<th>Species</th>
<th>N in plant excluding fibrous roots / N in entire plant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Broad bean</td>
<td>0.95</td>
</tr>
<tr>
<td>Carrot</td>
<td>0.95</td>
</tr>
<tr>
<td>Leek</td>
<td>0.95</td>
</tr>
<tr>
<td>Lettuce</td>
<td>0.95</td>
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<tr>
<td>Onion</td>
<td>0.95</td>
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<tr>
<td>Parsley</td>
<td>0.95</td>
</tr>
<tr>
<td>Peas</td>
<td>0.95</td>
</tr>
<tr>
<td>Potato</td>
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</tr>
<tr>
<td>Radish</td>
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</tr>
<tr>
<td>Red beet</td>
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<tr>
<td>Sugar beet</td>
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<td>Summer cabbage</td>
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<td>Spinach</td>
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<tr>
<td>Swede</td>
<td>0.95</td>
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<tr>
<td>Tumbler</td>
<td>0.95</td>
</tr>
<tr>
<td>Winter cabbage</td>
<td>0.95</td>
</tr>
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</table>

(b) 

Recovery factor

\[ y = 1.5947x - 0.6926 \]

\[ R^2 = 0.5032 \]
$y_{\text{red beet}} = 0.0587x$
$R^2 = 0.9924$

$y_{\text{radish}} = 0.0908x$
$R^2 = 0.9952$

Fig. 8
Fig. 9

(a) Excessive N fertiliser (kg N ha\(^{-1}\)) vs. Normalised W.

(b) Simulated W / W\(_{\max}\) vs. Measured W / W\(_{\max}\) with best fit lines for W4/W\(_{\max}\) and W5/W\(_{\max}\).

- Measurements
- Osmo correction factor = 1
- Osmo correction factor = 2
- Osmo correction factor = 3

Equations and R\(^2\) values:

- \(y_{W4} = 0.6331x + 0.3803\), \(R^2 = 0.4787\)
- \(y_{W5} = 0.9006x + 0.1635\), \(R^2 = 0.6707\)
(a) Cumulative N mineralisation (kg ha\(^{-1}\))

- Soil T-1973
- Air T-1973
- Soil T-1975
- Air T-1975

\[ y_{1973} = 0.909x + 0.7098 \quad R^2 = 0.9071 \]
\[ y_{1975} = 0.921x + 0.6556 \quad R^2 = 0.9034 \]

(b) Mean air temperature (°C) vs. Mean soil temperature (°C)

\[ y_{1973} = 0.909x + 0.7098 \quad R^2 = 0.9071 \]
\[ y_{1975} = 0.921x + 0.6556 \quad R^2 = 0.9034 \]

Fig. 10