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1 **Development and critical evaluation of a generic 2-D agro-hydrological model**  
2 **(SMCR\_N) for the responses of crop yield and nitrogen composition to nitrogen**  
3 **fertilizer**

4

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22

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1 **Abstract**

2

3 Models play an important role in optimizing fertilizer use in agriculture to maintain  
4 sustainable crop production and to minimize the risk to the environment. In this study,  
5 we present a new Simulation Model for Crop Response to Nitrogen fertilizer  
6 (SMCR\_N). The SMCR\_N model, based on the recently developed model EU-  
7 Rotate\_N for the N-economies of a wide range of crops and cropping systems,  
8 includes new modules for the estimation of N in the roots and an associated treatment  
9 of the recovery of soil mineral N by crops, for the reduction of growth rates by  
10 excessive fertilizer-N, and for the N mineralization from soil organic matter. The  
11 validity of the model was tested against the results from 32 multi-level fertilizer  
12 experiments on 16 different crop species. For this exercise none of the coefficients or  
13 parameters in the model was adjusted to improve the agreement between  
14 measurement and simulation. Over the practical range of fertilizer-N levels model  
15 predictions were, with few exceptions, in good agreement with measurements of crop  
16 dry weight (excluding fibrous roots) and its %N. The model considered that the entire  
17 reduction of soil inorganic N during growth was due to the sum of nitrate leaching,  
18 retention of N in fibrous roots and N uptake by the rest of the plant. The good  
19 agreement between the measured and simulated uptakes suggests that in this arable  
20 soil, losses of N from other soil processes were small. At high levels of fertilizer-N  
21 yields were dominated by the negative osmotic effect of fertilizer-N and model  
22 predictions for some crops were poor. However, the predictions were significantly  
23 improved by using a different value for the coefficient defining the osmotic effect for  
24 saline sensitive crops. The developed model SMCR\_N uses generally readily

1 available inputs, and is more mechanistic than most agronomic models and thus has  
2 the potential to be used as a tool for optimizing fertilizer practice.

3

4 **Abbreviations:** %N - percentage of N in  $W$ , %N<sub>crit</sub> - critical %N in  $W$ , i.e. the  
5 minimum %N at which growth is not restricted, %N<sub>max</sub> - maximum percentage of N in  
6  $W$ , %N<sub>spot</sub> - potential percentage of N in  $W_r$ , %N<sub>r</sub> - percentage of N in  $W_r$ ,  $\Delta W$  -  
7 maximum possible increment in growth on the day (t ha<sup>-1</sup>),  $\alpha$ ,  $\beta$  - parameters which  
8 relate critical %N to crop dry weight,  $\alpha_{osmo}$  - species specific correction factor for the  
9 osmotic effect of growth,  $\theta_{osmo}$  - average soil volumetric water content in the depth of  
10  $Z_{osmo}$ ,  $\rho_s$  - soil bulk density (g cm<sup>-3</sup>),  $a_x$ ,  $a_z$  - shape parameters controlling root  
11 distribution in  $x$  and  $z$  directions,  $ET_0$  - daily reference evapotranspiration (mm),  $ET_c$  -  
12 daily crop evapotranspiration under standard conditions (mm),  $f$  - soil fraction not  
13 covered by plants and exposed to evaporation,  $f_{Nmin}$  - response function for soil  
14 temperature,  $k$  - coefficient for the rate of organic matter oxidation (yr<sup>-1</sup>),  $K_1$  - value of  
15  $W$  at which the rate of increase is half the maximum (t ha<sup>-1</sup>),  $K_2$  - growth rate  
16 coefficient (t ha<sup>-1</sup> d<sup>-1</sup>),  $K_c$  - crop coefficient for calculating evapotranspiration from  
17  $ET_c$ ,  $K_{cb}$  - basal crop coefficient for transpiration,  $K_{emax}$  - maximum evapotranspiration  
18 coefficient,  $K_e$  - evaporation coefficient,  $K_{ri}$  - root growth rate in the corresponding  
19 direction (m day<sup>-1</sup> °C<sup>-1</sup>) ( $i = x, z$ ),  $L_0$  - total root length (m m<sup>-3</sup>),  $m_C$  - soil organic C  
20 content (%),  $M_{Nosmo}$  - mineral N in the depth of  $Z_{osmo}$  (kg ha<sup>-1</sup>),  $N_{smin}$  - daily N  
21 mineralization rate from soil organic matter (kg ha<sup>-1</sup>),  $Q_{10}$  - a factor for correcting  
22 rates of soil organic matter breakdown for differences in temperature,  $R_{CN}$  - C:N ratio  
23 of the soil organic matter,  $R_i$  - rooting width and depth (m) ( $i = x, z$ ),  $R_{istart}$  - starting  
24 rooting width and depth (m) ( $i = x, z$ ),  $R_{lux}$  - coefficient of crop luxury N consumption,  
25  $R_N$  - reduction coefficient of increment in  $W$  due to N deficiency in crop,  $R_{osmo}$  -

1 reduction coefficient of increment in  $W$  caused by the osmotic pressure,  $t$  - time (d),  $T$   
2 - daily mean air temperature ( $^{\circ}\text{C}$ ),  $T_{gmax}$  - temperature above which plant growth is the  
3 maximum ( $^{\circ}\text{C}$ ),  $T_{gb}$  - base temperature below which plant does not grow ( $^{\circ}\text{C}$ ),  $T_{0.5}$  - a  
4 half life of soil organic matter ( $y_r$ ),  $T_{lag}$  - threshold of cumulative day degree for root  
5 growth ( $^{\circ}\text{C d}$ ),  $T_s$  - base temperature at which  $f_{Nmin}(t)$  equals 1 ( $^{\circ}\text{C}$ ),  $T_{soil}$  - daily mean  
6 soil temperature ( $^{\circ}\text{C}$ ),  $U_N$  - potential N uptake ( $\text{kg ha}^{-1}$ ),  $U_{Nr}$  - potential N demand by  
7 fibrous roots ( $\text{kg ha}^{-1}$ ),  $W$  - dry weight of the entire plant excluding fibrous roots ( $\text{t ha}^{-1}$ )  
8  $^1$ ),  $W_r$  - dry weight of fibrous roots ( $\text{t ha}^{-1}$ ),  $Z_{osmo}$  - soil depth used in the calculation of  
9 mean osmotic pressure (cm),  $Z_{smin}$  - depth of soil below which no N mineralization is  
10 assumed to take place (cm),  $\Delta W_r$  - root dry weight increment ( $\text{t ha}^{-1}$ ).

11

12 **Key words:** simulation, agronomic model, crop response, nitrogen fertilizer, crop  
13 growth, SMCR\_N

14

## 15 **1. Introduction**

16

17 It is a common feature that agro-ecosystems, like many other ecosystems, receive  
18 excessive applications of nitrogen (Schlesinger et al., 2006). This has caused nitrate  
19 pollution to surface water (Schlesinger et al., 2006), to groundwater via leaching  
20 through soils (Neeteson and Carlton, 2001), and contributed to the rise in  $\text{N}_2\text{O}$   
21 emissions (Jungkunst et al., 2006). Imbalance in N supply relative to crop demand can  
22 also compromise growth and quality of produce. Therefore, it is important to develop  
23 effective systems to optimize fertilizer-N application in agricultural systems to  
24 maintain sustainable crop production and to minimize the risk to the environment.

25

1 The optimum levels of fertilizer-N are controlled by various dynamic factors such as  
2 the weather, soil conditions and the N demand for plant growth. It is generally  
3 impossible to obtain reliable estimates of optimum N levels by conventional statistical  
4 interpretation of a programme of field trials. Attempts have been made to use the  
5 knowledge of fundamental processes governing availability and acquisition of  
6 nutrient-N in the soil-plant system to devise mechanistic models for various crop  
7 species (Bergstrom et al., 1991; Hutson and Wagenet, 1991; Williams et al., 1993;  
8 Diekkruger et al., 1995; Jarvis, 1995; Hoogenboom et al., 1999; Brisson et al., 2003;  
9 Keating et al., 2003; Jones et al., 2003; Stöckle et al., 2003; van Ittersum et al., 2003;  
10 Liang et al., 2007; Rahil and Antonopoulos, 2007). The most prominent individual  
11 nutrient response models that cover a range of crops are the EPIC models (Williams et  
12 al., 1993; Sharpley and Williams, 1990a, b) and the DSSAT models (Hoogenboom et  
13 al., 1999; Jones et al., 2003). EPIC uses a single group of algorithms for simulating  
14 more than 20 crops, with each crop having its own unique parameter values. Versions  
15 of the model have been used widely to simulate soil-N dynamics on a large scale by  
16 many researchers (Huffman et al., 2001). The DSSAT group of models, on the other  
17 hand, focussed more on the physiological development of crops, dealing specifically  
18 with potential yields and their dependence on the environment. The models used  
19 different routines for the various crop types. This group of models includes CERES  
20 (Jones and Kiniry, 1986; Wu et al., 1989) for cereals, CROPGRO (Boote et al., 1998)  
21 for grain legumes, and SUBSTOR (Ritchie et al., 1995) for root and tuber crops. In all,  
22 they cover more than 16 different crops and most have been successfully evaluated in  
23 different climatic zones (Huffman et al., 2001). The EPIC and DSSAT models have  
24 been used in both basic and applied research to study the effects of climate and  
25 management on growth and yield. However, these models are generally species

1 dependent, and therefore different models are required for different crops to study N  
2 response on yield, causing difficulties in the application of model to devise  
3 environmentally friendly and sustainable fertilization strategies. Moreover, the  
4 required inputs of these models are generally difficult to obtain and the models can be  
5 difficult to run due to their complexity.

6

7 In order to overcome these problems, a new agronomic model named EU-Rotate\_N  
8 has been developed for N response of vegetable and arable crops (Rahn et al., 2007).  
9 The model inherits some routines used in the N\_ABLE (Greenwood et al., 1985;  
10 Greenwood and Draycott, 1989a, b; Greenwood et al., 1996) which has been  
11 independently tested in different countries (Riley and Guttormsen, 1993; Goodlass et  
12 al., 1997; Yang et al., 1999; Huffman et al., 2001; Yang et al., 2002) and served as a  
13 key component in the integrated model for N, P and K fertilizers (Zhang et al., 2007),  
14 but is much more advanced and more mechanistic in dealing with many soil and plant  
15 processes. Compared with other agronomic models, EU-Rotate\_N has the advantages  
16 of generality, 2-D which is able to simulate N dynamics in the soil domain in the  
17 horizontal and vertical directions, utilisation of readily available data, and the ability  
18 to simulate crop rotations. The generality of the model was made possible due to the  
19 discoveries that both crop critical %N for maximum growth and crop dry matter  
20 increments during growth could be described by unified equations (Greenwood et al.,  
21 1985). These discoveries have been used in the previous crop N models such as  
22 various versions of the N\_ABLE (Greenwood, 2001). By setting a pre-defined set of  
23 values for each crop, the model used the same algorithm to simulate N responses for  
24 different crops. The 2-D nature of the model makes it more accurate in simulating N-  
25 economy for row crops. However, although the EU-Rotate\_N model is one of the

1 most innovative models of its kind, it does not properly account for N allocated in  
2 fibrous roots during growth, and is unable to consider the depressive osmotic effect  
3 caused by excessive application of fertilizer-N on crop growth and therefore cannot  
4 reproduce some data collected from crop N response experiments (Zhang et al., 2007).  
5 Furthermore, the parametrization of the complex N mineralization routine for release  
6 of soil mineral N could be problematic. To address these problems, a new Simulation  
7 Model for Crop Response to Nitrogen fertilizer (SMCR\_N) based on the EU-  
8 Rotate\_N is developed in the study.

9

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

23

24 The objectives of this study are therefore: 1) to present the SMCR\_N model which  
25 rectifies the above-mentioned faults in the EU-Rotate\_N model by incorporating



1 newly developed modules to take account of N-partition into the roots and the osmotic  
2 effect of mineral N in the soil on crop growth, and to devise a simplified algorithm for  
3 calculating N mineralization based on soil organic C content and its C:N ratio and the  
4 half-lives of organic matter in different soils, 2) to rigorously test and validate the  
5 model against a comprehensive dataset collected from 192 sets of measurements  
6 obtained in 32 fertilizer-N field experiments on 16 different vegetable species.

7

## 8 **2. Model description**

9

### 10 *2.1. Model structure*

11

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

1

## 2 2.2. Plant growth

3

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

6

7 Potential maximum daily increments in dry weight  $W$  excluding fibrous roots are  
8 calculated by the main growth equation. It defines the growth rate until harvest and  
9 was derived from the notion that the interception of radiation increased asymptotically  
10 with increase in plant mass per unit area (Greenwood et al., 1977; 1985; Greenwood,  
11 2001). The equation is:

12

$$13 \frac{\Delta W}{\Delta t} = \frac{K_2 W}{K_1 + W} \quad (1)$$

14

15 where  $\Delta W$  ( $t \text{ ha}^{-1}$ ) is the maximum possible increment in growth on the day,  $W$  ( $t \text{ ha}^{-1}$ )  
16 is the dry weight of the entire plant excluding fibrous roots,  $t$  (d) is the time,  $K_2$  ( $t \text{ ha}^{-1}$   
17  $\text{d}^{-1}$ ) is a growth rate coefficient, and  $K_1$  is the semi-maximum  $W$  for growth rate.  $K_2/K_1$   
18 and  $K_2$  approximate to the specific growth rate when  $W \rightarrow 0$  and to the absolute growth  
19 rate when  $W \gg 0$ , respectively. Eq. (1) thus mimics initial exponential followed by  
20 near constant growth as  $W$  increases. By assuming plant growth is driven by air  
21 temperature, integrating Eq. (1) gives:

22

$$23 K_2 = \frac{K_1 \ln W_{\max} + W_{\max} - K_1 \ln W_0 - W_0}{\sum \max[\min(T, T_{g \max}) - T_{gb}, 0]} \quad (2)$$

24

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

7

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

10

$$11 \quad R_N = 1 - \min\left(\frac{\%N}{\%N_{crit}}, 1\right) \quad (3)$$

12

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

15

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

17

$$18 \quad \%N_{crit} = \alpha(1 + \beta e^{-0.26W}) \quad (4)$$

19

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

21

22 Some crops are able, when there is much soil mineral N, to take up more N than  
23 necessary for maximum growth. In these circumstances, the maximum crop  $\%N$  is  
24 calculated as follows:

1

$$2 \quad \%N_{\max} = R_{lux} \%N_{crit} \quad (5)$$

3

4 where  $R_{lux}$  is the coefficient of crop luxury N consumption.

5

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

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

9

$$10 \quad R_i = \min \{ R_{istart} + \max[0, (\sum T - T_{lag}) K_{ri}], R_{imax} \} \quad (6)$$

11

12 where  $i = x, z$  stands for the coordinates in the horizontal and vertical directions,  $R_i$  (m)  
13 is the rooting width and depth,  $R_{istart}$  (m) is the starting rooting width and depth,  $\sum T$   
14 ( $^{\circ}\text{C d}$ ) is the cumulative day degree,  $T_{lag}$  ( $^{\circ}\text{C d}$ ) is the threshold of cumulative day  
15 degree for root growth,  $K_{ri}$  ( $\text{m day}^{-1} \text{ }^{\circ}\text{C}^{-1}$ ) is the root growth rate in the corresponding  
16 direction.  $R_{imax}$  (m) is the maximum rooting depth and width restricted by physical  
17 barriers or the effective rooting width (= a half row width) for row crops. Eq. (6),  
18 given a proper parameterisation, gives a good description of root penetration of crops  
19 observed in a number of studies (Thorup-Kristensen, 1998, 2001, 2006; Thorup-  
20 Kristensen & Van den Boogaard, 1998, 1999; Kage et al., 2000; Kristensen &  
21 Thorup-Kristensen, 2004).

22

1 Crop total root length is calculated as a product of root dry weight and a fixed specific  
 2 root length. The increment in root dry weight  $\Delta W_r$  is a function of the increment in  
 3 crop dry weight  $\Delta W$ , crop dry weight  $W$ , and a parameter defining root class:

$$4 \quad \Delta W_r = \Delta W \times R_{root} \quad (7)$$

6  
 7 where  $R_{root}$  is the ratio of  $\Delta W_r$  to  $\Delta W$ , which declines with  $W$  and varies with the  
 8 root class parameter as shown in Fig. 2.

9  
 10 The root length declines logarithmically from the soil surface downwards, as  
 11 originally proposed by Gerwitz and Page (1974), and also logarithmically laterally  
 12 from the crop row to the inter-row soil. However, different from Gerwitz and Page's  
 13 (1974) the module extends the rooting depth by 30% from the calculated penetrating  
 14 depth where the root density declines from a calculated value at the penetrating depth  
 15 to zero, i.e.:

$$16 \quad L(x, z) = \begin{cases} L_0 e^{-(a_z z + a_x x)} & z < R_z \\ L_0 e^{-(a_z z + a_x x)} \left(1 - \frac{z - R_z}{0.3 R_z}\right) & R_z \leq z \leq 1.3 R_z \end{cases} \quad (8)$$

18  
 19 where  $L_0$  ( $\text{m m}^{-3}$ ) is the total root length,  $a_x$  and  $a_z$  are the shape parameters controlling  
 20 root distribution in  $x$  (horizontal) and  $z$  (vertical) directions, respectively.

### 21 22 2.3 *N* and water requirement

23

1 In the EU-Rotate\_N there is only one N compartment in crops, and the N partition to  
 2 the roots is ignored. This fault has been rectified in the SMCR\_N. SMCR\_N assumes  
 3 that there are two N compartments in crops, a top N compartment and a root N  
 4 compartment. The top N compartment contains N of the entire plant excluding N in  
 5 fibrous roots, whereas the root N compartment stores N allocated in fibrous roots. The  
 6 potential N requirement in the top compartment is calculated from its dry weight, N  
 7 concentration, the maximum possible concentration for a plant of the same mass and  
 8 its potential maximum increment in weight, i.e.:

9

$$10 \quad U_N = 10[(W + \Delta W) \times \%N_{\max} - W \times \%N] \quad (9)$$

11

12 where  $U_N$  (kg ha<sup>-1</sup>) is the potential N uptake of the entire plant excluding fibrous roots.

13

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

15

$$16 \quad U_{Nr} = 10[(W_r + \Delta W_r) \times \%N_{rpot} - W_r \times \%N_r] \quad (10)$$

17

18 where  $U_{Nr}$  (kg ha<sup>-1</sup>) is the potential N demand by fibrous roots,  $W_r$  and  $\Delta W_r$  are the  
 19 root dry weight on the previous day and the potential root dry weight increment on the  
 20 day, respectively,  $\%N_r$  is the actual percentage of N in  $W_r$ , and  $\%N_{rpot}$  is the root  
 21 potential %N, which is calculated from:

22

$$23 \quad \%N_{rpot} = 1 + \beta e^{-0.26W} \quad (11)$$

24

1 Eq. (11) was derived by assuming that the potential %N in the roots decreased with  
2 increase in crop dry weight, and the decrease rate followed the same pattern as the  
3 critical %N in  $W$ . The ratio of critical %N in  $W$  to that in  $W_r$  is  $\alpha$ , a parameter in  
4 calculating critical %N in  $W$  (Eq. 4) and always greater than 1.0. For crops with large  
5 yields,  $\%N_{rpot}$  approaches 1% at maturity. The derivation was based on the  
6 observations of %N in roots over a number of field crops made by Osaki et al., (1997)  
7 that root %N decreased during growth and the %N at maturity ranged from 0.5% to  
8 2.0% with wheat and maize having the value of about 1%.

9

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

12

$$13 \quad ET_c = K_c ET_0 \quad (12)$$

14

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

17

18 The crop coefficient method partitions the  $K_c$  factor into two separate coefficients:

19

$$20 \quad K_c = K_{cb} + K_e \quad (13)$$

21

22 where  $K_{cb}$ , dependent on crop species and its development stage, is the basal crop  
23 coefficient for transpiration, and  $K_e$  is the soil evaporation coefficient, which is  
24 defined as:

25

1 
$$K_e = \min(K_{c_{max}} - K_{cb}, fK_{c_{max}}) \quad (14)$$

2

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

7

#### 8 *2.4. N mineralization from soil organic matter*

9

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

20

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

22

23 
$$\frac{dm_C}{dt} = -km_C \quad (15)$$

24



1 where  $m_C$  ( $\text{g g}^{-1}$ ) is the organic C content, and  $k$  ( $\text{yr}^{-1}$ ) is a coefficient for the rate of  
2 organic matter oxidation.

3

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

5

$$6 \quad kT_{0.5} = -\ln(0.5) \quad (16)$$

7

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

9

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

16

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

19

$$20 \quad f_{N \min}(t) = Q_{10}^{\frac{T_{soil}(z) - T_s}{10}} \quad (17)$$

21

22 where  $f_{N \min}(t)$  is the response function for soil temperature,  $T_{soil}(z)$  is the soil  
23 temperature at the soil depth  $z$ ,  $T_s$  ( $^{\circ}\text{C}$ ) is the base temperature at which  $f_{N \min}(t)$  equals  
24 1, and  $Q_{10}$  is the factor change in rate with a 10 degree change in temperature.

25

1 Thus, provided the half life of organic matter breakdown is known, the daily N  
 2 mineralization from soil organic matter can be calculated:

3

$$4 \quad N_{s \min} = \frac{k}{\sum_{i=1}^{365} f_{N \min}(t_i)} f_{N \min}(t) \rho_s Z_{s \min} \frac{m_c}{R_{CN}} \times 10^5 \quad (18)$$

5

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

9

## 10 2.5. Effect of osmotic pressure on crop growth

11

12 To consider the negative osmotic effect caused by mineral N in the soil on crop  
 13 growth, a growth reduction coefficient  $R_{osmo}$  is introduced by modifying Zhang et al.  
 14 (2007):

15

$$16 \quad R_{osmo} = 1 - \alpha_{osmo} K_r \quad (19)$$

17

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

21

$$22 \quad K_r = \frac{1}{6.73} \times \frac{1.5 \times 273 \times 8.27}{14} \times \frac{M_{Nosmo}}{\theta_{osmo} Z_{osmo} \times 10^5} = 1.6 \times 10^{-3} \frac{M_{Nosmo}}{\theta_{osmo} Z_{osmo}} \quad (20)$$

23

1 in which  $Z_{osmo}$  (cm) is the soil depth where the osmotic pressure induced by mineral N  
2 is considered,  $M_{Nosmo}$  ( $\text{kg ha}^{-1}$ ) is the mineral N in the depth of  $Z_{osmo}$ ,  $\theta_{osmo}$  is the  
3 average soil volumetric water content in the depth of  $Z_{osmo}$  (30 cm). The equation was  
4 derived by considering that  $\text{NH}_4\text{NO}_3$  was incorporated in the upper 30 cm from the  
5 surface and was immediately nitrified and converted into  $\text{NO}_3^-$ . As in standard  
6 theory each gram mole ion per litre of soil solution increased the osmotic pressure by  
7  $8.27 \text{ (kPa)} \times$  the absolute temperature, (273 K); no correction was made for  
8 differences in temperature. It was assumed that  $K_r$  equalled the ratio of osmotic  
9 pressure in 6.73 kPa and that  $K_r = 1$  when the ratio  $\geq 1$  (Kramer, 1949; Mengel and  
10 Kirkby, 2001).

11

## 12 *2.6. Root N and water uptake and evaporation*

13

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

25

1    2.7. *Soil water and N movement*

2

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

14

15   2.8. *Model inputs*

16

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

19

- 20       • Site properties: altitude and latitude of the site.
- 21       • Weather data: air temperature, radiation, rainfall, relative humidity and wind  
22        speed.
- 23       • Soil properties: bulk density, volumetric soil water content at saturation, field  
24        capacity and the permanent wilting point, soil organic C content, CN ratio,  
25        half-life of soil organic matter, and the depth from the soil surface of any

- 1 barrier to rooting.
- 2 • Initial conditions: volumetric soil water content and mineral N concentration
  - 3 distributions in the soil profile and dates of measurement.
  - 4 • Fertilization and irrigation: dates and amounts of fertilizer-N and irrigation
  - 5 applied.
  - 6 • Crop data: species, spacings, sowing/planting and harvest dates, crop dry
  - 7 weight at planting, expected maximum crop dry weight excluding fibrous
  - 8 roots.

9

### 10 **3. Experiments and parameter setting**

11

#### 12 *3.1 Experimental set-up*

13

14 The validity of the model SMCR\_N was tested against a comprehensive dataset of the  
15 yield and N composition from historical field experiments on various crops at  
16 Wellesbourne, UK. Sixteen crops were grown in 32 fertilizer-N experiments during  
17 the period 1970-1975 on the same field: Big Ground of the National Vegetable  
18 Research Station, now Warwick-HRI (Greenwood et al., 1980). The soil was a sandy  
19 loam of the Wick series and is described in Whitfield (1974). The experiments  
20 followed the same general pattern. Six fertilizer-N treatments from N0 (the zero  
21 fertilizer-N) to N5 (the highest fertilizer-N) were tested in each crop. There were three  
22 plots in each fertilizer-N treatment, all with the expected optimum levels of P and K.  
23 In each plot there were three blocks or replicates. The plots were laid out  
24 systematically in order of fertilizer application. The direction of increase in fertilizer-  
25 N was chosen at random. The entire plant material excluding fibrous roots was

1 removed from each block and weighed at commercial maturity. All the plant material  
2 from three plots with the same fertilizer-N treatment was bulked together and treated  
3 as one sample. The dry weight and the N composition in the plant were then  
4 determined. The dates of sowing and harvest and the levels of fertilizer-N for each of  
5 the experiments are summarised in Table 1. Detailed description of the experiments  
6 can be seen elsewhere (Greenwood et al., 1980).

7

### 8 *3.2. Parameter setting*

9

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

16

17 At the time of planting the estimated distributions of mineral N were 30 kg N ha<sup>-1</sup> in  
18 the 0-30 cm layer, 15 kg N ha<sup>-1</sup> in 30-60 cm layer, and 5 kg N ha<sup>-1</sup> in the 60-90 cm  
19 layer (Zhang et al., 2007). The soil bulk density was 1.4 g cm<sup>-3</sup>, and the volumetric  
20 water content at saturation, field capacity and the permanent wilting point were 0.45,  
21 0.26 and 0.1 cm<sup>3</sup> cm<sup>-3</sup> (Zhang et al., 2007), respectively. As the soil moisture was not  
22 measured at the time of planting, the soil water distribution in the profile at planting  
23 was calculated by running the model from 1 January of the planting year when the soil  
24 water deficit was assumed to be zero. For the exercise of model validation, the  
25 maximum yield, obtained from the experiment on a crop grown at various fertilizer-N

1 on the same year, was taken to be the required input of maximum plant dry weight at  
2 harvest. However, if the model is used for prediction purposes, the maximum yield  
3 should be estimated independently based on previous experience or other measures.  
4 The minimum soil mineral N level below which plants were not able to take up N was  
5 set  $0.0035 \text{ kg m}^{-3}$ , and the species specific correction factor for the osmotic effect of  
6 growth was set 1.0 for all crops. Broad bean and pea differed from other crops in that  
7 they were able to fix atmospheric-N in these experiments when N supply from the soil  
8 was limited, although it was recognised that this ability was dependent on the  
9 presence of suitable strains of Rhizobium in soil.

10

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

21

#### 22 **4. Evaluation criteria**

23

24 The evaluation criteria used in the study were similar with those described previously  
25 by Greenwood et al. (2001) and Zhang et al. (2007). If  $Y$  is the value predicted by the

1 model and  $y$  is the experimentally determined treatment mean then  $Y$  may be a good  
2 predictor either absolutely or after a both shift and scale change i.e.  $a + bY$ .

3

4 The discrepancies in both cases are:

5

$$6 \quad D_1 = \sum(y - Y)^2 / K \quad (21)$$

$$7 \quad D_2 = \sum(y - a - bY)^2 / (K - 2) \quad (22)$$

8

9 where  $K$  is the number of comparisons, and

10

$$11 \quad a = \bar{y} - b\bar{Y} \quad (23)$$

$$12 \quad b = \sum y(Y - \bar{Y}) / \sum (Y - \bar{Y})^2 \quad (24)$$

13

14 where  $\bar{y}$  and  $\bar{Y}$  are the average measurements and predictions.

15

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

20

## 21 **5. Results**

22

23 Simulated values of plant %N were almost proportional to the measured values for all  
24 192 combinations of crops and fertilizer levels (Fig. 3). The model gave good



1 predictions of both  $W$  and %N for some crops over the whole range of fertilizer levels  
2 as illustrated for turnip, summer cabbage, parsnip, potato, radish and spinach, in Fig. 4.  
3 Figure 5 compares the measured responses of plant  $W$  to fertilizer-N for summer  
4 cabbage 70 and sugar beet 73 with the simulated values from the EU-Rotate\_N and  
5 the SMCR\_N models. A much better agreement was observed between measurement  
6 and simulation from the SMCR\_N model for both cases, illustrating that the  
7 SMCR\_N model performs better than the EU-Rotate\_N model.

8

9 Statistical comparison was carried out between the measured and simulated  $W$  and  
10 %N for 13 out of 16 crops (Table 3). No attempt of statistical analysis was made for the  
11 other 3 crops due to lack of degree of freedom resulting from the crops grown only in  
12 a single year. The discrepancies between the simulated and measured  $W$  at zero  
13 fertilizer-N which was crucial to test the model were less than 20% for 9 out of 13  
14 crops (Table 3). If the ratio of  $D_1$  or  $D_2$  to the residual variance in Table 3 is not  
15 significant at  $P < 0.05$  by the variance ratio test, all the discrepancies can be explained  
16 by experimental error (Greenwood et al., 2001; Zhang et al., 2007). Thus, it can be  
17 concluded that there was no significant difference between the measured and  
18 simulated values of  $W$  for turnip and of %N for lettuce, as the ratio of  $D_1$  to the  
19 residual variance was not significant at  $P < 0.05$ . The linear relationship between  
20 measured and simulated values of %N for winter cabbage accounted for the  
21 discrepancies between measurement and simulation, as the ratio of  $D_2$  to the residual  
22 variance was not significant at  $P < 0.05$ .

23

24 Since the maximum dry weight yield was obtained from the experiment on a crop  
25 grown at various fertilizer-N, it is important to test the model's ability to predict yield

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

21

22 The simulated ratios of N contained in the plant excluding fibrous roots to that in the  
23 whole plant including fibrous roots for different crops grown at sub-optimal N levels  
24 crops are plotted in Fig. 7(a). The ratio, varying with crop species, ranged from 0.77  
25 for crops with small yields to 0.93 for crops with big yields. The ratio calculated in

1 the study was correlated with a ‘recovery factor’ fairly well (Fig. 7b). The recovery  
2 factor was obtained by plotting crop N uptake against fertilizer-N and determining the  
3 gradient at near zero application for crops grown under conditions where there was no  
4 leaching (Greenwood et al., 1989). The measured recovery factor includes effects of  
5 loss of mineral by biological process such as denitrification which the simulated ratio  
6 did not. When fertilizer-N was over applied, crop yields declined linearly with  
7 increase in fertilizer-N (Fig. 8) as calculated using Eq. (19), and percentage reductions  
8 in yield were greater for crops having a low than a high yield. For example, 300 kg-N  
9 ha<sup>-1</sup> depressed yield by 27% for radish but only about 16% for red beet, respectively.

10

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

22

23 The simulated estimates of cumulative N mineralized from soil organic matter are  
24 plotted against time in Fig. 10(a) for years 1973 and 1975; they were calculated  
25 assuming that they were dominated either by measured mean daily soil or air

1 temperature. The differences between the simulated cumulative mineralization of N  
2 using each of the two types of temperature were always less than 7%. Inter-year  
3 differences were also small between 1973 and 1975. Figure 10(b) shows that there is a  
4 strong correlation between the measured temperature in top 30 cm soil and air  
5 temperature. The best regression lines for 1973 and 1975 are close to the 1:1 line.

6

7 **6. Discussion**

8

9 *6.1. Model general performance and its comparison with EU-Rotate\_N*

10

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

17

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

1 Rotate\_N would have been less satisfactory even for the positive effect of fertilizer-N  
2 on crop  $W$ .

3

#### 4 *6.2. Mechanistic account of fractional recovery of fertilizer-N by crop*

5

6 The routine for calculating the root N content is an important feature of the model.  
7 The ratio of the N content of the plant excluding fibrous roots to the N content of the  
8 plant including fibrous roots at sub-optimal levels of N for the different crops was  
9 strongly correlated with an independent measure of the recovery of fertilizer-N (Fig.  
10 7b) (Greenwood et al., 1989). Moreover, the ratio was close to the recovery for crops  
11 with large yields, whereas it was generally lower than the recovery for small crops.  
12 The recovery was obtained by plotting N uptake at harvest against the fertilizer-N  
13 level and determining the gradient when the fertilizer level tended to zero. The  
14 discrepancies between the ratio and the recovery for small crops might be due to the  
15 fact that the lateral distribution of mineral N in the soil was not considered in  
16 determining recovery. For a small crop even grown under a low fertilizer-N, a  
17 significant amount of mineral N could be left at harvest due to failure of the crop to  
18 fully explore the inter row soil and extract mineral N from it. The recovery also  
19 assumed that there was no loss of mineral N through soil processes such  
20 denitrification. The model assumes that the entire disappearance of fertilizer-N,  
21 excluding that lost by leaching, could be accounted for by uptake in the roots and in  
22 the remainder of the plant. Yet with this assumption the model gave good predictions  
23 of  $W$ , its %N content and the ratio in good agreement the recovery for crops with big  
24 yields. It therefore appears that N losses from low levels of fertilizer-N through soil  
25 processes such as denitrification, ammonia volatilization and ammonia fixation were

1 small. Though small, they may explain why the predicted values of  $W$  for some crops  
2 are higher than the measured ones at level N1.

3

4 *6.3. Mechanistic account of depressive osmotic effect on yield*

5

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

13

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

22

23 It is clear that the model with the osmotic correction factor of 1 did not work  
24 satisfactorily for the salt sensitive crops. The possibility of using the proposed  
25 approach with a different value for the correction factor for different crops to simulate

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

11

#### 12 *6.4. Evidence of satisfactory N mineralization routine for release of soil mineral N*

13

14 Rigorous validation of the N mineralization routine was not possible in the study as  
15 the soil mineral N concentration was not directly measured in the experiments.  
16 However the indirect assessment of the performance of the routine can be carried out  
17 based on the following facts. Firstly the relationship between measured and simulated  
18 values of  $W$  when fertilizer-N was withheld (Figs. 4 and 6) was near proportional.  
19 Secondly the measured %N (Figs. 3 and 4) was nearly 1:1 to the simulated values.  
20 This, together with the first point, indicates that prediction of crop N uptakes from the  
21 endogenous soil mineral N, was simulated correctly. Thirdly the model simulated that  
22 the unfertilized crops reduced soil inorganic N to around  $10 \text{ kg N ha}^{-1}$  in the top 0.3 m  
23 of the soil, in agreement with the previous studies (Thorup-Kristensen and Sørensen,  
24 1999; Thorup-Kristensen, 2006), suggesting that the minimum level of soil mineral N  
25 from which plant roots can extract mineral N was set correctly for most crops. Finally,

1 the simulated N leaching at 90 cm soil depth was small during crop growth, ranging  
2 from 0 to 2.5 kg-N ha<sup>-1</sup>, which was supported by the previous study that N leaching  
3 mainly occurred from late autumn to early spring on the Western European soils, out  
4 of growing periods for most of crops (Neeteson and Carton, 2001). Based on these  
5 lines of evidence, it is clear that the mineral N input from soil organic matter into the  
6 crop-soil systems during growth was properly accounted for, and therefore it could be  
7 concluded that the proposed algorithm for N mineralization from soil organic matter  
8 worked reasonably well for this sandy loam arable soil.

9

10 It was found that when the soil temperature is not available, air temperature can be  
11 used instead without great loss of accuracy of estimating soil N mineralization (Fig.  
12 10a) since the soil temperature in the top 30 cm depth is almost 1:1 related to the air  
13 temperature (Fig. 10b). This implies that in agronomic models the simulation of soil  
14 temperature might not be essential. Simulation of soil temperature concerns many  
15 complex processes such as heat transfer, moisture movement and water movement to  
16 the surface, and some of these processes are closely related to each other. Accurately  
17 modelling soil temperature has been proven extremely difficult (Akinyemi and  
18 Mendes, 2007).

19

## 20 **7. Conclusions**

21

22 A new generic model SMCR\_N for nitrogen response on yield and N composition for  
23 vegetable and arable crops has been developed. The model gave predictions of the  
24 responses of crop dry weight  $W$  and its %N to fertilizer-N that with few exceptions  
25 were in close agreement with the measured values over the practical range of fertilizer



1 applications. This suggests that the model framework and the major modules  
2 including newly developed ones for N allocation in roots, the depressive effect of  
3 excessive fertilizer-N application on crop yield and the simplified N mineralization  
4 algorithm for release of soil mineral N work reasonably well. Therefore, the  
5 SMCR\_N model can be used as a platform for optimizing fertilizer-N application in  
6 crop production.

7

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

19

20 The future work includes the further development of the EU-Rotate\_N with the  
21 obtained improvements in the study. Opportunities also exist to enhance the  
22 performance of the SMCR\_N model in predicting N leaching by replacing the current  
23 cascade type algorithm for soil water movement with the one developed by Yang et al.  
24 (2009) which, using an integration strategy on the basic flow equation, is simple and  
25 highly accurate in hydrological simulations.

1

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3

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Table 1: Experimental details

Crop <sup>a</sup>	Sowing/planting date	Harvest date	Fertilizer rate (kg N ha <sup>-1</sup> )
Broad bean 72	26/04/72	10/08/72	0, 56, 140, 224, 308, 392
Broad bean 73	13/03/72	19/06/72	0, 56, 140, 224, 308, 392
Carrot 70	05/05/70	28/09/70	0, 56, 140, 224, 308, 392
Leek 70	29/04/70	09/11/70	0, 90, 224, 359, 493, 628
Leek 71	02/04/71	11/11/71	0, 90, 224, 359, 493, 628
Lettuce 70	15/06/70	07/08/70	0, 56, 140, 224, 308, 392
Lettuce 75	12/06/75	20/08/75	0, 56, 140, 224, 308, 392
Onion 70	29/04/70	01/09/70	0, 90, 224, 359, 493, 628
Onion 73	23/08/72	03/07/73	0, 56, 140, 224, 308, 392
Parsnip 70	01/05/70	02/12/70	0, 90, 224, 359, 493, 628
Parsnip 72	03/05/72	13/12/72	0, 90, 224, 359, 493, 628
Parsnip 73	26/03/73	05/11/73	0, 90, 224, 359, 493, 628
Pea 71	24/03/71	23/06/71	0, 67, 168, 269, 370, 471
Potato 71	19/04/71	16/08/71	0, 67, 168, 269, 370, 471
Potato 72	16/05/72	05/09/72	0, 67, 168, 269, 370, 471
Potato 73	16/05/73	11/09/73	0, 67, 168, 269, 370, 471
Radish 71	23/06/71	23/07/71	0, 90, 224, 359, 493, 628
Radish 72	21/06/72	24/07/72	0, 90, 224, 359, 493, 628
Red beet 70	19/05/70	19/10/70	0, 112, 280, 448, 616, 785
Red beet 73	04/06/73	08/10/73	0, 112, 280, 448, 616, 785
Spinach 71	20/04/71	22/06/71	0, 112, 280, 448, 616, 785
Spinach 72	17/05/72	11/07/72	0, 112, 280, 448, 616, 785
Sugar beet 73	16/04/73	27/11/73	0, 112, 280, 448, 616, 785
Sugar beet 74	18/04/74	27/11/74	0, 112, 280, 448, 616, 785
Summer cabbage 70	20/05/70	18/08/70	0, 90, 224, 359, 493, 628
Swede 71	04/05/71	28/09/71	0, 90, 224, 359, 493, 628
Swede 72	17/05/72	04/10/72	0, 90, 224, 359, 493, 628
Swede 73	27/03/73	26/09/73	0, 90, 224, 359, 493, 628
Turnip 71	06/04/71	07/07/71	0, 90, 224, 359, 493, 628
Turnip 72	03/05/72	01/08/72	0, 90, 224, 359, 493, 628
Winter cabbage 70	16/07/70	21/12/70	0, 112, 280, 448, 616, 785
Winter cabbage 72	13/07/72	04/01/73	0, 112, 280, 448, 616, 785

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<sup>a</sup> two digits in the crop names represent the year of experiment, for example 72 stands for year 1972.

1 Table 2: Crop parameter values used in the simulations

Crop	N fixation	$\alpha^a$	$\beta^a$	$R_{lux}^b$	$T_{lag}^c$ (day °C)	$K_{rz}^d$ (m day <sup>-1</sup> °C <sup>-1</sup> )	$a_z^e$	Root class	$K_{cb}^f$		
									Initial stage	Middle stage	Mature stage
Broad bean	Yes	2	3	1	100	0.0007	3	1	0.15	1.1	1.05
Summer cabbage	No	2.6	1.1	1	100	0.001	2	1	0.15	0.95	0.85
Winter cabbage	No	2.6	1.1	1	100	0.001	1.5	2	0.15	0.95	0.85
Carrot	No	1.2	1.26	1.5	250	0.0007	3	1	0.15	0.95	0.85
Leek	No	1.35	1.77	1.2	350	0.0003	8	2	0.15	0.9	0.9
Lettuce	No	1.35	1.35	1	100	0.001	3	1	0.15	0.9	0.9
Onion	No	1.35	2.42	1	250	0.0003	8	2	0.15	1.05	0.75
Parsnip	No	1.35	1.26	1	250	0.0007	3	1	0.15	0.95	0.85
Potato	No	1.35	3	1	100	0.0007	3	1	0.15	1.1	0.9
Radish	No	1.35	1.87	1.2	100	0.001	3	1	0.15	0.85	0.75
Red beet	No	1.53	3	1.35	250	0.001	2	1	0.15	0.95	0.85
Spinach	No	1.35	3	1	100	0.001	3	1	0.15	0.9	0.85
Sugar beet	No	1.11	1.38	1.65	250	0.001	2	1	0.15	1.15	0.5
Swede	No	1.35	3	2	100	0.001	1.5	1	0.15	1	0.85
Turnip	No	1.35	3	2	100	0.001	2	1	0.15	1	0.85
Peas	Yes	1.35	3	1	100	0.001	3	1	0.15	1.1	1.05

2 <sup>a</sup>  $\alpha$  and  $\beta$  are the parameters which relate critical %N to crop dry weight.

3 <sup>b</sup>  $R_{lux}$  is the luxury N consumption coefficient.

4 <sup>c</sup>  $T_{lag}$  (°C d) is the threshold of cumulative day degree for root growth.

5 <sup>d</sup>  $K_{rz}$  is the vertical root growth rate.

6 <sup>e</sup>  $a_z$  is the shape parameter controlling root distribution in the soil depth.

7 <sup>f</sup>  $K_{cb}$  is the basal crop coefficient for transpiration.



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Table 3: Statistical comparison between measured and simulated crop DW yield and %N

Crop	Range		$D_1^a$	$D_2^a$	<i>d. f.</i> for $D_1$	Residual variance <sup>b</sup>	
	Simulated	Measured					
Broad bean	W (t ha <sup>-1</sup> ) <sup>c</sup>	5.29 - 7.07	5.22 - 7.3	0.82	0.53	0.200	
	%N <sup>d</sup>	2.59 - 3.5	2.62 - 3.58	0.23	0.11	12	0.013
Leek	W (t ha <sup>-1</sup> )	5.13 - 16.6	9.62 - 16.82	5.63	3.90		0.711
	%N	0.73 - 1.9	0.99 - 2.06	0.06	0.05	12	0.018
Lettuce	W (t ha <sup>-1</sup> )	1.1 - 2.92	0.93 - 2.63	0.15	0.14		0.009
	%N	1.59 - 2.72	1.72 - 2.81	0.01*	0.01*	12	0.026
Onion	W (t ha <sup>-1</sup> )	3.36 - 6.7	2.28 - 6.29	1.56	1.29		0.133
	%N	1.34 - 2.35	1.05 - 2.6	0.13	0.15	12	0.026
Parsnip	W (t ha <sup>-1</sup> )	5.84 - 9.91	6.09 - 9.35	0.84	0.57		0.297
	%N	1.04 - 1.72	0.96 - 2.3	0.09	0.09	18	0.036
Potato	W (t ha <sup>-1</sup> )	3.55 - 12.7	3.46 - 13.21	3.47	3.38		0.174
	%N	0.89 - 2.68	0.37 - 2.55	0.36	0.18	18	0.038
Radish	W (t ha <sup>-1</sup> )	0.43 - 1.48	0.62 - 1.32	0.03	0.01		0.001
	%N	1.99 - 4.33	2.75 - 4.42	0.19	0.13	12	0.043
Red beet	W (t ha <sup>-1</sup> )	4.25 - 13.3	5.28 - 13.46	3.16	2.98		0.415
	%N	1.09 - 2.71	1.25 - 2.7	0.05	0.05	12	0.007
Sugar beet	W (t ha <sup>-1</sup> )	10.5 - 20.3	9.77 - 20.65	3.78	3.82		0.608
	%N	0.62 - 1.92	0.81 - 1.82	0.19	0.06	12	0.011
Spinach	W (t ha <sup>-1</sup> )	0.8 - 2.92	0.86 - 2.83	0.06	0.06		0.012
	%N	1.8 - 4.64	2.14 - 4.7	0.47	0.26	12	0.044
Swede	W (t ha <sup>-1</sup> )	4.93 - 10.2	4.94 - 10.48	1.39	1.14		0.308
	%N	1.06 - 3.83	1.23 - 3.96	0.54	0.54	18	0.099
Turnip	W (t ha <sup>-1</sup> )	2.71 - 9.9	3.62 - 10.0	0.73*	0.62*		0.456
	%N	0.97 - 4.19	1.23 - 3.97	0.21	0.09	12	0.009
Winter cabbage	W (t ha <sup>-1</sup> )	3.29 - 6.36	1.73 - 5.9	1.23	1.21		0.243
	%N	1.64 - 3.65	2.18 - 3.85	0.16	0.12*	12	0.055

4

<sup>a</sup>  $D_1$  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).

8

<sup>b</sup> *d.f.* for residual variance  $\geq 20$ .

10

<sup>c</sup>  $W$  is the dry weight of the entire plant excluding fibrous roots.

12

<sup>d</sup> %N is the concentration of N expressed as a percentage of  $W$ .

14

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

16

17

1

2 Captions to figures:

3

4 **Fig. 1.** Schematic representation of the SMCR\_N model.

5

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

7

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

11

12 **Fig. 4.** Comparison of crop  $W$  and %N between the measured and simulated results of  
13 turnip 72 and summer cabbage 70 (a) (d), of parsnip 70 and potato 71 (b) (e), and of  
14 radish 71 and spinach 71 (c) (f). Lines represent the simulations. Symbols  $\square$  and  $\diamond$  in  
15 (a) and (d) represent measurements for turnip 72 and summer cabbage 70,  $\Delta$  and  $\times$  in  
16 (b) and (e) represent measurements for parsnip 70 and potato 71, and \* and + in (c)  
17 and (f) represent measurements for radish 71 and spinach 71, respectively.

18

19 **Fig. 5.** Comparison of responses of crop  $W$  to fertilizer-N between the measured and  
20 simulated by the EU-Rotate\_N model and the SMCR\_N model for summer cabbage  
21 70 (a) and sugar beet 73 (b).

22

23 **Fig.6.** Comparison between the measured and simulated  $W$  at different fertilizer-N  
24 levels normalised by  $W_{max}$  from all fertilizer-N levels: N0 level (a) (0 fertilizer-N), N1  
25 level (b), N2 level (c), N3 level (d), N4 level (e) and N5 level (f) (max. fertilizer-N).

1 Solid lines are the linear regressions for all crops, and dotted lines represent the linear  
2 regressions for the crops excluding the low salt tolerant crops of broad bean, carrot,  
3 pea and onion.

4

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

9

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

13

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

19

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

23

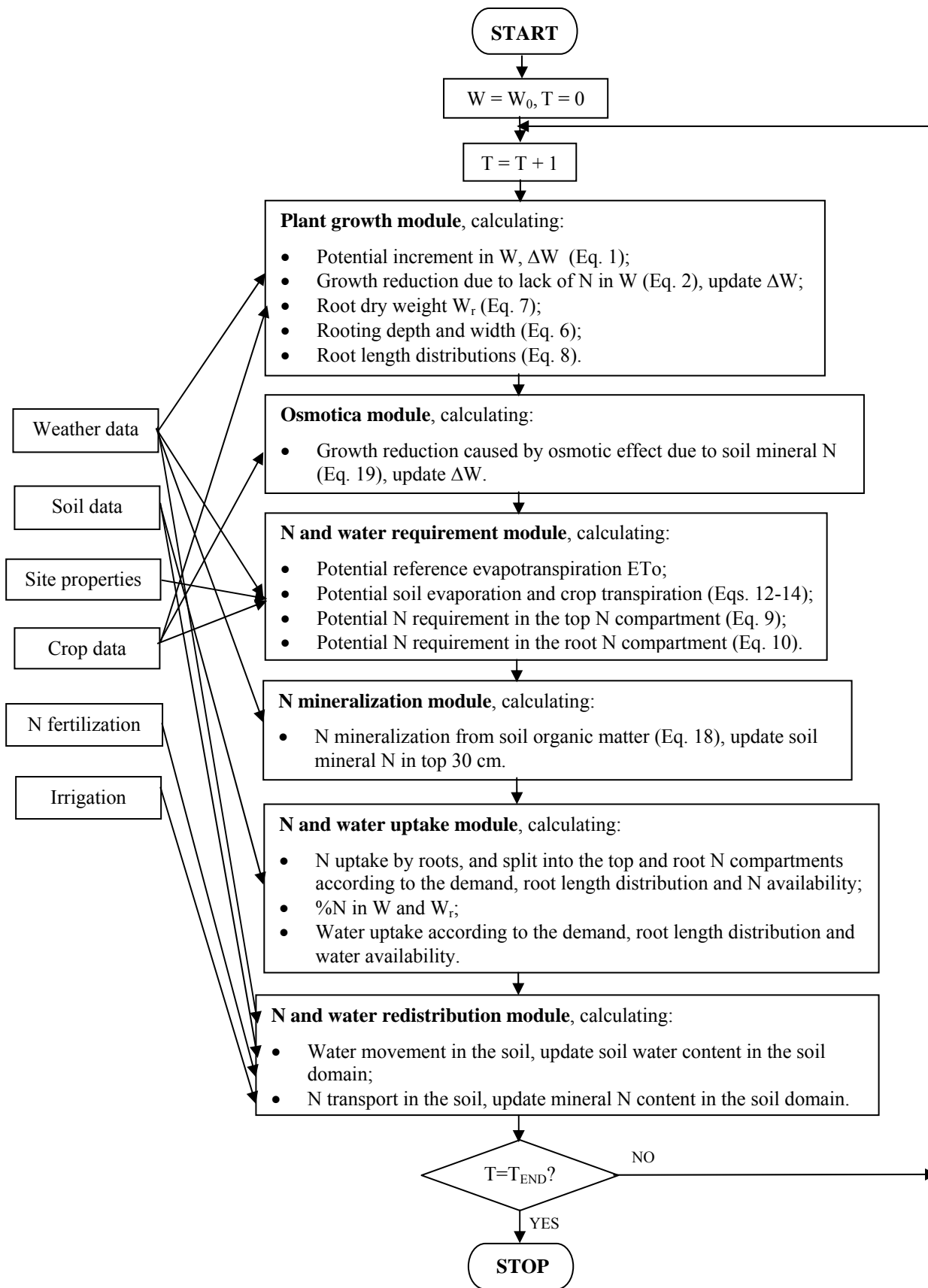


Fig. 1

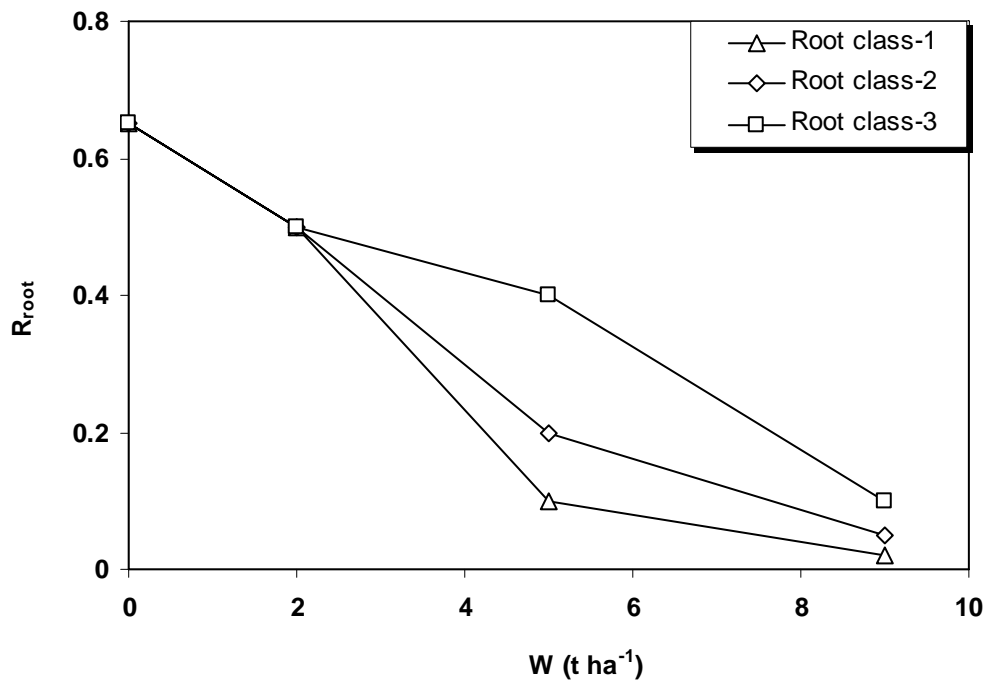


Fig. 2

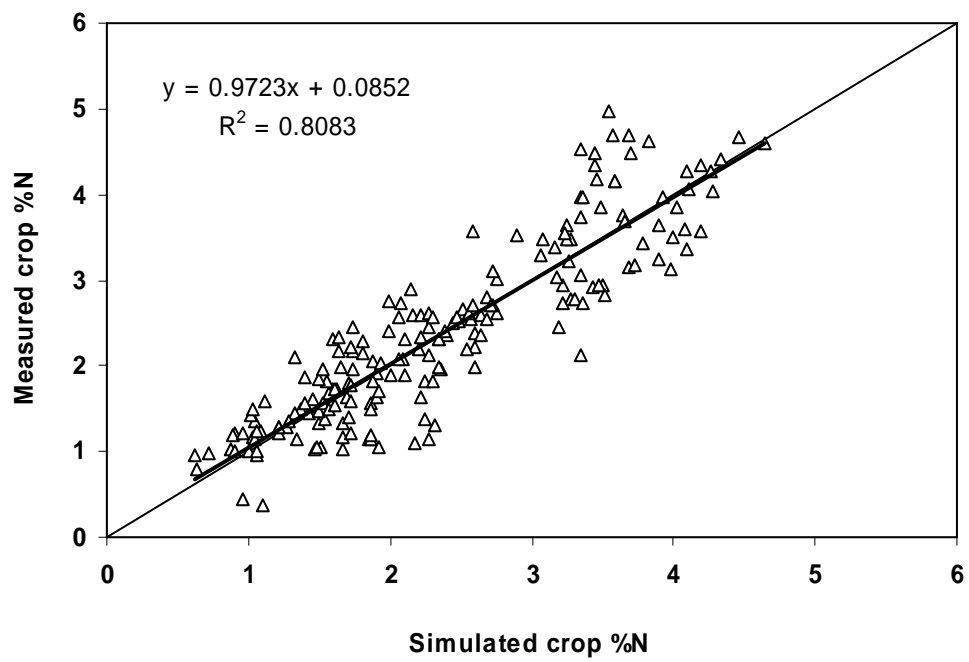


Fig. 3

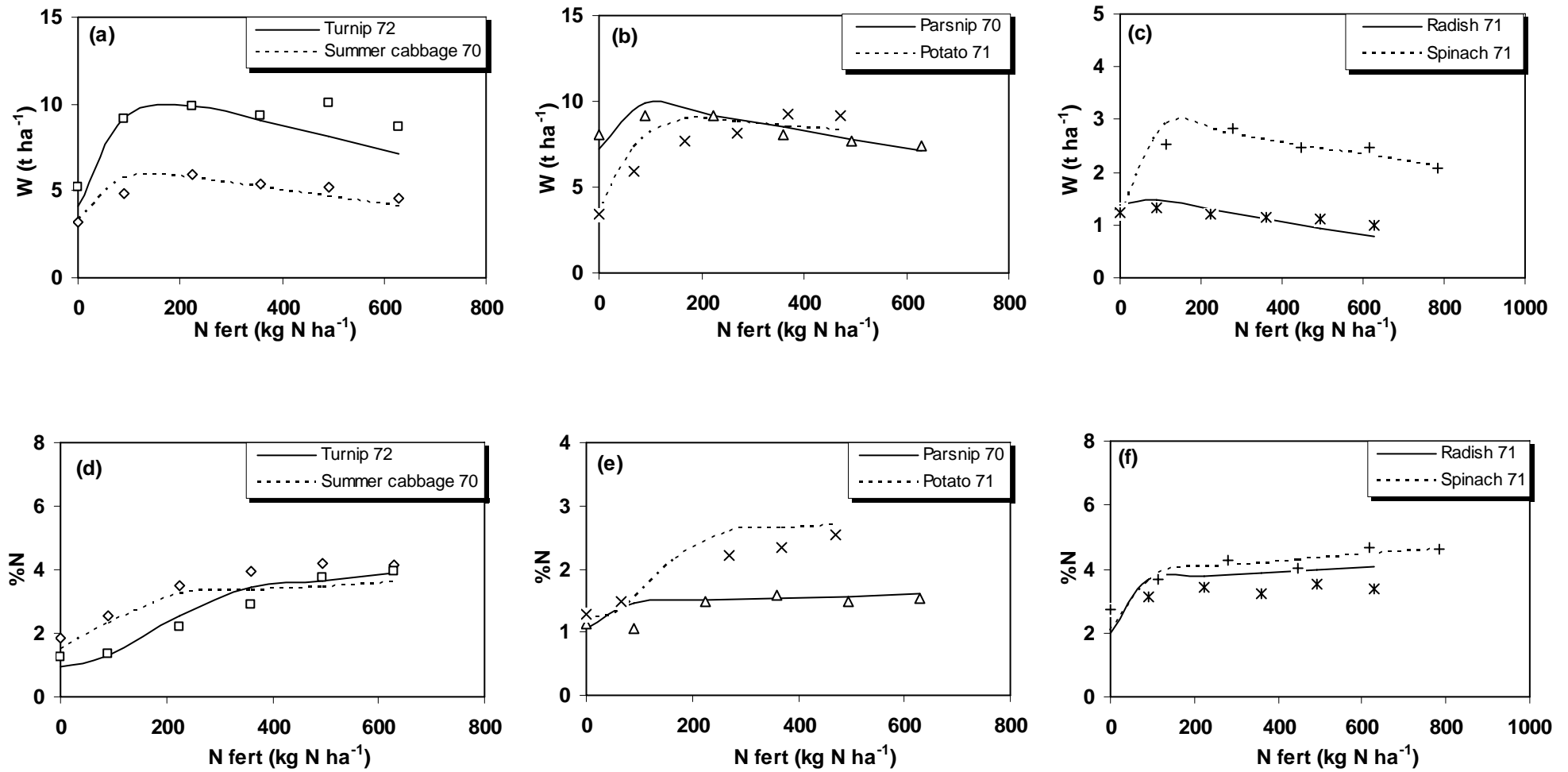
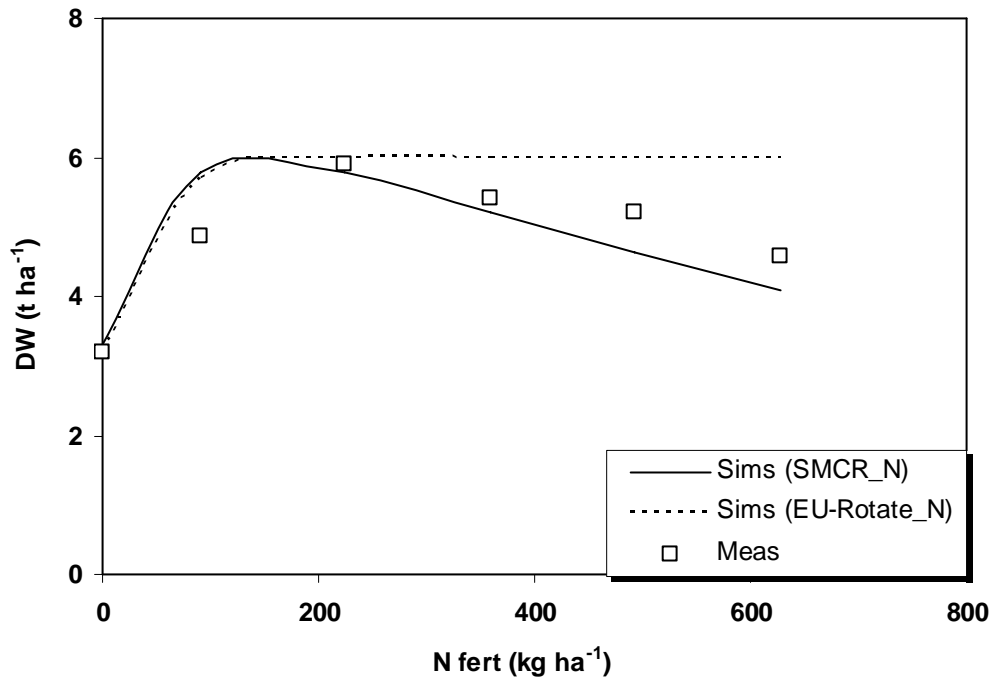
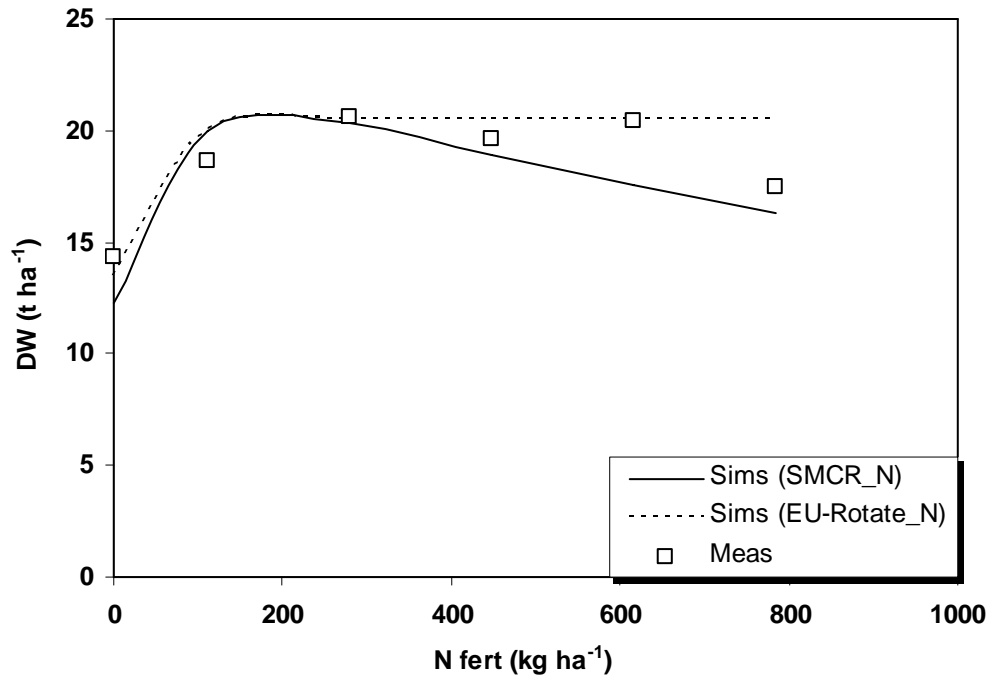


Fig. 4



(a)



(b)

Fig. 5



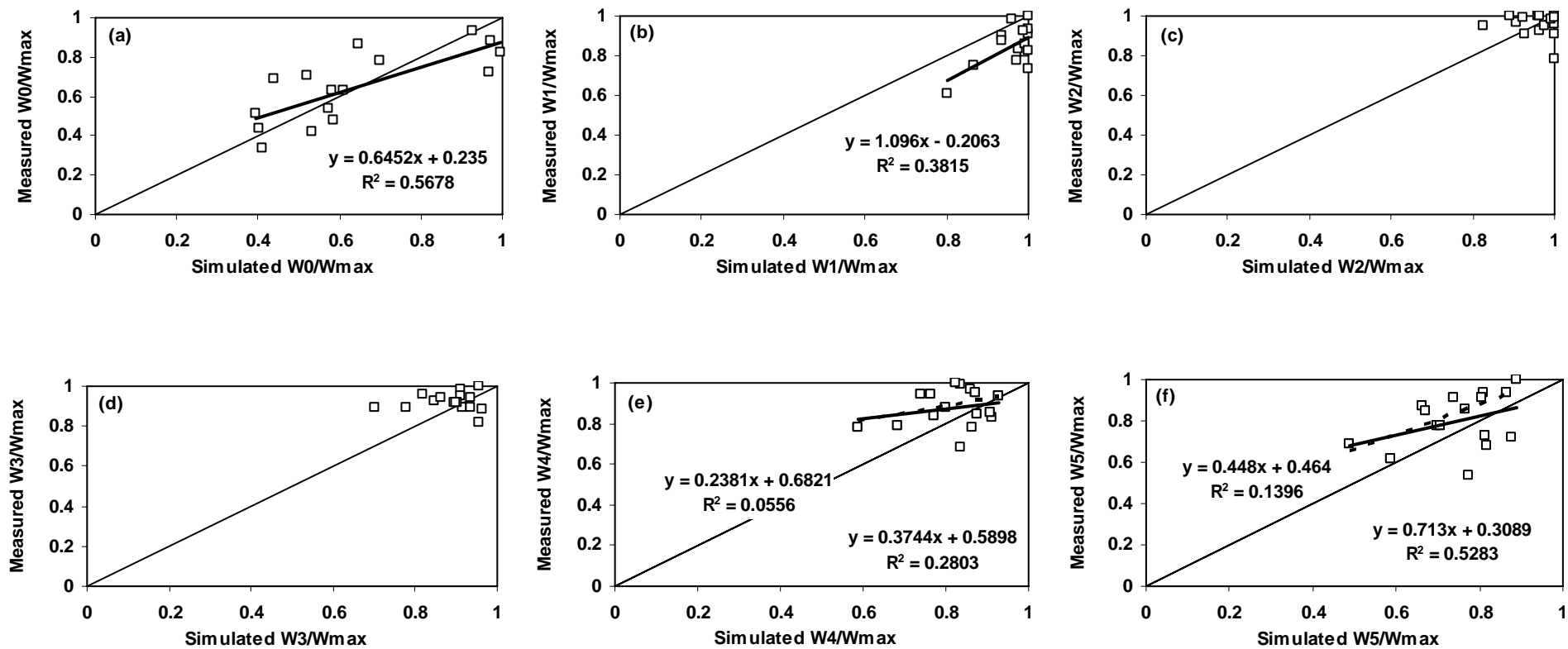
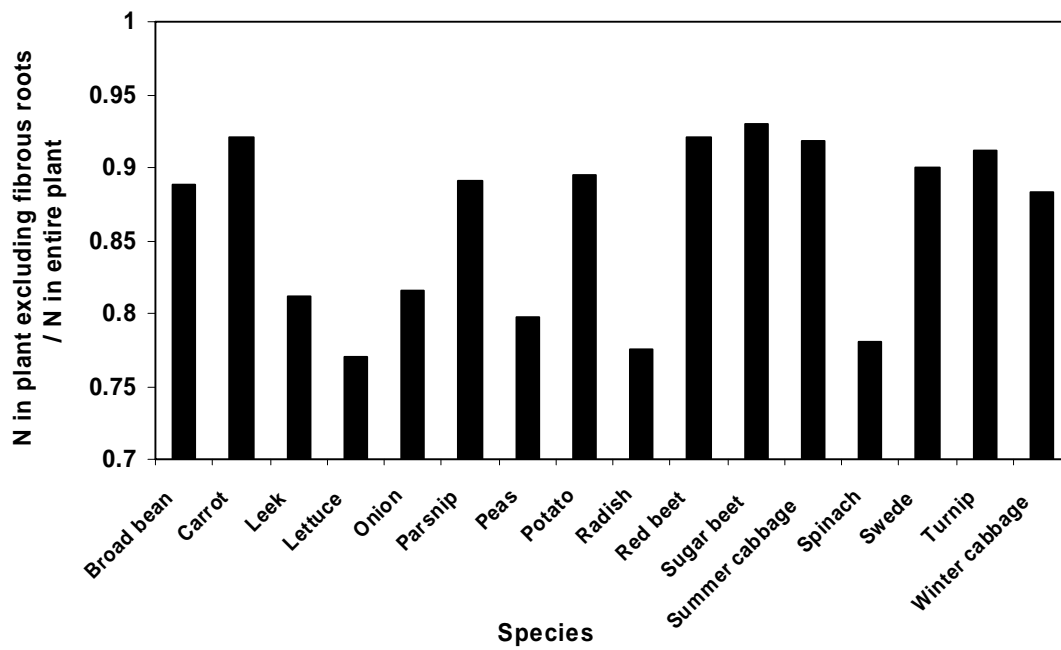
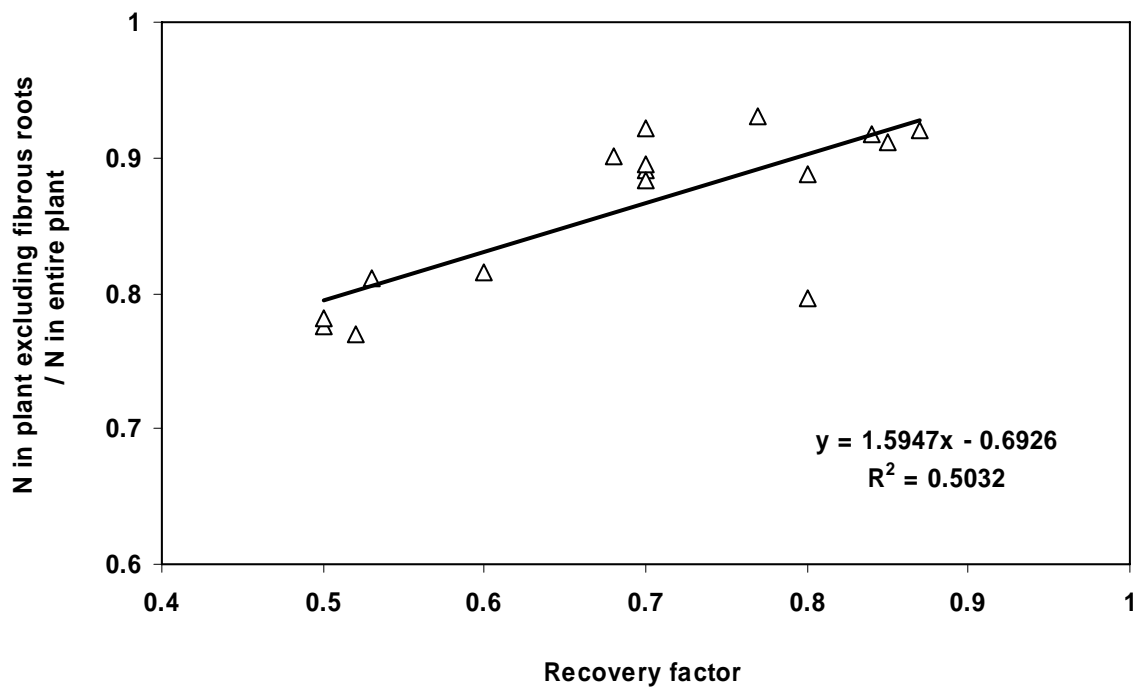


Fig. 6



(a)



(b)

Fig. 7

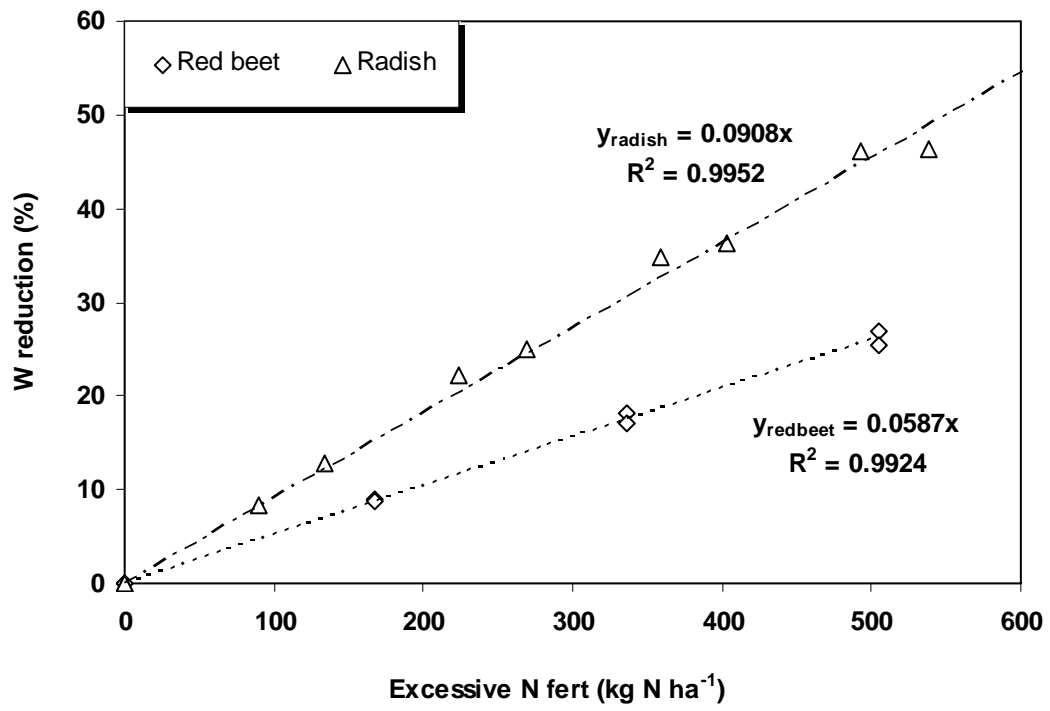
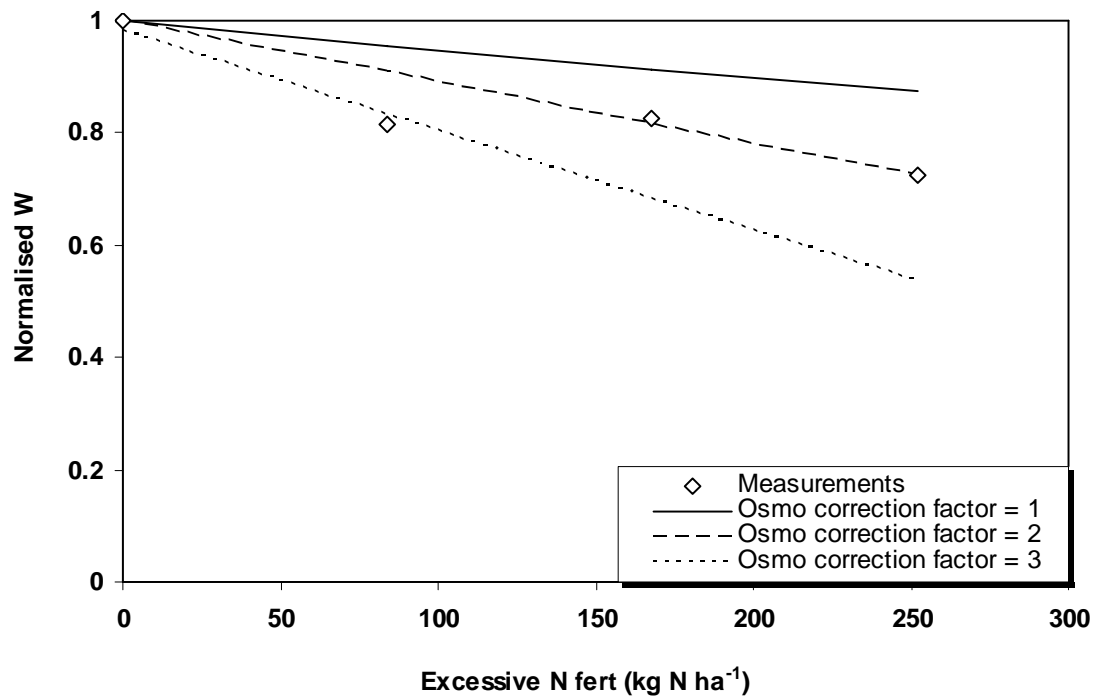
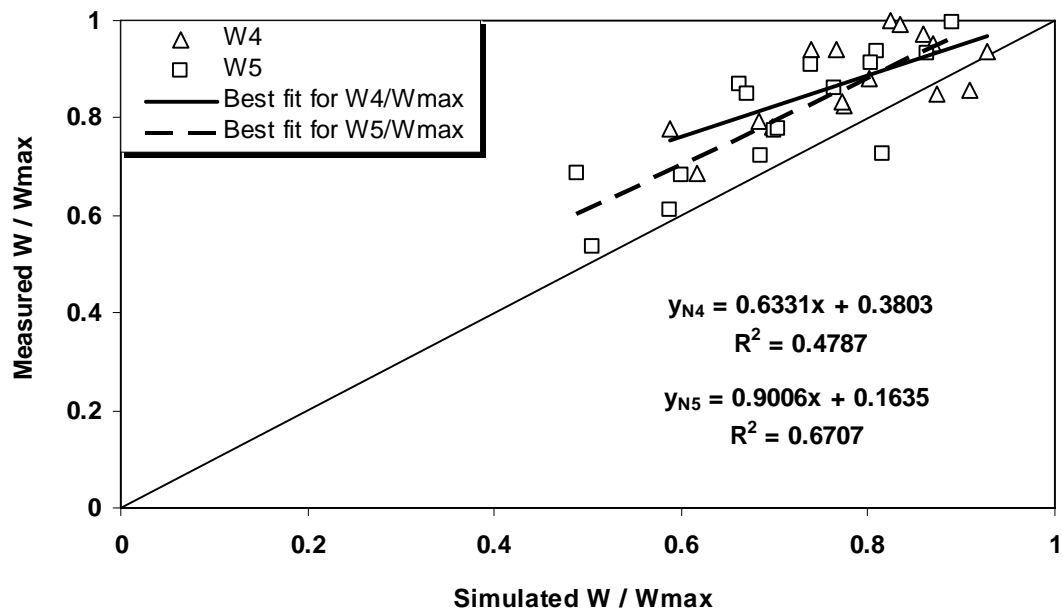


Fig. 8

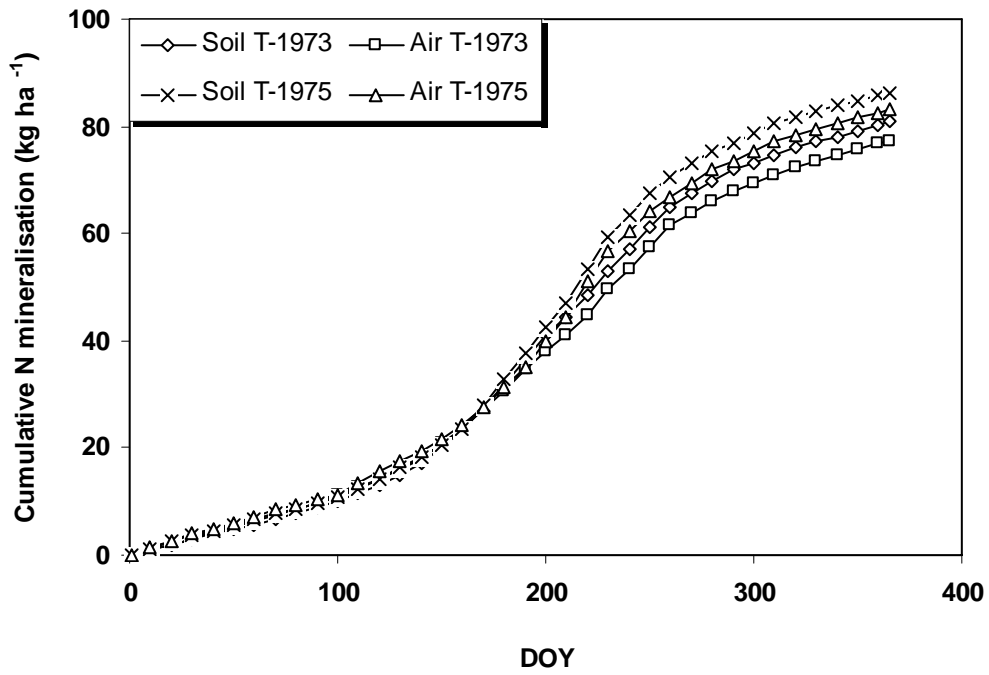


(a)

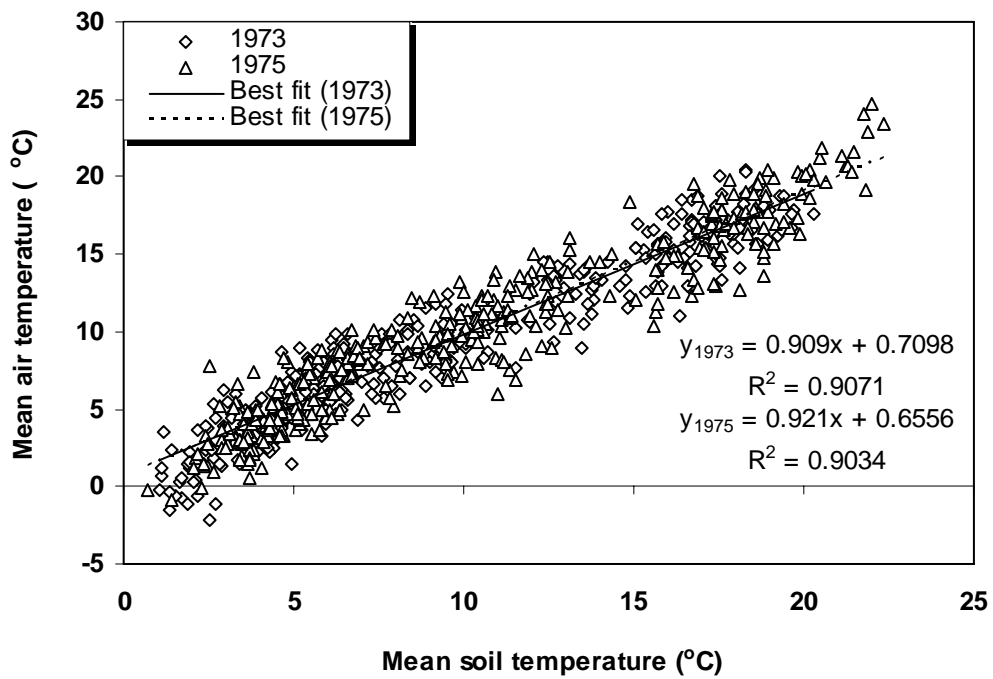


(b)

Fig. 9



(a)



(b)

Fig. 10