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1 **Evaluation of a generic agro-hydrological model for water and nitrogen**

2 **dynamics (SMCR_N) in the soil-wheat system**

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10

11 **Abstract**

12

13 Agro-hydrological models have widely been used for optimizing resources use in

14 agriculture for maximum crop growth and minimum environmental consequences.

15 The SMCR_N model is a recently developed, process-based, multi-crop and

16 management-oriented agro-hydrological model for water and nitrogen dynamics in

17 the soil-crop system, and has been validated against data from field experiments over

18 a range of vegetable crops. In this study, the model is further tested against the

19 comprehensive measured datasets from field experiments conducted under different

20 circumstances on wheat. It has been found that given the proper parameterization of

21 the simple growth equation, which worked well with vegetable crops, the model was

22 able to simulate wheat growth accurately. The predicted relative root length density

23 distributions at various development stages agreed with the measurements and those

24 modeled by alternative approaches in the literature. The explicit hydrological

25 algorithm for the basic equations governing water and nitrogen transport in soil

performed well. Compared with other conventional numerical schemes, the algorithm used in the study was much simpler and easy to implement. The simulated spatial-temporal soil water content was in good agreement with the measurements, given the information of groundwater table was known. The model was also capable of reproducing the data of nitrogen uptake and soil mineral nitrogen concentration measured at depths and at time intervals. This indicates that the key equations for various processes governing water and nitrogen dynamics in the soil-wheat system were correctly formulated, and the model was properly parameterized. The results from this exercise, together with the model's previous validation over 16 vegetable crops, make the model a good candidate to be used for water and nitrogen management for growing diverse crops.

Key words: SMCR_N model, soil-crop system, wheat, water and nitrogen dynamics, resources management.

1. Introduction

Mechanistic agro-hydrological models are powerful tools in managing water and fertilizer use for optimal crop growth, and in evaluating the consequences of different farming practices on the environment. Numerous agro-hydrological models have been developed for assisting irrigation scheduling (Bastiaanssen et al., 2007) and assessing the effects of fertilizers on crop growth for various crop species and the environmental impacts, with a large proportion of models developed solely for nitrogen (N) fertilizer (Cannavo et al., 2008).

1   With the advance in computing power and the increasingly understanding on

2   soil and plant sciences, many of the developed agro-hydrological models have

3   become extremely sophisticated. These models include the most prominent ones such

4   as the EPIC models that cover a range of crops (Williams et al., 1993) and the DSSAT

5   models (Hoogenboom et al., 1999). While the models of such are useful for basic

6   research and studying the effect of climate on crop growth, the models are generally

7   too complicated to use for water and N management purposes. These models are crop

8   specific, and require parameter values which are difficult to determine for a given

9   crop. This is a common feature for the majority of crop N models. Cannavo et al.

10   (2008) surveyed 62 crop N models, and found that only 2 models were able to

11   simulate N cycle for 4 crops families, while the rest were only able to deal with a

12   single crop. Efforts have been made to develop a generic crop N model which could

13   be used for growing a wide range of crops. The SMCR_N model, based on N_ABLE

14   (Greenwood, 2001) and EU-Rotate_N (Rahn et al., 2010), has been devised for crop

15   N response and N leaching in arable soils (Zhang et al., 2009). Compared with most

16   models of its kind, the SMCR_N model strikes a balance between generality and

17   complexity. The generality of the model was made possible due to the discoveries that

18   both crop critical %N for maximum growth and crop dry matter increment during

19   growth could be described by unified equations (Greenwood et al., 1985). By setting a

20   pre-defined set of values for each crop, the model used the same algorithm to simulate

21   N responses for different crops. Rigorous and systematic validation of the model has

22   revealed that the SMCR_N model was able to reproduce the measurements of

23   responses of crop yield and mineral N composition to fertilizer N from 32 field

24   experiments over 16 vegetable crops (Zhang et al., 2009). However, the ability of the

25   model to simulate the similar responses has not been tested yet for cereal crops, a

1   major and important crop family in crop production. To make the model to be

2   applicable for water and N management for growing diverse crops, it is essential to

3   validate the model for cereal crops.

4

5   The model SMCR_N concerns many processes in the soil-crop systems such

6   as plant growth, N turnover, water and N transfers etc.. Rigorous validation of the

7   model requires frequent measurements in the above-ground biomass and in the soil

8   during growth. Such measurements from field experiments on crops are labor-

9   intensive and rarely available. Therefore the systematic evaluation of the model for all

10   cereal crops is difficult due to the lack of appropriate data. However, fortunately there

11   were measured datasets available from the experiments on wheat for testing the model

12   (Groot and Verberne, 1991). The experiments were conducted under various

13   circumstances ranging from different soil textures in profiles to different groundwater

14   tables. Unlike those from many other field crop experiments, the measurements from

15   these experiments (Groot and Verberne, 1991) were comprehensive and systematic,

16   including above-ground dry weight and its N composition, soil water content and

17   mineral N concentration at various depths, and the groundwater table at time intervals,

18   which enabled to examine the model rigorously in many key aspects.

19

20   The aim of the study was to validate the SMCR_N model against the data

21   mentioned above from the field experiments on wheat to assess the ability of the

22   model in predicting water and N dynamics in the soil-wheat system. To enable the

23   validation to be carried out more accurately, the simple equations describing crop dry

24   matter accumulation and root growth, which greatly influences water and N dynamics

1   in the soil-crop system, were first calibrated using the sequential measurements of

2   crop dry weight and rooting depth during growth from independent experiments.

3

4   **2. Materials and methods**

5

6   *2.1 The SMCR_N model*

7

8   SMCR_N is a recently developed, generic and mechanistic model for water

9   and N dynamics in the soil-crop system (Zhang et al., 2009). Here a brief description

10   of major modules in the model, i.e. including those for plant growth, water and N

11   requirements, actual water and N uptake, N mineralization, and soil water and mineral

12   N re-distributions, is given in order to assist the reader to understand the framework

13   of the model. Also, to help the model parameterization the key equations employed in

14   the model are listed in the Appendix (Tables A1, A2). Detailed description of the

15   model is given in Zhang et al. (2009).

16

17   Plant growth module simulates daily dry weight increments in plant excluding

18   fibrous roots and root growth (see Eqs. A1-A6). The potential maximum increments

19   in plant dry weight excluding fibrous roots and in root dry weight and rooting depth

20   are driven by daily air temperature. The reduction in dry weight increment due to N

21   deficiency in crop is also considered. The root length is assumed to decline

22   logarithmically from the soil surface downwards. Crops are considered to have two N

23   compartments, a top N compartment and a root N compartment. The top N

24   compartment contains N in the above ground dry weight W, whereas the root N

25   compartment stores N allocated in fibrous roots. The potential N requirement in both

1   compartments are calculated from plant dry weight, root dry weight, N concentrations,

2   and the critical N concentration for a plant of the same mass and its potential

3   maximum increment in dry weight (Eqs. A7, A8). The potential water demand is the

4   crop evapotranspiration, which is calculated using a dual crop coefficient method

5   recommended by the FAO (Allen et al., 1998) (Eqs. A10, A11). The actual root water

6   uptake is dependent on crop water demand, root length distribution and soil water

7   availability (Eq. A12). The detailed procedure in modeling root water uptake can be

8   seen in Yang et al. (2009) and Zhang et al. (2010). The actual N uptake, which relates

9   with the crop N demand, root length distribution, soil mineral N concentration and the

10   minimum soil mineral N concentration for root uptake, is formulated in Eqs. (A13)

11   and (A14) based on the work by Pedersen et al. (2010). Soil N mineralization is

12   quantifies by assuming that the organic matter breakdown rate is in first-order. The

13   effect of air temperature on N soil mineralization is considered according to Johnsson

14   et al. (1987) (Eq. A15). Unlike that in the previous version of the model where a

15   cascade approached was employed (Zhang et al., 2009), modeling water and N

16   dynamics in soil is carried out using the basic flow theory (Eqs. A16-A17). The

17   governing flow and transport equations are solved using an explicit algorithm

18   formulated in Eqs. (A18) and (A19). The approach considers that water movement

19   and mineral N transport in a 5 cm soil layer is only influenced by its adjacent layers in

20   a small time step of 0.001 d. Detailed steps of implementing such an algorithm have

21   been reported in Yang et al. (2009).

22

23   *2.2 Experiments*

24

1   The experiments used for calibration and validation in the study were

2   conducted on three different farms with two contrasting soils cropped with winter

3   wheat at the Institute for Soil Fertility Research, Netherlands from 1982 to 1984

4   (Groot and Verberne, 1991). The three experimental farms were: the Bouwing farm,

5   the EEST farm and the PAGV farm. The soil in the Bouwing farm was silty clay loam,

6   while the soil in the EEST and PAGV farms was silty loam. In total six experiments

7   with three fertilizer N treatments each were carried out, namely BOUW_83,

8   BOUW_84, PAGV_83, PAGV_84, EEST_83, EEST_84 (Table 1). The

9   measurements included spatial-temporal soil water content, soil mineral N as well as

10   above-ground dry matter accumulation, and N content in various organs during

11   growth. The measurements of soil water content and mineral N concentration in the

12   layers of 0-30, 30-60 and 60-90 cm in the BOUW_83, PAGV_83 and EEST_83

13   experiments and of 0-20, 20-40, 40-60, 60-80 and 80-100 cm in the BOUW_84,

14   PAGV_84 and EEST_84 experiments were made at intervals of three weeks. The

15   above-ground dry weight and mineral N content in different organs were measured at

16   the same time as these for soil water content and mineral N concentration. Also the

17   time-course of groundwater tables were measured in the BOUW_84, PAGV_84 and

18   EEST_84 experiments, but no efforts were made for measuring the groundwater table

19   in the other experiments. The summary of the experiments is given in Table 1. Details

20   of the experimental set-up together with the time-course measurements of above-

21   ground dry weight, rooting depth and root length distribution, groundwater table and

22   weather variables can be seen in Groot and Verberne (1991).

23

24   **3. Model calibration and validation**

25

1   The measured data of wheat above-ground dry weight and rooting depth at

2   time intervals during growth from the experiments on the EEST farm, i.e. the

3   EEST_83 and EEST_84 experiments, was used for calibrating the equations

4   describing crop growth and root development. The data from other 4 experiments on

5   the Bouwing and the PAGV farms, i.e. the BOUW_83, BOUW_84, PAGV_83 and

6   PAGV_84 experiments, was used for model validation.

7

8   *3.1 Calibration of the equations for plant above-ground and root growth*

9

10   The plant above-ground growth equation Eq. (A1) was constructed based on

11   the sequential measurements of W of mainly vegetable crops grown under optimum

12   conditions during the main growing season in the UK from seeding until the onset of

13   senescence (Greenwood et al., 1977). It was found that Eq. (A1) with $K_1 = 1$ t ha^{-1}

14   reproduced the measurements of W reasonably well. However, the suitability of such

15   a parameterization for wheat growth requires to be examined. In order to obtain the

16   appropriate growth coefficient K_1, the sequential measurements of above ground dry

17   weight in the EEST experiments under the N2 and N3 treatments from the first

18   measurement to the maximum biomass were used. The exclusion of the data from the

19   N1 treatment from the procedure of finding optimum K_1 was due to the possibility of

20   the crop grown under N-limiting conditions.

21

22   Since only one parameter was involved in the fitting procedure, it was not

23   difficult to find the optimum value of K_1. A simple procedure was employed to

24   establish the relationship between the sum of the squares of the differences between

25   the measured and simulated dry weight at intervals and the growth coefficient, and the

1   optimum value of K_1 was found to be 0.38 t ha^{-1}. It can be seen that the simulated dry

2   weights with the optimum value of K_1 agree well with the measurements throughout

3   growth (Fig. 1), indicating that the calibrated growth equation is sufficiently accurate

4   to describe wheat growth.

5

6   Calibration was also carried out for determining the root penetration rate. To

7   do so the information from the measured rooting depth was considered (Groot and

8   Verberne, 1991). By using the measured rooting depths at different intervals and the

9   calculated cumulative day degree, the penetration rate K_{rz} in Eq. (A4) was determined

10   as 0.097 cm d^{-1} ^{o}C^{-1}, close to that of some vegetable crops (Pedersen et al., 2010;

11   Zhang et al., 2009). The maximum rooting depth at the maximum above-ground

12   biomass was calculated as 1.2 m, in line with the guidance of the maximum rooting

13   depth of 1.5 m for wheat by the FAO (Allen et al., 1998).

14

15   *3.2 Model validation*

16

17   Soil water retention curves for different layers in the Bouwing experiments (0-

18   40 and 40-100 cm) and the PAGV experiments (0-25, 25-40 and 40-100 cm) were

19   given in Groot and Verberne (1991). The values of the van Genuchten hydraulic

20   parameters used in the study to describe the soil water retention curves were fitted

21   using the RETC software (van Genuchten et al., 1991) and are listed in Table 2.

22   Considering the fact that there were layers of gravel at the depth of about 100-120 cm

23   in the Bouwing experiments (Groot and Verberne, 1991), it was decided that the

24   calculated soil domain was 120 cm down from the surface, and set the boundary

25   condition at the bottom as free drainage. In the PAGV experiments, the calculated soil

1   domain was down to 200 cm and set the water content at saturation in the soil below

2   the measured groundwater table. The soil hydraulic properties below 100 cm for both

3   cases were taken as the same as those in the layers immediately above. Other

4   parameter values used in the simulations are given in Table A1.

5

6   The crop was sown in October in the previous year in all the experiments, but

7   no measurements of soil water content and mineral N concentration were taken until

8   the following February. Thus the dates and values of the first measurements of soil

9   water and mineral N concentration were used as the starting points and the initial

10 conditions in the simulations. The used weather information was from Groot and

11 Verberne (1991).

12

13 **4. Results**

14

15   The simulated values of crop dry weight and N uptake were strongly

16 correlated with the measured values throughout growth in all the experiments (Fig. 2).

17 Regressions of simulated and measured values gave high R^2 of 0.97 to the dry weight

18 and of 0.89 to the N uptake. Further, the regression coefficients of 0.90 and 1.04 for

19 the dry weight and N uptake are close to 1.0, indicating that the model is capable of

20 reproducing the measured values well.

21

22   The simulated relative root length density was compared with the

23 measurements at different time intervals in all the experiments (Fig. 3). Good

24 agreement between measurement and simulation was observed (R^2 = 0.82). Also

25 shown in Fig. 3 are the relative root length distributions for wheat calculated using the

1   available equations in the literature (Wu et al., 1999; Zuo et al., 2004). Zuo et al.

2   (2004) described the root length distribution using a highly non-linear equation with

3   four parameters, while Wu et al. (1999) formulated the distribution with a third-order

4   polynomial equation. Both equations were derived based on comprehensive datasets

5   made up from measurements. It can be seen that the simulated relative root length

6   distribution in the study was in good agreement with these calculated by Wu et al.

7   (1999) and Zuo et al. (2004).

8

9   The simulated values of soil water content also agreed well with the measured

10 values (Fig. 4a) ($R^2 = 0.68$). Over the 160 comparisons only 30 differed by more than

11 $0.05 \text{ cm}^3 \text{ cm}^{-3}$ and 3 by more than $0.1 \text{ cm}^3 \text{ cm}^{-3}$. Compared with soil water content,

12 the simulated soil mineral N concentration was less satisfactory (Fig. 4b), although

13 statistically the simulated values of soil mineral N concentration was still correlated

14 fairly well with the measured values ($R^2 = 0.41$). However, the value of R^2 increased

15 greatly to 0.66 if the regression without the data from the PAGV_83 experiment was

16 carried out.

17

18   The simulated dry weight, N uptake, soil water content and mineral N

19 concentration in various layers at intervals were compared in detail with the

20 measurements. Fig. 5 illustrates such comparisons for the N2 treatment in the

21 PAGV_84 experiment as an example. The agreement between measurement and

22 simulation was good. Similar agreement was also simulated for other experiments

23 (data not shown), except for the PAGV_83 experiment where considerable

24 discrepancies between measurement and simulation were observed from the soil water

25 content and soil mineral N concentration as demonstrated in Fig. 6. The simulated soil

11

1 water content in the 60-90 cm layer was markedly lower than the measured values

2 (Fig. 6a), while the simulated soil mineral N concentration in the 0-30 cm layer was

3 much higher than the measured values (Fig. 6b).

4

5   Water dynamics in the various processes in the soil-wheat system was

6 simulated as illustrated in Fig. 7(a) for the BOUW_84 experiment. In this case, crop

7 evapotranspiration was mainly met by rainfall during the growing season and soil

8 water originally contained in the soil column. The cumulative rainfall during the

9 period was 244 mm, which accounts for a large proportion of water to meet crop

10 evapotranspiration. At the end of the simulation 93 mm of water originally contained

11 in the soil was depleted. The opposite changes in the cumulative rainfall and the

12 cumulative water flux from the soil column show that the charge of water to the soil

13 column occurred when rainfall events intensified. Water percolation at 1 m from the

14 soil surface was not great. The cumulative water percolation was 17 mm and only

15 occurred at the early stages of crop development when the soil was relatively wet.

16

17   The simulated cumulative N uptake, N mineralization from soil organic matter,

18 N leaching at 1 m depth together with the cumulative applied fertilizer-N under the

19 N3 treatment in the BOUW_84 experiment are shown in Fig. 7(b). N uptake by the

20 crop before Day 100 was small, and followed by a stead increase. N mineralized from

21 soil organic matter accumulated with time, and the accumulation rate increases with

22 time as well. During the growing period, the total N mineralized from soil organic

23 matter was about 97 kg ha^{-1}. At the end of the simulation the simulated cumulative N

24 uptake was 307 kg ha^{-1}, which was mainly met by the fertilizer-N and the mineralized

1 N from the soil. N leaching at 1m depth was ignorable as the total simulated value

2 was only 2.5 kg ha^{-1}.

3

4 **5. Discussion**

5

6 *5.1 Model overall performance*

7

8 Good agreement was achieved between measurement and simulation for

9 various variables including above-ground dry matter accumulation, relative root

10 length distribution, N uptake, spatial-temporal water content and mineral N

11 concentration in the soil profile in all the experiments with few exceptions. This

12 suggests that the overall model performance was satisfactory, indicating that the

13 various processes governing water and N dynamics in the soil-crop system were

14 reasonably quantified, and the parameterization of the model was properly carried out.

15 Thus the proposed model has the potential to be adopted for optimal management of

16 water and fertilizer N in wheat production.

17

18 *5.2 Major discrepancies and possible explanations*

19

20 Despite overall satisfactory performance of the model, there were still marked

21 discrepancies between measurement and simulation. The main discrepancies concern

22 soil water content in the 60-90 cm layer (Fig. 6a) and soil mineral N concentration in

23 the 0-30 cm layer (Fig. 6b) in the PAGV_83 experiment. The simulated soil water

24 content in the 60-90 cm layer was considerably lower than the measurement. This

25 might be due to the fact that groundwater effect was not properly considered in the

1 simulation. According to the measurements in the PAGV_84 experiment which was

2 conducted on the same site, the groundwater table was high, ranging from 86 cm to

3 173 cm from the surface. This inevitably has a significant effect on soil water in the

4 profile, especially in the region near the groundwater table. However the groundwater

5 information in the PAGV_83 experiment was not available. This has led to the

6 assumption of free drainage at the lower boundary, which may not reflect the reality

7 of the case, resulting that the simulated soil water content was lower than the

8 measurement.

9

10 In the 0-30 cm soil layer in the PAGV_83 experiment, the model simulated a

11 sharp increase in soil mineral N after the fertilizer-N application (Fig. 6b). However

12 this was not materialized in the measurement. Such a phenomenon of 'disappearance'

13 of the applied fertilizer-N was observed elsewhere (Nielsen and Jensen, 1986), and

14 might be attributed to the microbial immobilization (Kersebaum and Richter, 1991)

15 which was not considered in the study. The deviation of the simulated soil mineral N

16 concentration from the measurement at late crop development stages may be due to

17 the assumed minimum soil N concentration below which the roots cannot take up N

18 from the soil. The minimum N concentration was set to be 0.0035 kg m^{-3}, equivalent

19 to about 10 kg-N ha^{-1} in a 30 cm soil layer. This was supported by the experimental

20 evidence (Thorup-Kristensen and Sørensen, 1999; Thorup-Kristensen, 2006) and

21 worked well for many vegetable crops (Zhang et al., 2009), but might be too high for

22 wheat since the measured soil mineral N concentration was frequently close to zero

23 (Fig. 6b). This indicates that wheat might have a greater capacity of depleting mineral

24 N from the soil than many vegetable crops.

25

1   *5.3 Advantages of using the explicit algorithm for hydrological simulation*

2

3   Hydrological simulation plays a crucially important role in the agro-

4   hydrological models. Many agro-hydrological models adopt the cascade approaches

5   in simulating soil water movement (Cannavo et al., 2008; Ranatunga et al., 2008).

6   These approaches, simple though, are not capable of producing satisfactory

7   predictions of soil water on a daily basis (Ranatunga et al., 2008). Further, they are

8   not able to simulate capillary flow, and thus cannot be applied to the circumstances of

9   high groundwater table. The algorithm used in the study for hydrological simulations

10 was recently proposed by Yang et al. (2009). The distinctive feather of the algorithm

11 is that it uses an explicit numerical scheme to the basic equations for soil water

12 movement and N transport in uniform 5 cm soil layers and a small time step of 0.001

13 d. Compared with the traditional schemes such as finite element method (Šimůnek et

14 al., 2008), the employed algorithm is much simpler and easy to implement. The

15 simplicity of the algorithm helps to use the basic theory of soil water flow and solute

16 transport in the agro-hydrological models for accurate simulations. Moreover, the

17 small time step provides the potential to use the weather information collected at

18 small time intervals (Yang et al., 2009).

19

20 *5.4 Wheat above-ground growth*

21

22   The growth equation for crop dry weight excluding fibrous roots used in the

23 study was simple and air temperature driven. It gave good description of growth for

24 many vegetable crops from seeding to the onset of senescence with the growth

25 coefficient K_1 being 1 t ha^{-1} (Greenwood et al., 1977). However it has been shown that

1 for wheat the coefficient has a smaller value of 0.38 t ha^{-1}. This suggests that while

2 the growth equation with the default value of K_1 of 1 t ha^{-1} can generally simulate

3 growth reasonably for various crops, the growth coefficient should be calibrated

4 individually for different crops when data is available since the crop growth is one of

5 key factors controlling water and N dynamics in the soil-crop system. Also, it should

6 be pointed out that the growth equation only describes wheat above-ground dry matter

7 accumulation with the specified dry weight at harvest, it is not able to predict the

8 grain yield, nor the final total dry weight. Therefore it cannot be used to study the

9 effect of climate on wheat growth and grain yield as some specifically designed

10 models for cereal crops do, for example CERES-wheat (Ritchie et al., 1988) and

11 CropSyst (Stockle et al., 2003) where the simulation of crop physiology forms a main

12 part of the models. However, under normal circumstances, the final dry weight yield

13 for a given crop grown in a specific location can be estimated with certainty in

14 advance according to the previous experience. Thus the model presented in the study

15 is robust enough for the purposes of water and fertilizer N management in wheat

16 production.

17

18 *5.5 Root development*

19

20   Root development simulation is a key part in modeling water and N transfer in

21 the soil-crop systems. Accurate modeling of root dynamics is extremely difficult since

22 the development and proliferation of roots in soil are affected by a number of factors

23 such as the supply of photosynthates from the shoot, the nutrient status of the plant,

24 soil type and compaction, water potential at the root surface and availability and

25 distribution of nutrients (Forde and Lorenzo, 2001; Bloom et al., 2003; Hammond and

White, 2008). Dynamic root architecture models including detailed modeling of individual roots have been developed (Pages et al., 2004; Kohl et al., 2007). Such models are useful for basic research to understand the mechanisms of resource uptake by roots, but are generally not suitable for ago-hydrological models because of a lack of data to evaluate the models. In the soil-wheat system, Wu et al. (1999) and Zuo et al. (2004) empirically formulated the distribution of wheat root length based on experimental measurements. Good agreement between the modeled relative root length distribution in the study and the results from the experiments and calculated by the equations of Wu et al. (1999) and Zuo et al. (2004) (Fig. 3) indicates that the employed simple approach for root dynamics is able to describe root length distribution in the soil for wheat. However, it should be pointed out that the model used in the study is rather simple. It does not take into consideration of other factors such as soil structure, soil water content and nutrients status. Although the model gave good descriptions of root development of crops observed in a number of studies in humid conditions (Kage et al., 2000; Kristensen and Thorup-Kristensen, 2004; Thorup-Kristensen, 2006), cautions need to be taken to apply the root model for crops grown under complex situations such as dry climates where low soil water content could be a limiting factor controlling root growth (Yang et al., 2009).

5.6 Water and N dynamics in the soil-wheat system

The simulations in the study highlighted the importance of considering the effect of groundwater table in water transfer in the soil-crop system. Yang et al. (2009) have demonstrated that the groundwater table has a profound influence on soil water and crop evapotranspiration. This has been confirmed in the study. Since the

1   groundwater table was not considered properly in the PAGV_83 experiment, the

2   simulated soil water content deviated markedly from the measurements (Fig. 6a).

3   Therefore it is critically important to have the information of groundwater table on the

4   experimental site, and the agro-hydrological models capable of considering the effect

5   of groundwater on water dynamics in the soil-crop system to enable the simulations to

6   be carried out reliably.

7

8   Rigorous assessment of the algorithms for N dynamics in the soil-wheat

9   system was difficult since there were processes where N dynamics was not measured

10   such as N incorporation in roots, and the processes which were not considered such as

11   N transformation in the soil. Nevertheless, it is possible to make some assessment of

12   the performance of the model on N dynamics. The simulated values of N uptake in the

13   above-ground dry weight (Fig. 2b) and mineral N in various layers (Fig. 4b) were

14   nearly 1:1 to the simulated values. The simulated N incorporated in the roots could

15   not be quantitatively validated due to unavailable experimental data, but the approach

16   for considering N partitioned in roots was reasonable for many crops as demonstrated

17   in Zhang et al. (2009). Further, the critical %N curve for roots during growth is

18   supported by the experimental evidence (Osaki et al., 1997). The used soil organic

19   matter breakdown rate is similar to those used in other models (Mueller et al., 1996;

20   Fu et al., 2000; Fang et al., 2005). The simulated N leaching at 90 cm soil depth was

21   small (Fig. 7b), which was supported by the finding of Neeteson and Carton (2001)

22   that N leaching mainly occurred from late autumn to early spring on the Western

23   European soils, out of crop growing seasons. Based on the above it is reasonable to

24   conclude that for this soil, losses of N from processes such as ammonia volatilization

25   and N transformation in the soil were generally small, in agreement with the previous

1   studies on a similar soil in the UK (Zhang et al., 2007; 2009). However, it appears that

2   the PAGV_83 experiment was an exception where N losses from these processes

3   might be significant for some reason (Fig. 6b).

4

5   *5.7 Model application and future development*

6

7   The model presented in this study, based on its previous version (Zhang et al.,

8   2009), improves the hydrological predictions by replacing the cascade approach with

9   the basic flow theory which was solved by a newly developed simple and explicit

10 algorithm (Yang et al., 2009). Thus the model is more accurate in modeling water and

11 N transport in soil, especially under the circumstances such as high groundwater table.

12 Compared with the similar models of N_ABLE (Greenwood, 2001) and EU-Rotate_N

13 (Rahn et al., 2010), the model mechanistically accounts for N partitioned in the roots

14 and employs a new relationship quantifying N mineralization from soil organic matter

15 as reported in Zhang et al. (2009), in addition to the more accurate hydrological

16 predictions. The model also differs from many available crop N models reviewed by

17 Cannavo et al. (2008) in that it is able to simulate water and N dynamics in the soil-

18 crop system over a wide range of crops. This makes the model a good candidate for

19 managing water and N use more precisely in crop production where diverse crops are

20 grown.

21

22   This work and the test of the previous version of the model on 16 vegetable

23 crops (Zhang et al., 2009) indicate that the model performs well for N transfer in the

24 soil-crop system if the final dry weight yield is known. It is realized that crop growth

25 is affected by the environment and the determination of the final dry weight yield

could be problematic. Therefore, there is a need to further develop the model so that the effect of the environment on the final crop dry weight yield can be taken into consideration. Also the model requires extending its function to model N transformation in soil and deal with organic fertilizers to widen its application.

6. Conclusions

The generic agro-hydrological model SMCR_N has been parameterized and validated against data from field experiments on wheat. The overall performance of the model was satisfactory. The model was able to reproduce the measurements including crop dry matter accumulation, cumulative N uptake, and the spatial-temporal soil water content and soil mineral N concentration. This suggests that the model can be used reliably for water and N dynamics in the soil-wheat system. Thus the model has the potential to be used as a good platform for optimal management of water and fertilizer N use not only in vegetable production as shown previously (Zhang et al., 2009), but also in wheat production.

Although the model performs reasonably well in predicting dry matter accumulation with a pre-defined dry weight yield by using a simple and general growth equation and default parameter values for various crops, it is beneficial to calibrate the equation for individual crops when data is available since the growth equation is a major factor controlling water and N dynamics in the soil-crop system. This also applies to the air-temperature-driven root growth equation. If the maximum rooting depth, for a given crop, and cumulative day temperature during growth can be estimated with certainty in advance, simple calibration of the root growth equation

1 should be carried out to facilitate more accurate simulations of water and N dynamics

2 in the soil-crop system.

3

4   Finally it should be pointed out that groundwater plays an important role in

5 meeting crop evapotranspiration under the circumstances of high groundwater table. It

6 is, therefore, crucial to gather the groundwater information from the experimental site

7 and use agro-hydrological models capable of simulating capillary flow for water

8 dynamics in the soil-crop system.

9

10 **Acknowledgements**

11

16

1 **Appendix: Abbreviations and key equations in the model**
2
3 Table A1: Abbreviations and parameter values used in the simulations

Symbol	Description	Unit	Value
Θ	relative saturation	-	
$\%N$	actual %N in crop dry weight	-	
$\%N_{crit}$	critical %N in crop dry weight	-	
$\%N_{max}$	max. %N in crop dry weight	-	
$\%N_{rpot}$	potential %N in root dry weight	-	
$\%N_r$	actual %N in root dry weight	-	
$\Delta c_{i+1,i}$	difference in soil mineral N concentration between layers $i+1$ and i	kg m^{-3}	
$\Delta h_{i+1,i}$	difference in soil pressure head between layers $i+1$ and i	cm	
Δt	time step for hydrological simulation	d	0.001
ΔW	daily dry weight increment	t ha^{-1}	
ΔW_r	daily root dry weight increment	t ha^{-1}	
Δz	soil layer thickness	cm	5.0
$\Delta \theta_i$	layer-average soil water content change in layer i	cm^3 cm^{-3}	
a_z	shape parameter controlling root distribution down the profile	-	3.0
c	mineral N concentration in soil	kg m^{-3}	
c_0	mineral N concentration constant	kg m^{-3}	0.007
c_i	soil mineral N concentration in soil layer i	kg m^{-3}	
c_{min}	min. soil mineral N concentration below that no N uptake is possible	kg m^{-3}	0.0035
E_0	potential soil evaporation	cm d^{-1}	
ET_0	reference evapotranspiration	cm d^{-1}	
f	soil fraction not covered by plants and exposed to evaporation	-	
h	soil pressure head	cm	
i	soil layer number	-	
K_1	crop growth coefficient	t ha^{-1}	
K	soil hydraulic conductivity	cm d^{-1}	
K_{cb}	basal crop coefficient for transpiration	-	
K_{cmax}	maximum value of crop coefficient	-	
K_e	evaporation coefficient	-	
k_{min}	rate of organic matter oxidation	d^{-1}	0.00015
k_N	plant N uptake coefficient	g m^{-1}d^{-1}	0.07
K_{rz}	vertical root growth rate	cm d^{-1} ^{o}C^{-1}	0.097
K_s	saturated hydraulic conductivity	cm d^{-1}	
L	root length density	m m^{-3}	
L_0	total root length	m	
m_c	soil organic C content	-	
n	shape parameters of the retention and conductivity functions	-	
N_{pot}	potential N uptake	kg ha^{-1} d^{-1}	
N_{smin}	daily N mineralization rate from soil organic matter	kg ha^{-1} d^{-1}	
Q_{10}	factor change in rate with a 10 degree change in temperature	-	3.0
R_{CN}	C:N ratio of the soil organic matter	-	
R_{lux}	coefficient of crop luxury N consumption	-	1.2
R_z	rooting depth	cm	
R_{z0}	rooting depth at planting	cm	
S_c	sink term for N uptake	kg m^{-3} d^{-1}	
S_r	specific root length density	m kg^{-1}	300000
S_w	sink term for water uptake	d^{-1}	
T	mean daily air temperature	^{o}C	
T_{gb}	base temperature below which plant does not grow	^{o}C	4.0
T_{gmax}	temperature above which plant growth is the maximum	^{o}C	20.0
T_{lag}	threshold of cumulative day degree for root growth	^{o}C d	100.0
t	time	d	
T_0	potential crop transpiration	cm d^{-1}	
T_s	base temperature at which Q$_{10}$ function equals 1	^{o}C	20.0
U_N	N demand in the above-ground biomass	kg ha^{-1} d^{-1}	
U_{Nr}	N demand in the root biomass	kg ha^{-1} d^{-1}	

v_{ci+1}	mineral N transport between soil layers $i+1$ to i in Δt	kg m^{-3}	
v_{wi+1}	water flux between soil layers $i+1$ to i in Δt	cm d^{-1}	
v_z	water flux	cm d^{-1}	
W	dry weight of the entire plant excluding fibrous roots	t ha^{-1}	
W_0	crop dry weight at planting	t ha^{-1}	
W_{max}	crop dry weight at onset of senescence	t ha^{-1}	17.0
W_r	dry weight of fibrous roots	t ha^{-1}	
W_{r0}	root dry weight at planting	t ha^{-1}	
z	vertical coordinate	cm	
Z_{smin}	soil depth where N mineralization takes place	cm	30.0
α	shape parameters of the retention and conductivity functions	-	
α_N	parameter relating critical %N to crop dry weight	-	1.35
α_w	root water stress reduction factor	-	
β_N	parameter relating critical %N to crop dry weight	-	3.0
θ_i	volumetric soil water content in soil layer i	cm^3 cm^{-3}	
θ_r	residual soil water content	cm^3 cm^{-3}	
θ_s	saturated soil water content	cm^3 cm^{-3}	
θ	volumetric soil water content	cm^3 cm^{-3}	
ρ	bulk density	g cm^{-3}	

Table A2: Key equations

Process	Equations
Plant growth	Daily dry weight increment (above-ground)

$$\Delta W = \frac{K_2 W}{K_1 + W} \; [1 - \min(\frac{\%N}{\%N_{crit}}, 1)] \tag{A1}$$

$$K_2 = \frac{K_1 \ln W_{max} + W_{max} - K_1 \ln W_0 - W_0}{\sum \max[\min(T, T_{g\,max}) - T_{gb}, 0]} \tag{A2}$$

$$\%N_{max} = R_{lux} \quad \%N_{crit} = R_{lux}\alpha_N (1 + \beta_N e^{-0.26W}) \tag{A3}$$

Rooting depth

$$R_z = R_{z0} + \max[0, (\sum T - T_{lag}) K_{rz}] \tag{A4}$$

Total root length

$$L_0 = W_r S_r = (W_{r0} + \Sigma \Delta W_r) S_r \tag{A5}$$

Root length distribution

$$L(z) = L_0 e^{-a_z z} \qquad z \le R_z \tag{A6}$$

N and water requirement

Above-ground

$$U_N = 10[(W + \Delta W) \times R_{lux} \times \%N_{crit} - W \times \%N] \tag{A7}$$

Root

$$U_{Nr} = 10[(W_r + \Delta W_r) \times \%N_{rpot} - W_r \times \%N_r] \tag{A8}$$

$$\%N_{rpot} = 1 + \beta_N e^{-0.26W} \tag{A9}$$

Soil evaporation

$$E_0 = K_e ET_0 = \min(K_{c\,max} - K_{cb}, fK_{c\,max}) ET_0 \tag{A10}$$

Crop transpiration

$$T_0 = K_{cb} ET_0 \tag{A11}$$

Water and N uptake

Crop transpiration

$$S_w = \alpha_w(h) \; L(z)T_0 / \Sigma L(z) \tag{A12}$$

N uptake

$$S_c = (U_N + U_{Nr})(1 - e^{-\frac{N_{pot}}{U_N + U_{Nr}}}) \times 10^{-4} \tag{A13}$$

$$N_{pot} = \int_0^{R_z} \frac{0.1L(z)k_N (c - c_{min})}{c + c_0} dz \tag{A14}$$

N mineralization from soil organic matter

$$N_{s\,min} = k_{min} Q_{10}^{\frac{T - T_s}{10}} \rho Z_{s\,min} m_c / R_{CN} \times 10^5 \tag{A15}$$

Soil water and mineral N re-distributions

Soil water movement

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[K(\theta)(\frac{\partial h}{\partial z} + 1)] - S_w \tag{A16}$$

Mineral N transport (diffusion term not included)

$$\frac{\partial \theta c}{\partial t} = -v_z \frac{\partial c}{\partial z} + N_{s\,min} - S_c \tag{A17}$$

Solutions to Eqs. A16, A17

$$\frac{\Delta \theta_i}{\Delta t} = \frac{1}{\Delta z}(v_{wi+1} - v_{wi}) - S_w \tag{A18}$$

$$\frac{\Delta \theta_i c_i}{\Delta t} = \frac{1}{\Delta z}(v_{ci+1} - v_{ci}) - N_{s\,min} - S_c \tag{A19}$$

$$v_{wi+1} = K_{i+1}(\Delta h_{i+1,i} / \Delta z + 1) \tag{A20}$$

$$v_{ci+1} = -v_{zi+1} c_{i+1} \tag{A21}$$

similarly v_{wi} and v_{ci} can be obtained by changing the subscript *i+1* to *i* and *i* to *i-1* in Eqs (A20)(A21).

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24

Table 1
Summary of the experiments

Experiment	Sowing and harvest dates	Date of 1st measurement	Date and N fertilizer amount yymmdd (kg N ha⁻¹)
BOUW_83	21 Oct., 1982 01 Aug., 1983	07 Feb., 1983	N1: no fertilizer N applied N2: 830513 (60) N3: 830513 (120), 830622 (40)
BOUW_84	27 Oct., 1983 21 Aug., 1984	13 Feb., 1984	N1: 840217 (70) N2: 840217 (70), 840509 (60), 840606 (40) N3: 840217 (70), 840506 (120), 840606 (40)
PAGV_83	25 Oct., 1982 02 Aug., 1983	08 Feb., 1983	N1: 830216 (80) N2: 830216 (60), 830510 (80) N3: 830216 (60), 830510 (140), 830610 (40)
PAGV_84	21 Oct., 1983 20 Aug., 1984	14 Feb., 1984	N1: 840217 (80) N2: 840217 (80), 840514 (60), 840608 (40) N3: 840217 (80), 840514 (120), 840608 (40)
EEST_83	19 Oct., 1982 03 Aug., 1983	09 Feb., 1983	N1: no fertilizer N applied N2: 830511 (60) N3: 830511 (120), 830621 (40)
EEST_84	21 Oct., 1983 09 Aug., 1984	16 Feb., 1984	N1: 840217 (50), 840511 (60) N2: 840217 (50), 840511 (60), 840621 (40) N3: 840217 (60), 840511 (60), 840621 (40)

Table 2
Fitted van Genuchten soil hydraulic parameter values[a] in the BOUW and PAGV experiments using the RETC software[b]

	Bouwing experiments		PAGV experiments		
	0–40 cm	40–100 cm	0–25 cm	25–40 cm	40–100 cm
θ_s (cm³ cm⁻³)	0.51	0.49	0.42	0.50	0.53
θ_r (cm³ cm⁻³)	0.00	0.00	0.04	0.06	0.06
α (−)	0.0266	0.0046	0.0162	0.0096	0.0098
n (−)	1.1841	1.1835	1.299	1.3460	1.3193
K_s (cm d⁻¹)	40.0	2.0	160.0	33.0	200.0

[a] The van Genuchten soil hydraulic functions are: $\Theta = (\theta - \theta_r)/(\theta_s - \theta_r) = (1+ |\alpha h|^n)^{-1/m}$
and $K(\theta) = K_s \Theta^{0.5}[1-(1-\Theta^{1/m})^m]^2$ (van Genuchten, 1980).
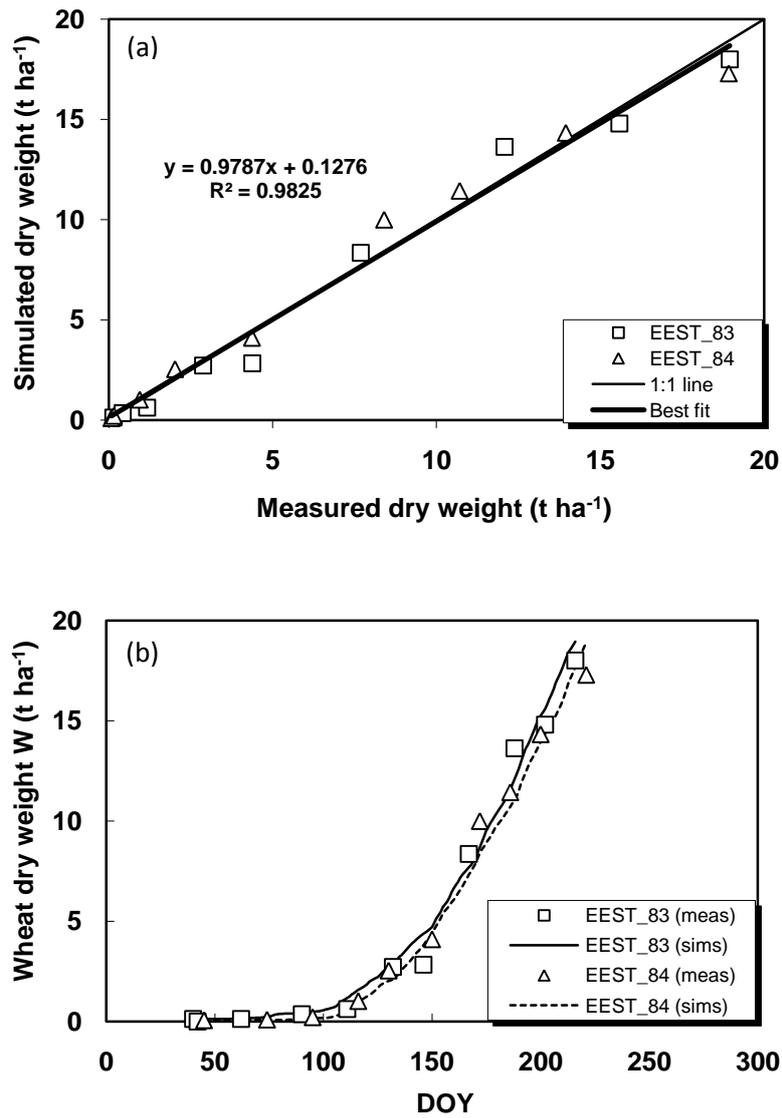[b] The RETC software was developed by van Genuchten et al. (1991).

Fig. 1. Overall (a) and detailed comparison (b) of crop dry weight between measurement and simulation using the optimum crop growth coefficient in the EEST_83 and EEST_84 experiments.
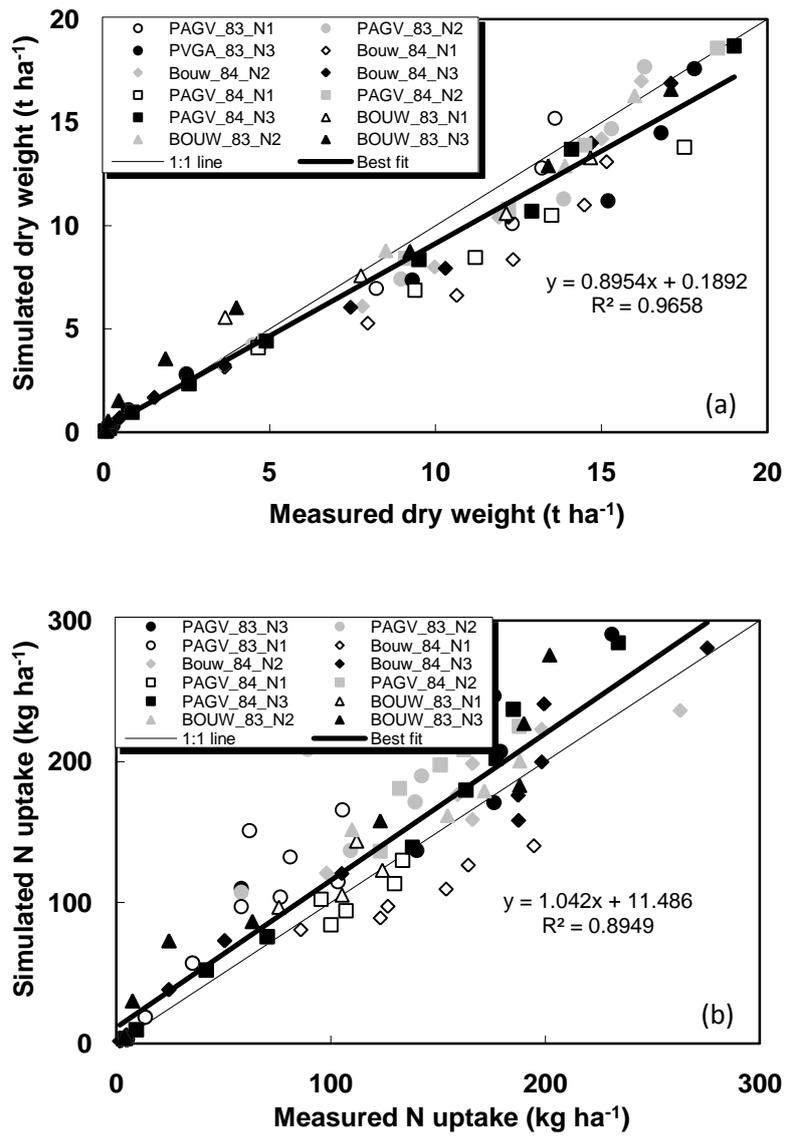
Fig. 2. Comparison of crop dry weight (a) and N uptake (b) between measurement and simulation.
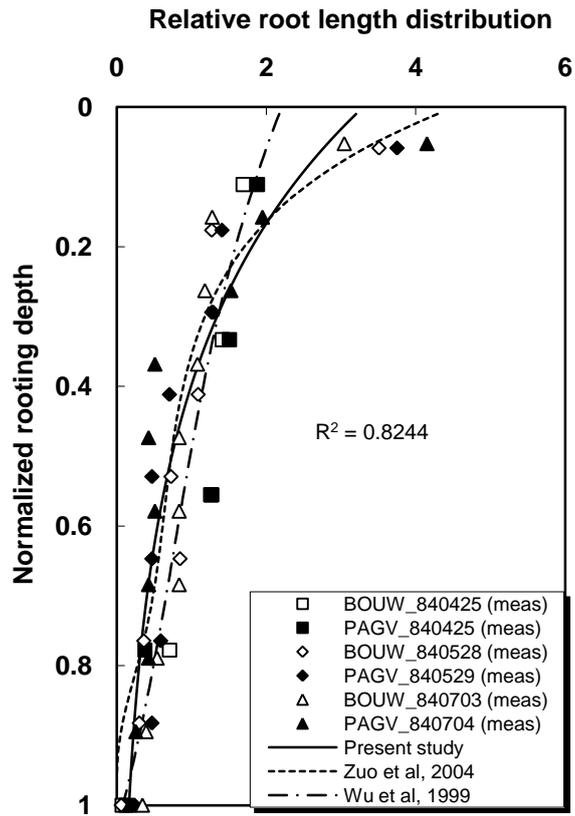
Fig. 3. Comparison of the simulated relative root length distributions at intervals with the measurements and those modeled with alternative approaches.
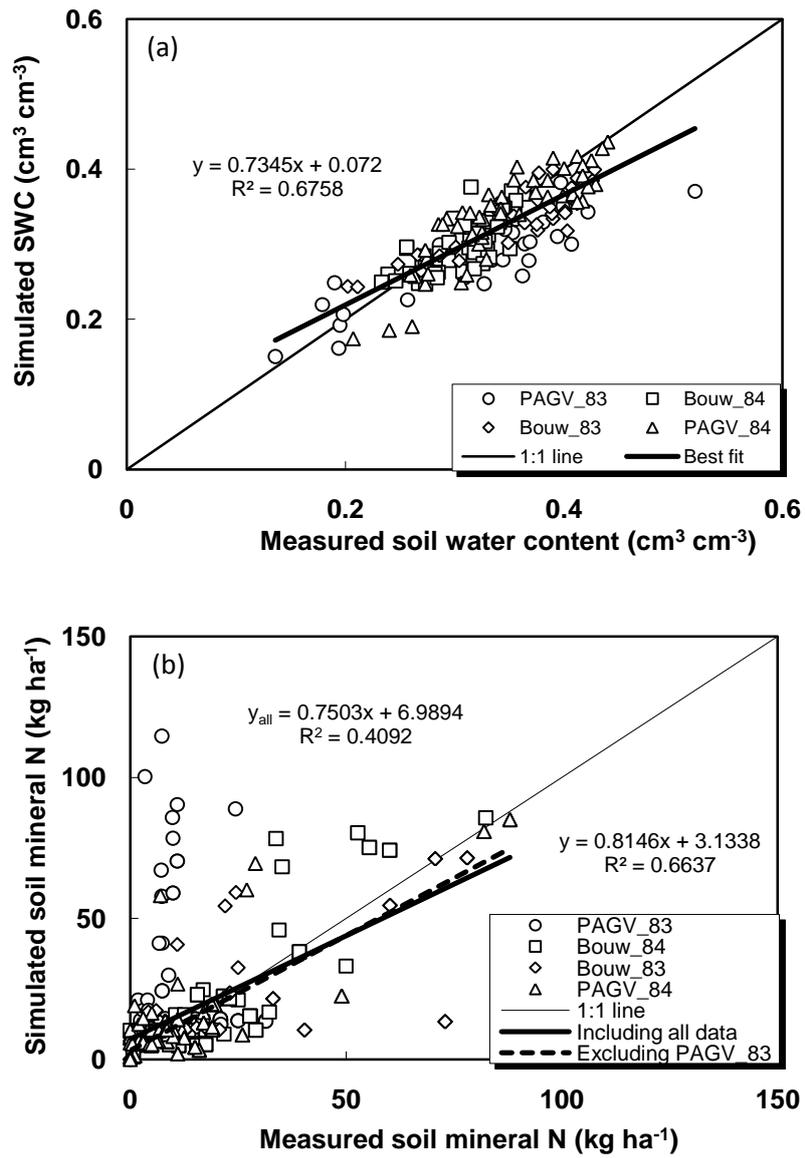
Fig. 4. Comparison of soil water content (a) and soil mineral N (b) in the different layers between measurement and simulation.
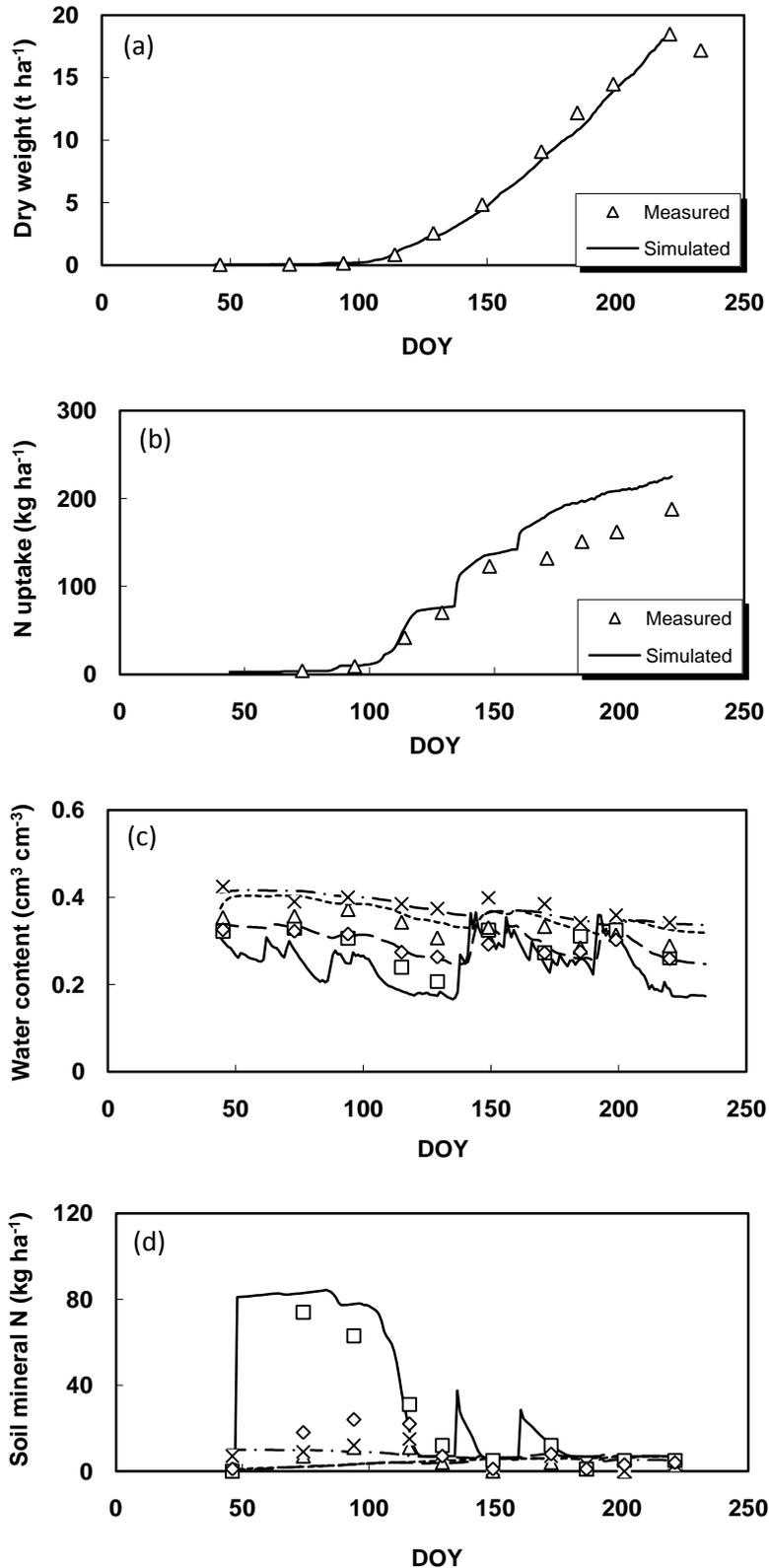
Fig. 5. Comparison between the measured and simulated crop dry weight (a), N uptake (b), soil water content (c) and soil mineral N (d) under the N2 treatment in the PAGV_84 experiment. Solid, dashed, dotted and dash-dotted lines in (c) and (d) represent the simulated values in the 0-20, 20-40, 40-60 and 60-80 cm soil layers, and the measured values are represented by symbols of □, ◊, Δ and x, respectively.
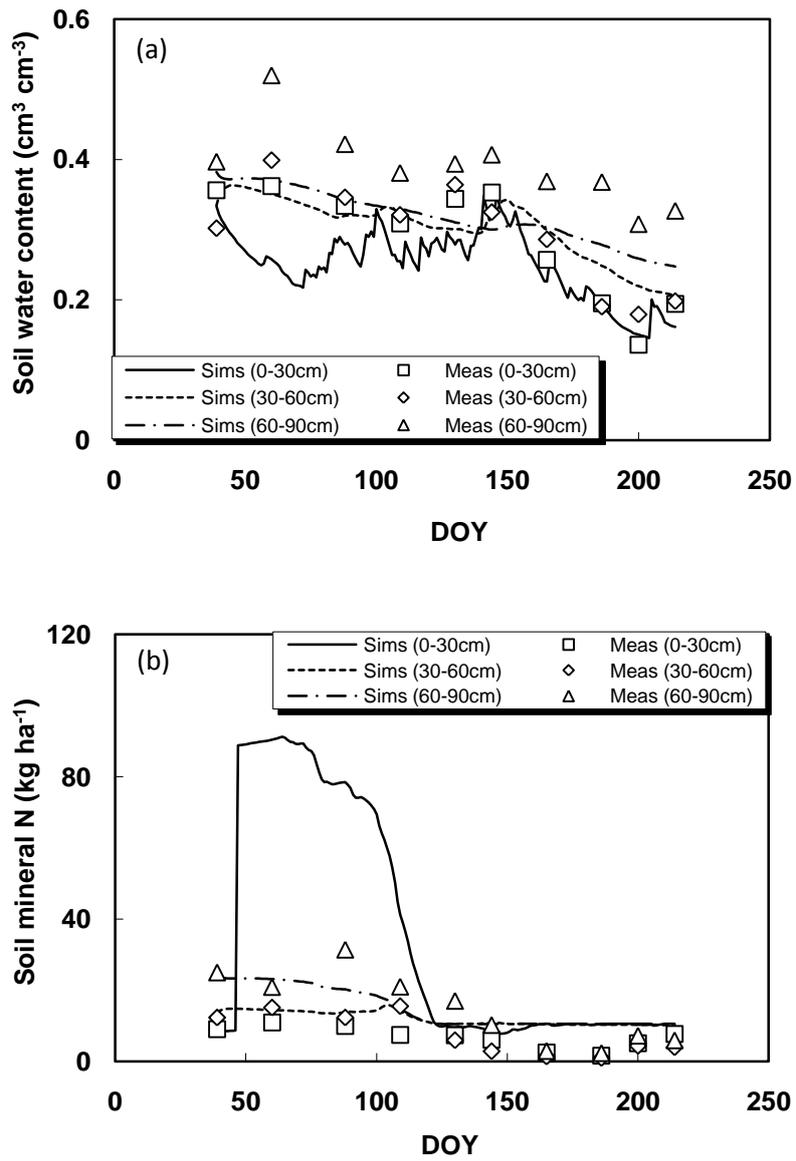
Fig. 6. Comparison between the measured and simulated soil water content (a) and soil mineral N (b) in different layers under the N1 treatment in the PAGV_83 experiment.
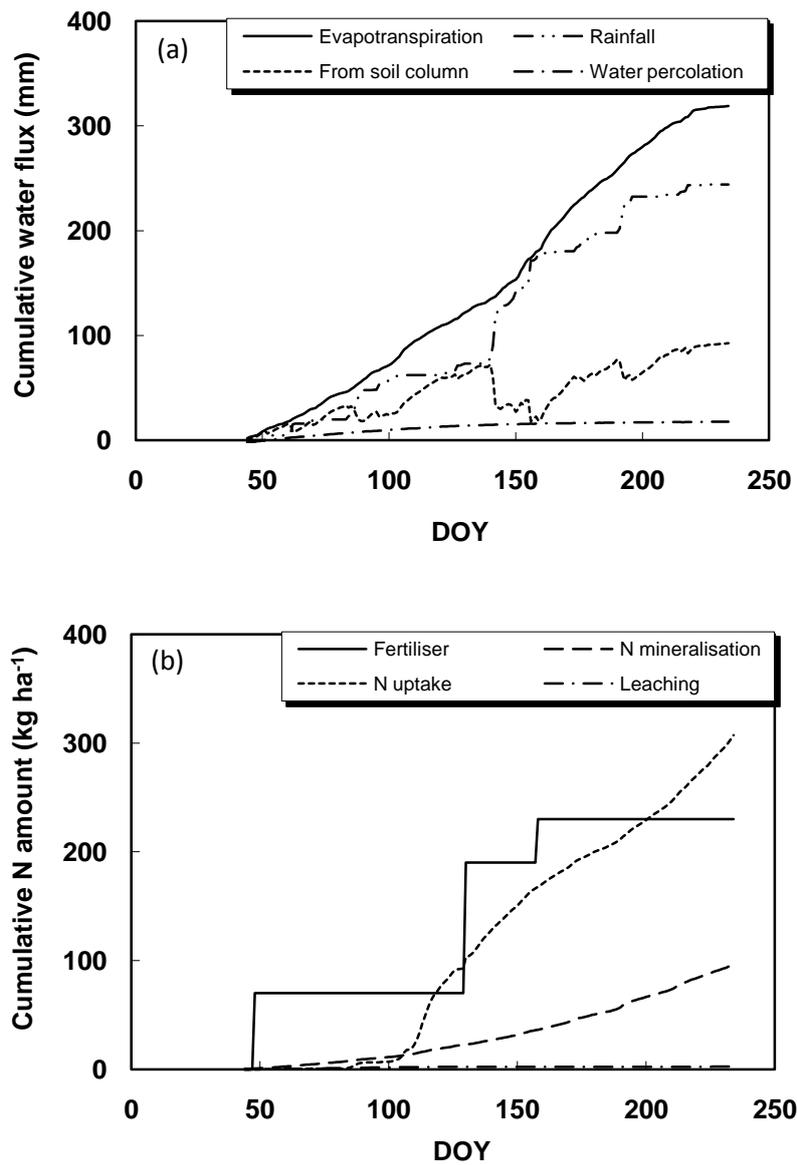
Fig. 7. Cumulative rainfall and simulated various water fluxes (a) and cumulative applied N fertilizer, N mineralization, N uptake and N leaching at 1 m depth (b) under the N3 treatment in the Bouwing_84 experiment. Soil column is 1 m in depth.