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Expanding the WOFOST crop model to explore options for sustainable nitrogen management: A study for winter wheat in the Netherlands

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ABSTRACT

Nitrogen (N) management is essential to ensure crop growth and to balance production, economic, and environmental objectives from farm to regional levels. This study aimed to extend the WOFOST crop model with N limited production and use the model to explore options for sustainable N management for winter wheat in the Netherlands. The extensions consisted of the simulation of crop and soil N processes, stress responses to N deficiencies, and the maximum gross CO_2 assimilation rate being computed from the leaf N concentration. A new soil N module, abbreviated as SNOMIN (Soil Nitrogen for Organic and Mineral Nitrogen module) was developed. The model was calibrated and evaluated against field data. The model reproduced the measured grain dry matter in all treatments in both the calibration and evaluation data sets with a RMSE of 1.2 Mg ha^{-1} and the measured aboveground N uptake with a RMSE of 39 kg N ha^{-1}. Subsequently, the model was applied in a scenario analysis exploring different pathways for sustainable N use on farmers' wheat fields in the Netherlands. Farmers' reported yield and N fertilization management practices were obtained for 141 fields in Flevoland between 2015 and 2017, representing the baseline. Actual N input and N output (amount of N in grains at harvest) were estimated for each field from these data. Water and N-limited yields and N outputs were simulated for these fields to estimate the maximum attainable yield and N output under the reported N management. The investigated scenarios included (1) closing efficiency yield gaps, (2) adjusting N input to the minimum level possible without incurring yield losses, and (3) achieving 90% of the simulated water-limited yield. Scenarios 2 and 3 were devised to allow for soil N mining (2a and 3a) and to not allow for soil N mining (2b and 3b). The results of the scenario analysis show that the largest N surplus reductions without soil N mining, relative to the baseline, can be obtained in scenario 1, with an average of 75%. Accepting negative N surpluses (while maintaining yield) would allow maximum N input reductions of 84 kg N ha^{-1} (39%) on average (scenario 2a). However, the adjustment in N input for these pathways, and the resulting N surplus, varied strongly across fields, with some fields requiring greater N input than used by farmers.

1. Introduction

Nitrogen (N) is, together with water, the most yield-limiting factor in crop production (Chukalla et al., 2020). Therefore, farmers rely on N fertilizers to increase crop yield. Sometimes, farmers apply larger amounts of N than recommended to minimize risk of yield losses due to N stress (Sheriff, 2005; Yadav et al., 1997; Silva et al., 2021b). Applied N not taken up by crops can get lost to the environment leading to undesired economic and environmental problems. First, N losses from applied fertilizers translate into economic losses for farmers as applied N is not efficiently used for crop production (Sheriff, 2005). Second, N losses also contribute to soil acidification, eutrophication of surface waters, and emission of greenhouse gases (van Grinsven et al., 2019).

The European Union Nitrogen Expert Panel (EUNEP) developed guidelines to benchmark N-use efficiency (NUE) and identify opportunities to minimize N losses while ensuring high crop yields (EU Nitrogen Expert Panel, 2015). Such guidelines acknowledge different performance indicators and different pathways for sustainable N use in relation to yield gap closure (i.e., the ratio of actual yield to the water-limited potential yield), NUE (i.e., kg N output per unit of N input), and N surplus (Quemada et al., 2020; Silva et al., 2021a; Zhang et al., 2015). Here, N output is defined as the amount of N in the

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harvestable part of the crop. One possible pathway to increase NUE is to adjust fertilizer application rates so that NUE reaches a desirable target (Schulte-Uebbing and de Vries, 2021). Another possible pathway is to increase crop yield through improved agronomy in relation to the timing, space, and form of applied N and other inputs (Silva et al., 2017). The latter strategy contributes to increase both crop yield and NUE, since N input remains unchanged. A third pathway combining the previous two is also possible, as in some contexts there are opportunities to reduce applied N while improving crop yield with better management of other factors beyond N.

It is challenging to identify the minimum amount of N required to achieve a desirable NUE, while maintaining crop yield. It is also challenging to estimate yield increases due to improved crop management practices using farmer field data alone (Chukalla et al., 2020; Silva et al., 2021b). Crop growth models can be used to explore pathways towards improved NUE and crop yield (Silva et al., 2017), and to provide operational advice to farmers when packaged in decision support systems or digital twins (Divya et al., 2021; Pylianidis et al., 2021; McNunn et al., 2019). Many crop growth models can simulate crop and N dynamics. The simplest ones, like M^3 (Berghuijs et al., 2020) or the Greenwood model (Greenwood et al., 1991), describe the crop N state with the total aboveground N uptake as a single state variable. These models have low input requirements, which makes them attractive in contexts for which few input data are available. However, they do not allow to simulate N dynamics separately for different organs. This limitation is particularly relevant for wheat as its grain N concentration is an important measure for baking quality (Osman et al., 2012). Furthermore, these models do not allow to calculate NUE from their output, as its calculation requires the amount of N in the harvestable part of the crop. Many other more complex crop growth models implement modules that can simulate N dynamics in separate plant parts. Examples are APSIM WHEAT (Zheng et al., 2014) in APSIM (Holzworth et al., 2014; Holzworth et al., 2018), CERES WHEAT (Ritchie et al., 1998) in DSSAT (Hoogenboom et al., 2019), and NCROP in ORYZA (Bouman et al., 2001).

The WOFOST crop growth model has been widely applied in agricultural research (Paudel et al., 2021; Reidsma et al., 2015; Schils et al., 2018; Knibbe et al., 2022; Overweg et al., 2021; Ten Den et al., 2022b). It is publicly available and has been calibrated for a large number of crop species within various pedoclimatic zones in Europe (Boons-Prins et al., 1993). It is also a key component of the MARS (Monitoring Agricultural ResourceS) crop yield forecasting system in support of decisions regarding agricultural markets throughout the European Union (EU) (van der Velde et al., 2019). This model is thus widely used in both research and policy making, but its current release version does not simulate crop growth under N-limited conditions dynamically (Boogaard et al., 2021; Van Diepen et al., 1988). This makes it challenging to explore the impact of different N management practices on crop growth and yield. The first objective of this study was therefore to extend WOFOST with the required modules to simulate crop N uptake and N stress responses.

Enabling the simulation of N-limited production in WOFOST requires a soil N module that simulates the amount of soil N available for crop uptake. There is a large variety in complexity of existing models or modules for soil N (Manzoni and Porporato, 2009; Shibu et al., 2006). The simplest soil N modules included in M^3 (Berghuijs et al., 2020) and LINTUL-3 (Shibu et al., 2010) consist of a single state variable for the amount of soil N available for uptake, do not distinguish between different soil layers, and assume a constant mineralization rate. Such modules calculate the effective N fertilizer application rate as the product of the total amount of N applied (kg N applied ha^{-1}) and its recovery fraction (kg N available kg^{-1} N applied) (Hijbeek et al., 2018; Silva et al., 2021b). Again, their low input requirements are attractive, but they cannot simulate various processes relevant for sustainable N use. First, the use of a constant mineralization rate does not allow to consider the effects of various environmental factors like temperature (Yang and Janssen, 2000; Janssen, 1986; Eckersten et al., 2011) and soil moisture (Groenendijk et al., 2005) on mineralization. Second, recovery fractions lump various processes that result in N loss to the environment in a single parameter. These processes include volatilization (Huijsmans et al., 2001), denitrification (Heinen, 2003) and run-off, and N leaching (Wang and Li, 2019). Since the recovery fractions are fixed input parameters, models relying on them cannot be used to simulate soil N losses dynamically. Finally, such models cannot simulate the gradual release of inorganic N from organic fertilizers by mineralization as they assume that all effective applied N is readily available for uptake. In contrast, more complex soil N modules like ANIMO (Groenendijk et al., 2005), SoilN (Hansen et al., 1991), RothC (Coleman and Jenkinson, 1996) and the soil N modules of APSIM (Holzworth et al., 2018) and DSSAT (Hoogenboom et al., 2019) simulate processes related to mineralization and N loss explicitly. They subdivide both the soil organic matter and the applied organic fertilizers and crop residues in different pools of organic matter (Verberne et al., 1990). These pools differ in their C:N ratios and first order decomposition rates. State variables include the amounts of organic matter, carbon (C) and N of each pool and layer and the amounts of soil inorganic N in each layer. A disadvantage of such an approach is that, although the total amounts of soil organic matter, C and N in soil, crop residues, and fertilizers can be measured, their relative contributions to each of these pools cannot be easily quantified and need to be parametrized through model calibration. An alternative approach that avoids this disadvantage is to simulate the amounts of organic matter, C, N in each organic amendment and in each soil layer as separate state variables. The decomposition rate of organic matter and the corresponding mineralization rates of organic C and N from each amendment are then calculated dynamically from the moment they are applied. The decomposition rate of organic matter in each amendment is determined by its so-called apparent age (Janssen, 1984), which depends on when the amendment was applied and on its specific initial apparent age. The latter variable can be easily estimated from measurements of the decomposition of that type of amendment (Janssen, 1984). Such approach was applied in the stand-alone soil N models MINIP (Heinen and De Willigen, 2005) and NDICEA (Van der Burgt et al., 2006). Yet, these models are challenging to use, because they either do not distinguish soil layers (MINIP) or distinguish only two soil layers with fixed thicknesses (NDICEA). They have also not been coupled to crop growth models. The second aim of this study was therefore to develop a new soil N module with a custom number of soil layers and depths and couple it to the WOFOST crop growth model. This module calculates the mineralisation from soil organic matter dynamically, according to the approach of MINIP and NDICEA. It also simulates the dynamics of inorganic soil N.

Since crop growth models and soil C and N models can only be relevant for real-world applications if they have been thoroughly evaluated (Berghuijs et al., 2023; Silva and Giller, 2020), the third objective of this study was to calibrate the extended version of WOFOST and to evaluate its performance of reproducing measurements of crop dry matter and partitioning, crop N uptake and partitioning, soil water, and soil N in two comprehensive Dutch field experiments with winter wheat (Berghuijs et al., 2023; Groot and Verberne, 1991). Finally, the extended model was used to assess the ambition of the EU to reduce N surplus of crop production with at least 50%, which is a part of their Farm to Fork strategy (European Commission, 2020) The last objective of this study is to explore more sustainable N management options for winter wheat in the Netherlands using scenario analysis.

This study introduces a new version of the WOFOST crop model to simulate crop and N soil processes, including a new soil N module, abbreviated as SNOMIN (Soil Nitrogen for Organic and MIneral Nitrogen module). This widens the applicability of WOFOST to address new applied research questions concerning N management in crop production. The improved model was further calibrated and evaluated against two high-quality datasets of field data for winter wheat crops in different time periods (Groot and Verberne, 1991; Berghuijs et al., 2023), hence providing a thorough calibration and evaluation of model performance against independent data. The model was finally applied in combination with farmer field data to explore options for sustainable N management, which illustrates the usefulness and relevance of crop models in applied agronomy research. Our approach is an example of the importance of coupling simulation and experimentation to guide crop model development and application (Silva and Giller, 2020) and provides a comprehensive assessment of modelling crop and soil N dynamics for arable crops.

2. Material and methods

2.1. Model overview

WOFOST was originally implemented in the FORTRAN programming language (Van Diepen et al., 1988). Recently, the model was reimplemented in the Python programming language and incorporated in a modelling framework called Python Crop Simulation Environment (De Wit et al., 2019). The full source code of PCSE is openly available at https://github.com/ajwdewit/pcse. Default crop parameter values to simulate potential and water-limited yields with WOFOST for 22 crop species are also publicly available at https://github.com/ajwdewit/WOFOST_crop_parameters. The PCSE source code includes the Python implementation of WOFOST 7.2 for potential and water-limited production, which was set as a starting point of this study. Detailed information on the implementation of WOFOST 7.2 is documented elsewhere (De Wit et al., 2020).

In this study, WOFOST was extended to simulate crop and soil N dynamics and their effect on crop dry matter production. Model extensions included a soil N module, a crop N module, a N stress module, and a new assimilation module that calculates the gross rate of leaf CO_2 assimilation from the N concentration in leaves. The new soil N module simulates soil inorganic and organic N dynamics and the movement of inorganic N across different soil layers. Since inorganic N moves between soil layers with the waterflow, and the current, free drainage soil water balance WaterBalanceFD (De Wit et al., 2020) does not consider different soil layers, we also replaced the existing soil water module with the layered soil water module WATFDGW (Rappoldt et al., 2012). In the remainder of this article, we refer to the extended version of the model as WOFOST. Its source code will be made publicly available at https://github.com/ajwdewit/pcse.

2.2. Model improvements

2.2.1. Soil water module

The soil water module WATFDGW (Rappoldt et al., 2012) was originally implemented in the FORTRAN programming language. The module was reimplemented in Python and incorporated in PCSE. In summary, the module distinguishes a user-defined number of soil layers with a user-defined depth. Each layer contains a state variable for the soil moisture content. There is also a state variable for the amount of soil water in the surface storage, which can be filled by rainfall and irrigation water and emptied by percolation and runoff. For the upper soil layer, a source of water consists of water infiltration from the surface. In all soil layers, water can be added and removed by water flows from adjacent soil layers. In saturated soil layers, the net flow is entirely determined by gravity and is always downward. However, in unsaturated soil layers, water flows are also influenced by the water flow driven by the gradient of the matrix suction, which can be both upward and downward. In each layer, water can be moved upward by soil evaporation or, if the layer is rooted, removed by crop transpiration. For each soil layer, input parameters consist of two tabular functions (Rappoldt and Van Kraalingen, 1989) describing the response of the soil moisture content (SMfromPF: m^3 water m^{-3} soil) and of the 10-base logarithm of the unsaturated soil hydraulic conductivity (CONDfromPF: $^{10}\log(\text{cm d}^{-1})$) to the pF, i.e., the 10-base logarithm of the suction pressure of water. Furthermore, there is a parameter for the maximum surface storage (SSMAX: cm water). The time step of the model is 1 day. For a full description of the model, we refer to Rappoldt et al. (2012).

2.2.2. Soil N module

The new soil N module, abbreviated as SNOMIN (Soil Nitrogen for Organic and MIneral Nitrogen module), is subdivided into a submodule for the dynamics of organic N in different soil layers and ammendments and a submodule for the dynamics of inorganic N in different soil layers (Fig. 1). The soil layers must have the same depths as defined in the soil water module. Supplementary Texts S1 and S2 provide a full mathematical description of SNOMIN.

2.2.2.1. Submodule organic matter, organic C, and organic N. SNOMIN describes the dynamics of organic matter (OM), organic carbon (C) and organic N. The module is largely based on the Janssen model (Janssen, 1984; Janssen, 1986) for the simulation of organic matter decomposition and on the NDICEA (Van der Burgt et al., 2006), MINIP-C, and MINP-N models (Heinen and De Willigen, 2005) for the simulation of organic C and N dissimilation. The most important difference between SNOMIN and these other models is that SNOMIN distinguishes different soil layers, which have the same depths as the previously described soil water module. In each soil layer, the initial amounts of organic matter, organic C, and organic N in each soil layer need to be specified at the start of the simulation. Additional organic matter, C, and N can also be added as amendments containing organic matter over the duration of the simulation. For each amendment in each layer, separate state variables are defined for the amounts of organic matter (ORGMAT,: kg OM m^{-2}), organic C (CORG: kg C m^{-2}) and organic N (NORG: kg N m^{-2}) as specified in Supplementary Text S1.2. The initial organic matter is considered as an amendment as well and state variables for the amounts of organic matter, C, and N are defined for the initial organic matter.

Organic matter, C, and N in the amendments are introduced at user-defined application dates. From the moment of application of an amendment until the end of the simulation, organic matter in this amendment is decomposed. This decomposition is described by the Janssen model (Janssen, 1984; Janssen, 1986), which assumes that the relative decomposition rate decreases exponentially over time. The initial relative decomposition rate depends on the so-called “initial apparent age” of the amendment, which is an amendment specific property. Initial apparent ages of different organic materials were derived in previous work (Groenendijk et al., 2005; Janssen, 1984; Yang and Janssen, 2000). The relative decomposition rate of organic matter in an amendment decreases with an increase in apparent age of the amendment. To simulate apparent ageing, separate state variables were defined for the apparent age of each amendment. There is also a state variable defined for the age of the soil organic matter at the start of the simulation, which is assumed to be 24 years (Van der Burgt et al., 2006). Supplementary Texts S1.3.1 and S2 provide a full description on how the decomposition of organic material is simulated.

The dissimilation rate of organic C in an amendment is proportional to the decomposition rate of organic matter and is the net result of the release of C from the amendment and assimilation of the released C by the microbial biomass in the amendment (Berghuijs - Van Dijk et al., 1985). The fraction of dissimilation to assimilation is assumed to be constant, i.e., 0.5 kg C kg^{-1} C (Heinen and De Willigen, 2005) (Supplementary Text S1.3.2). During the release of C in the amendment, organic N is released in inorganic form (i.e., ammonium or NH_4^+-N) through mineralization. The mineralization rate from an amendment is proportional to the release rate of C from that amendment and the proportionality factor is the inverse of the C:N ratio of the amendment at the time of C release. During assimilation, the microbial biomass in an amendment takes up the exact amount of NH_4^+ required to maintain its C:N ratio, which is assumed to be 10 (Heinen and De Willigen, 2005), a process called immobilization. If the immobilization rate from an amendment in a soil layer is larger than the mineralization rate of the

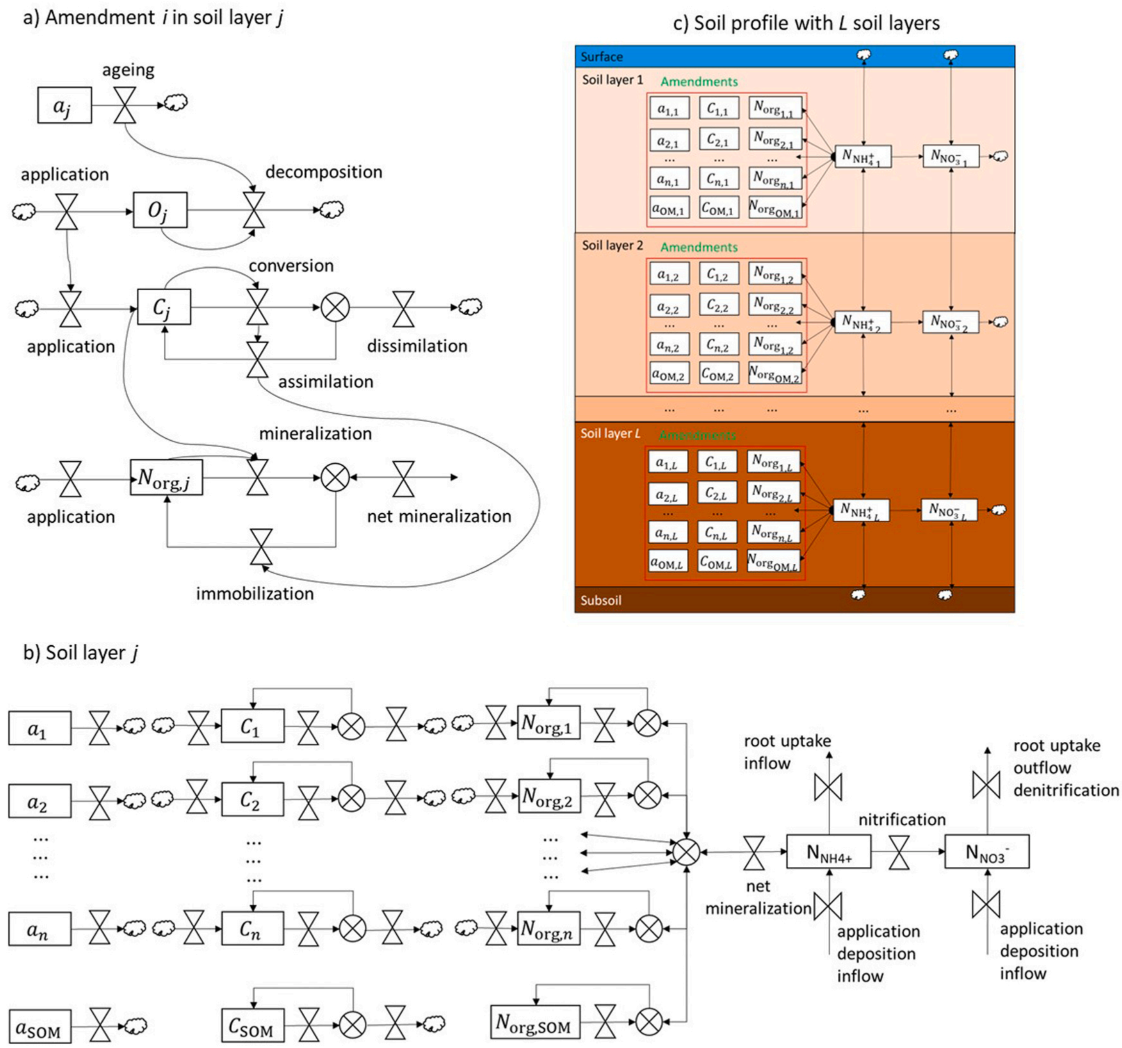

Fig. 1. Relational diagrams of the soil N module SNOMIN at different hierarchical levels: (a) amendment, (b) soil layer, and (c) soil profile. Each single amendment *i* in each soil layer *j* is described by four state variables (a): apparent age a_j and the amounts of organic matter ($O_{i,j}$), organic carbon ($C_{i,j}$), and organic N ($N_{org,ij}$). The organic matter in the amendment is applied during the simulation is decomposed over time. During decomposition, C and N are released from the organic matter and can either be reintegrated into the amendment (assimilation/immobilization) or released (dissimilation/net mineralization) in the soil profile. One soil layer has many amendments, applied at different times, and the amounts of the initial organic matter ($O_{SOM,i,j}$), organic C ($C_{SOM,i,j}$), and organic N ($N_{org,SOM,i,j}$) are simulated as a separate amendment (b). The net mineralization rate from all amendments in a layer contributes to the amount of NH_4^+-N ($N_{NH_4^+,i,j}$) in this layer or, if negative (net immobilibzation), converted back into organic form by assimilation. NH_4^+-N can also be introduced by application, deposition, and inflow and be removed by outflow or root uptake. It can also be converted into NO_3^--N ($N_{NO_3^-i,j}$) by nitrification. Finally, inflow, application, and deposition can add NO_3^--N, while root uptake, outflow, and denitrification remove it. The soil in the model consists of various layers (c) and each soil layer *j* has its own state variables for its amendments (O_{ij}, C_{ij}, $N_{org,ij}$) and the amount of NH_4^+-N and NO_3^--N.

same amendment in that soil layer, the microbial biomass in that amendment takes up additional NH_4^+-N from that soil layer to maintain its C:N ratio. If the sum of the mineralization rates of all amendments in a soil layer is larger than the sum of immobilization rates in the soil layer, there is a net release of NH_4^{+-N} in that soil layer. Else, there is net immobilization and there is a net removal of NH_4^+-N in that soil layer (Verberne et al., 1990) (Supplementary Text S1.3.3).

2.2.2.2. Submodule inorganic N. SNOMIN calculates the dynamics of the amounts of N in the form of ammonium (NH_4^+-N) (Supplementary Text S1.4) and nitrate (NO_3^--N) (Supplementary Text S1.5) in each soil layer, similarly to the SWAP model (Groenendijk et al., 2016; Kroes et al., 2017) with, again, the important difference that SNOMIN distinguishes different soil layers. Sources of NH_4-N include mineralization of organic matter from the soil and the amendments and the application of amendments that contain NH_4^+-N. Furthermore, NH_4-N can be added in the upper soil layer through infiltration of rainwater with dissolved NH_4^+-N (i.e., N deposition). NH_4^+-N can be both added and removed by mass transport, depending on the direction of the net water flow. Sinks for NH_4^+-N consist of nitrification (i.e., into NO_3^--N) and, if the soil layer is rooted, root uptake. It is assumed that there is an instantaneous equilibrium between dissolved NH_4^+-N and NH_4^{+-N} that is bound to negatively charged soil particles (Groenendijk et al., 2016). Only NH_4^+-N dissolved in water is used for crop N uptake.

Sources of NO_3^--N include the application of NO_3^--N-containing amendments, nitrification, and N deposition in the upper layer. Furthermore, also NO_3^--N can be added or removed from a soil layer by mass transport. Sinks for NO_3^--N transport are denitrification (Heinen, 2003) and root uptake. The submodule also calculates per soil layer the amount of N available for root uptake as the sum of the amounts of NO_3^--N and NH_4^+-N dissolved in water in the rooting zone. This information is then used by the crop model (see Section 2.2.3 and

Supplementary Text S3) to calculate the actual root uptake.

2.2.3. Crop N module

Crop N dynamics are described by the amount of N in grains, leaves, stems, and roots (see Supplementary Text S3). Sources of N in any organ consist of crop N uptake and N_2 fixation (in case of legume crops). Sinks of N in the vegetative organs (i.e., roots, leaves, and stems) consist of N loss due to senescence and N translocation to the storage organs. For storage organs, N translocation is thus a source. WOFOST calculates the daily N demand of each organ, i.e., the amount of N uptake to maintain the maximum N concentration in each organ. If N demand is both lower than the crop's maximum daily N uptake rate and the amount of soil available N, then crop N uptake equals N demand. If there is not enough N available in the soil to fulfil N demand for crop uptake, then crop uptake equals the remaining amount of soil N available. N is further distributed over the different organs after crop uptake. Translocation of N occurs if N demand of the storage organs cannot be met by root uptake and N_2 fixation only. N is then transferred from the vegetative organs to the storage organs until either the grain N demand is fulfilled or exceeds the maximum daily translocation rate.

2.2.4. CO_2 assimilation module

In the previous versions of WOFOST (Boogaard et al., 2021; De Wit et al., 2020; Van Diepen et al., 1989), the effect of the decrease of leaf N on the maximum reference gross CO_2 assimilation rate, $A_{\mathrm{mx,rf}}(t)$, was implicitly considered with a tabular function (AMAXTB,: kg CO_2 ha^{-1} leaf h^{-1}) calculating the maximum rate of photosynthesis at reference conditions (360 ppm ambient CO_2, optimal temperature) for a given development stage $\delta(t)$ (DVS) at time t. In the version of WOFOST presented here, the tabular function $A_{\mathrm{mx,rf}}(t)$ from the previous versions of WOFOST was discarded. Instead, the maximum gross CO_2 assimilation rate is now calculated from the leaf N concentration in a similar way as the ORYZA crop model (Bouman et al., 2001); see Supplementary Text S4 for details.

2.2.5. Crop N stress module

Besides a reduction of the gross CO_2 assimilation rate (Supplementary Text S4), WOFOST also accounts for other effects of N deficiencies on crop growth, namely a reduction of the leaf area index growth in juvenile plants and an increased relative leaf death rate. Further details about how these processes were modelled can be found in Supplementary Text S5.

2.2.6. Reallocation of aboveground dry matter

WOFOST was recently extended with reallocation of dry matter from aboveground vegetative organs to storage organs (Ten Den et al., 2022a). This reallocation module assumed that conversion efficiencies can be inverted to estimate the assimilates available for reallocation. The drawback of this approach is that it leads to high reallocation efficiency with no losses. As this is unrealistic, we modified the reallocation module in the model used in this study. The new module (Supplementary Text S6) calculates the amount of reallocatable dry matter in the stem and leaves as a fraction of the stem and leaf dry matter once a certain development stage is reached. From this development stage until maturity, a fixed fraction of the initial amount of reallocatable dry matter is daily translocated to the grains assuming a fixed reallocation efficiency.

2.3. Model calibration

2.3.1. Field trials and weather data for model calibration

The Groot and Verberne (1991) data set was used to calibrate WOFOST, hence we will refer to it as "calibration data set". This data set was used for model calibration because it contained detailed N uptake data for individual crop organs over the growing season, which is required for detailed calibration of the crop N module (see Section 2.2.2), as opposed to the more recent evaluation data set described in Section 2.4 for which only total N uptake data was available. Winter wheat field trials were conducted in the growing seasons 1982–1983 and 1983–1984 at three different sites in the Netherlands (De Bouwing, De Eest, PAGV). At each site, winter wheat cultivar Arminda (released in 1977) was cultivated under three N-fertilizer regimes: a low (N1), intermediate (N2), and a high N-fertilization regime (N3) (Supplementary Table S1). No irrigation was applied. The data set includes measurements of crop phenological stages, crop dry matter and partitioning, crop N amounts and partitioning, soil moisture measurements, soil N measurements, and soil textural data. Measurements were taken 10 and 11 times during the first and second growing seasons, respectively. We refer to Groot and Verberne (1991) for a full description of the data set and the raw data.

WOFOST requires daily observations of minimum temperature (°C), maximum temperature (°C), global radiation (kJ m^{-2} d^{-1}), precipitation (mm d^{-1}), vapour pressure (kPa), and wind speed (m s^{-1}). For simulations for the site De Bouwing, we used weather data from the Veenkampen weather station located near Wageningen. For simulations of the site De Eest and PAGV, weather data from the Swifterbant weather station (Groot, 1987; Groot and De Willigen, 1991) were used. Annual ambient CO_2 concentrations (CO2: ppm; Fig S1) were obtained from NOAA (2021).

2.3.2. Soil input data for model calibration

The soil water module requires tabular functions for the response of the soil moisture content and of the unsaturated hydraulic conductivity to the pF (10-base logarithm of suction pressure in hPa). For each site and each soil layer, first soil textural properties (Supplementary Table S2) were firstly obtained from the Dutch BOFEK soil map (Heinen et al., 2021). Secondly, the soil textural properties were rescaled such that the configuration of the soil layers matched the layer configurations of the soil N and soil water observations (Supplementary Table S3). Third, Van Genuchten parameters (Van Genuchten, 1980) were estimated for each rescaled soil layer using Wösten pedotransfer functions (Wösten and Nemes, 2004) (Supplementary Table S4). Finally, the Van Genuchten equations were used to calculate the tabular response functions of soil moisture content and unsaturated hydraulic conductivity to pF. Supplementary Text S7 describes the full details of these procedures.

Supplementary Text S8 describes how the input values for SNOMIN were obtained and how the initial amounts of NO_3^--N and NH_4^+-N were estimated. In summary, bulk density, mass fractions of organic matter, and C:N ratios for each soil layer (Supplementary Table S3) were obtained from BOFEK (Heinen et al., 2021) and rescaled to match the layer configurations in the soil N observations (Supplementary Table S4). Year- and site-specific values for the NO_3^--N and NH_4^+-N concentrations in rainwater (Supplementary Table S5) were calculated from the local annual precipitation and the annual national N deposition values (CLO, 2022). Values for other input variables were considered constant for different years and locations (Supplementary Table S6) and were obtained from various other studies (Groenendijk et al., 2016; Heinen and De Willigen, 2005; Janssen, 1984; Van der Burgt et al., 2006). Finally, we assumed an application depth of 10 cm for each fertilization event.

2.3.3. Crop parameters

Unless mentioned otherwise, all crop parameters used for the simulations presented in this study have the same value as in Boons-Prins et al. (1993). Newly introduced WOFOST crop parameters and re-estimated parameters were either obtained from literature, directly calculated from the experimental data or estimated by non-linear optimization. All newly introduced and re-calibrated model parameters are listed in Table 1 and Supplementary Text S9-S11 give a full description on how they were obtained. In summary, phenological parameters were calculated from the phenological observations, daily minimum and maximum temperature observations, and assumed responses to vernalization state (Supplementary Text S10). Tabular biomass partitioning

Table 1
WOFOST crop parameters for winter wheat. Only parameters that are either new or for which the value was adjusted for the simulations presented in this study are shown. The remaining WOFOST parameters were the same as determined by Boons-Prins et al. (1993).

Crop parameter	Definition	Value		Unit
		Original	Modified	
AMAX_LNB	Specific leaf nitrogen below which there is no CO_2 assimilation	absent[a]	0.0	kg ha^{-1}
AMAX_REF	Maximum possible reference gross leaf CO_2 assimilation rate under reference conditions	absent[b]	39.7	kg ha^{-1} h^{-1}
AMAX_SLP	Slope of relationship between maximum gross leaf CO_2 assimilation rate and specific leaf N content	absent[a]	3.24	kg CO_2 kg^{-1} N h^{-1}
AMAXTB	Maximum gross leaf CO_2 assimilation as a function of development stage	$\begin{pmatrix} 0.0 & 40 \\ 1.0 & 40 \\ 2.0 & 20 \end{pmatrix}$	absent[c]	-, kg ha^{-1} h^{-1}
DLO	Day length above which the vernalization rate is no longer reduced by daylength	not applicable[d]	16.3	h
DTSMTB	Vernalization rate as a tabular function of daily average temperature	not applicable[d]	$\begin{pmatrix} 0 & 0 \\ 30 & 30 \\ 45 & 30 \end{pmatrix}$	d^{-1}
FLTB	Fraction of newly produced dry matter that is allocated to leaves	$\begin{pmatrix} 0.000 & 0.65 \\ 0.100 & 0.65 \\ 0.250 & 0.70 \\ 0.500 & 0.50 \\ 0.646 & 0.30 \\ 0.950 & 0.00 \\ 1.00 & 0.00 \\ 2.00 & 0.00 \end{pmatrix}$	$\begin{pmatrix} 0.00 & 0.51 \\ 0.25 & 0.51 \\ 0.74 & 0.00 \\ 1.00 & 0.00 \\ 1.01 & 0.00 \\ 2.00 & 0.00 \end{pmatrix}$	-, kg kg^{-1}
FOTB	Fraction of newly produced dry matter that is allocated to grains	$\begin{pmatrix} 0.000 & 0.00 \\ 0.100 & 0.00 \\ 0.250 & 0.00 \\ 0.500 & 0.00 \\ 0.646 & 0.00 \\ 0.950 & 0.00 \\ 1.00 & 1.00 \\ 2.00 & 1.00 \end{pmatrix}$	$\begin{pmatrix} 0.00 & 0.00 \\ 0.25 & 0.00 \\ 0.74 & 0.00 \\ 1.00 & 0.00 \\ 1.01 & 100 \\ 2.00 & 1.00 \end{pmatrix}$	-, kg kg^{-1}
FSTB	Fraction of newly produced dry matter that is allocated to stems	$\begin{pmatrix} 0.000 & 0.35 \\ 0.100 & 0.35 \\ 0.250 & 0.30 \\ 0.500 & 0.50 \\ 0.646 & 0.70 \\ 0.950 & 1.00 \\ 1.00 & 0.00 \\ 2.00 & 0.00 \end{pmatrix}$	$\begin{pmatrix} 0.00 & 0.49 \\ 0.25 & 0.49 \\ 0.74 & 1.00 \\ 1.00 & 1.00 \\ 1.01 & 0.00 \\ 2.00 & 0.00 \end{pmatrix}$	-, kg kg^{-1}
KN	Extinction coefficient of leaf N in canopy	absent[a]	0.40	m^{2} m^{-2}
NFIX_FR	Fraction of crop N demand that can be met by N_2 fixation	absent[a]	0.00	kg kg^{-1}
NMAXRT_FR	Ratio of maximum N concentration in roots to maximum N concentration in leaves	absent[a]	0.383	kg kg^{-1}
NMAXST_FR	Ratio of maximum N concentration in stems to maximum N concentration in leaves	absent[a]	0.383	
NMAXLV_TB	Maximum N concentrations in leaves as a function of development stage	absent[a]	$\begin{pmatrix} 0.00 & 0.060 \\ 0.40 & 0.040 \\ 0.70 & 0.030 \\ 1.00 & 0.020 \\ 2.00 & 0.014 \\ 2.01 & 0.014 \end{pmatrix}$	kg kg^{-1}
NMAXSO	Maximum N concentration in storage organs	absent[a]	0.020	kg kg^{-1}
NSLLV_TB	Tabular function of enhancement factor of leaf ageing as a function of N stress index	absent[a]	$\begin{pmatrix} 0.00 & 1.0 \\ 1.1 & 1.0 \\ 1.5 & 1.4 \\ 2.0 & 1.5 \\ 2.5 & 1.5 \end{pmatrix}$	-, -
NRESIDLV	Residual N concentration in leaves	absent[a]	0.004	kg kg^{-1}
NRESIDRT	Residual N concentration in roots	absent[a]	0.002	kg kg^{-1}
NRESIDST	Residual N concentration in stems	absent[a]	0.002	kg kg^{-1}
RDRSTB	Relative death rate of stem as a function of development stage	$\begin{pmatrix} 0 & 0.00 \\ 1.50 & 0.00 \\ 1.5001 & 0.02 \\ 2.00 & 0.02 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 \\ 1.50 & 0 \\ 1.5001 & 0 \\ 2.00 & 0 \end{pmatrix}$	-, kg kg^{-1}
REALLOC_EFFICIENCY	Efficiency of dry matter reallocation	absent[a]	0.95	kg kg^{-1}
REALLOC_DVS	Development stage above which reallocation starts	absent[a]	1.5	-
REALLOC_LEAF_FRACTION	Fraction of leaf dry matter at anthesis that will be available for reallocation	absent[a]	0.00	kg kg^{-1}
REALLOC_STEM_FRACTION	Fraction of stem dry matter at anthesis that will be available for reallocation	absent[a]	0.20	kg kg^{-1}
REALLOC_STEM_RATE	Relative rate of reallocation of reallocatable dry matter in the stems	absent[a]	0.043	d^{-1}
RGRLAI_MIN	Relative growth rate of LAI under maximum N stress during the juvenile growth stage	absent[a]	0.0040	ha ha^{-1}d^{-1}
RNUPTAKEMAX	Maximum daily root N uptake	absent[a]	5.0	kg ha^{-1} d^{-1}
TCNT	Time coefficient for N translocation to storage organs	absent[a]	10	d
TDWI	Initial total dry weight	100.0	538	kg ha^{-1}
TMNFTB	Reduction factor of the leaf gross CO_2 assimilation rate due to low temperatures as a tabular function of minimum temperature	$\begin{pmatrix} 0 & 0 \\ 3 & 1 \end{pmatrix}$	$\begin{pmatrix} -3 & 0 \\ 0 & 1 \end{pmatrix}$	°C, -
TSUM1	Growing degree days between emergence to anthesis if the crop phenology would not be sensitive to daylength and vernalization	1255	886 / 880[e]	°C d
TSUM2	Growing degree days between anthesis and maturity	909	870 / 909[e]	°C d
VERNBASE	Base vernalization requirement	not applicable[d]	9	d
VERNSAT	Saturated vernalization requirement	not applicable[d]	44	d

[a] The previous versions of WOFOST did not include parameters for N dynamics in the crop.
[b] New parameter added to WOFOST to consider that crops can take up more N than needed for potential growth.

[c] WOFOST no longer calculates $A_{\max,\mathrm{rf}}(t)$ from a tabular function. Instead, $A_{\max,\mathrm{rf}}(t)$ is calculated from the specific leaf N concentration.
[d] The original calibration of WOFOST (Boons-Prins et al., 1993) did not consider sensitivity of crop phenology to daylength, temperature, or vernalization.
[e] TSUM1 and TSUM2 were estimated separately for cv Arminda in the Groot and Verberne (1991) data set and for the cultivars Julius, Ritmo, and Tabasco in the Berghuijs et al. (2023) data set

fractions (FOTB, FLTB, and FSTB) were estimated simultaneously with the parameters TDWI and AMAX_REF. This was done using the Berghuijs et al. (2020) biomass partitioning model (see also Supplementary Text S11), following the procedure described by Berghuijs et al. (2023) and Ten Den et al. (2022a). This procedure minimizes the normalized RMSE of the leaf area index and yield. Third, the reallocation parameters and RNUPTAKEMAX, NMAXST_FR, and NMAXSO were calculated from the experimental data.

2.3.4. Evaluation of the calibrated model

WOFOST was used to simulate all N treatments in the calibration data set, assuming that crop growth is limited by both water and nitrogen. The quality of the calibration was evaluated with the root mean squared error (RMSE), the mean bias estimate (MBE), and the coefficient of determination (r^2), which are calculated as (Quinn and Keough, 2006):

$$\mathrm{MBE} = \frac{\sum_{i=1}^{n}\left(y_{\mathrm{obs,i}} - y_{\mathrm{sim,i}}\right)}{n} \tag{1}$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(y_{\mathrm{obs,i}} - y_{\mathrm{sim,i}}\right)^2}{n}} \tag{2}$$

$$r^2 = \left(\frac{n \bullet \sum_{i=1}^{n}\left(y_{\mathrm{obs,i}} \cdot y_{\mathrm{sim,i}}\right) - \sum_{i=1}^{n}\left(y_{\mathrm{obs,i}}\right) \cdot \sum_{i=1}^{n}\left(y_{\mathrm{sim,i}}\right)}{\sqrt{\left(\sum_{i=1}^{n}\left(y_{\mathrm{obs,i}}^2\right) - \left(\sum_{i=1}^{n}\left(y_{\mathrm{obs,i}}\right)\right)^2\right) \cdot \left(\sum_{i=1}^{n}\left(y_{\mathrm{sim,i}}^2\right) - \left(\sum_{i=1}^{n}\left(y_{\mathrm{sim,i}}\right)\right)^2\right)}}\right)^2 \tag{3}$$

where $y_{\mathrm{obs,i}}$ is the observed value of variable y at index i and $y_{\mathrm{sim,i}}$ is the corresponding simulated value. n is the number of observations. For MBE, a positive value indicates that WOFOST underestimates variable y while a negative value indicates that WOFOST overestimates variable y. RMSE quantifies the overall difference between the observed and simulated values of y. The r^2 indicates how much variation in the observations was explained by the model.

2.4. Model evaluation

The aim of this model evaluation was to assess the capability of WOFOST to reproduce observations from a truly independent data set at a different location and collected during a more recent period (2013–2015) than the calibration experiments (1982–1984). For this purpose, observations from a recent field experiment conducted in Wageningen during the growing seasons 2013–2014 and 2014–2015 (https://doi.org/10.5281/zenodo.10439170), described by Berghuijs et al. (2023), were used. We refer to these data as "evaluation data set".

In summary, during both growing seasons, three different cultivars, namely Julius (released in 2009), Ritmo (released in 1992), and Tabasco (released in 2008), were grown during both growing seasons under three different N-fertilization regimes: low (N1), intermediate (N2), and high N-application treatment (N3). N application dates and amounts are provided in Supplementary Table S1. During the growing season of 2013–2014, there were two irrigations of 15 mm on July 1 and July 4. No irrigation was supplied in the 2015 growing season. The data set includes measurements of crop phenological stages, crop dry matter and partitioning, whole crop N concentration, and soil water retention. Measurements were taken 10 times during the growing season. For the simulations of the field experiments in the 2013–2014 growing season, weather data from a weather station on the experimental site were used (51.956° N, 5.634° E). For the simulations in the 2014–2015 growing season, weather data from the Veenkampen weather station (2 km from the experimental site) were used.

The crop phenological parameters TSUM1 and TSUM2 were re-estimated for the evaluation data set to account for different cultivars in this experiment (Julius, Ritmo, Tabasco) than the one used in the calibration data set (Arminda), following the same procedure as for the calibration data set (see Supplementary Text S10). There were no phenological differences reported between the different cultivars in the evaluation data set (Berghuijs et al., 2023), hence the values of TSUM1 and TSUM2 for Julius, Ritmo and Tabasco are identical. All other crop parameters were assumed the same as for Arminda. Supplementary Text S12 describes how the input data for soil water and N were obtained. The MBE and RMSE were used to quantify the residual error in the calibration dataset and the capability of the model to simulate total aboveground dry matter, yield, and N uptake in the evaluation data set.

2.5. Scenario analysis

2.5.1. Farmer field data for model application

The data set described by Silva et al. (2020) contains detailed management data and crop yield for a large number of farmers' fields throughout the Netherlands over the growing seasons of 2014–2015, 2015–2016, and 2016–2017. Management data recorded for each field included the sowing date, harvest date, and fertilization dates, types, and amounts, among others. In this study, we focused on the fields located in the province of Flevoland due to its importance for national wheat production.

The initial number of field-year combinations for winter wheat in Flevoland consisted of 185 records. Yet, 44 field-year combinations were discarded due to one of the following reasons: 1) missing values for fertilizer amounts, 2) unknown fertilizer type, 3) fertilization events reported after the harvest date, 4) two or more years difference between harvest and sowing date, and 5) occurrence of duplicated fertilization events. The final dataset for model application thus included wheat yield and management data for 141 field-year combinations. In each of these field-year combinations, there was at least one N application with mineral fertilizer. In 51 fields, there were also one or more applications of organic amendments, which were either cattle slurry, cattle manure, pig slurry, or pig manure. Supplementary Table S7 displays values from Groenendijk et al. (2016) for the initial apparent ages, C:N ratios, and mass fractions of organic matter fractions, ammonium and nitrate fractions that were used to simulate N available from these organic amendments.

2.5.2. Simulation of water -and N-limited yields at field level

The aim of the WOFOST simulations was to determine the maximum wheat yield that could have been achieved under rain-fed conditions in Flevoland for a given N input (i.e., water- and N-limited yields, Y_{WN}, as simulated by WOFOST). For this purpose, the growth of winter wheat for each field-year combination was simulated to quantify the yield and N output (i.e., amount of N in the grains) at harvest time. The simulations were run for both water-limited growth (no N limitation) and water- and N limited growth. The crop parameters used in these simulations were those derived from the evaluation data set for cultivar Julius. Data from the BOFEK soil map for the calibration site PAGV, which is also located in Flevoland, were used to establish the input values for the soil water and nitrogen modules for each field-year combination (see Supplementary Text S13).

2.5.3. Post processing of WOFOST outputs

The field-specific site and management input data, the crop input data, and the weather data were used to simulate the growth of winter wheat for each field-year combination. For each simulated field-year combination i, the effective annual N input $N_{\text{in,i}}$ was estimated as (Silva et al., 2021b):

$$N_{\text{in,i}} = N_{\text{seed}} + N_{\text{bckg}} + \sum_{f=1}\left(f_{\text{rep,f}} \cdot N_{i,f}\right) \tag{4}$$

where N_{seed} is the amount of N in sown seeds assumed to be 3.5 kg N ha^{-1} (Silva et al., 2021b). N_{bckg} is the annual daily atmospheric N deposition rate (kg N ha^{-1}), which was calculated from the daily precipitation rates and the national N deposition statistics (Supplementary Fig S2, Supplementary Text S8). $f_{\text{rep,f}}$ is the replacement fraction of the applied fertilizer or manure type f, which corresponds to the fraction of the total amount of N in the fertilizer that becomes available for crop uptake in the year of application (Hijbeek et al., 2018). We adopted the values for $f_{\text{rep,f}}$ from Silva et al. (2021b). From each simulated field-year combination i, the wheat yield ($Y_{\text{WN,i}}$) was determined as the simulated grain dry matter at the harvest date and the N output ($N_{\text{out,WN,i}}$) as the simulated amount of N in the grains at the harvest date. The following equation was fitted (Fig. 2a) to the estimates of Y_{WN} and N_{in}:

$$Y_{\text{WN}} = Y_{\text{WL}} - \left(Y_{\text{WL}} - Y_{\text{WN,0}}\right) \cdot e^{-c_1 \cdot N_{\text{in}}} \tag{5}$$

where Y_{WL} (kg DM ha^{-1}) is the simulated water-limited yield and c_1 (ha kg^{-1} N) is a coefficient. The following equation was fitted (Fig. 2b) to the estimates of N output and N input:

$$N_{\text{out,WN}} = \begin{cases} N_{\text{out,0}} + c_2 \cdot N_{\text{in}} & \mid \quad N_{\text{in}} \le \dfrac{N_{\text{out,WL}} - N_{\text{out,0}}}{c_2} \\ N_{\text{out,WL}} & \mid \quad N_{\text{in}} > \dfrac{N_{\text{out,WL}} - N_{\text{out,0}}}{c_2} \end{cases} \tag{6}$$

where $N_{\text{out,0}}$ is the N output that would be obtained in the absence of N fertilization. $N_{\text{out,WL}}$ (kg N ha^{-1}) is the N output obtained under water-limited growth c_2 (ha kg^{-1} N) is the slope of the relationship between $N_{\text{out,WN}}$ and N_{input} when $N_{\text{out,WN}}$ is smaller than $N_{\text{out,WL}}$.

2.5.4. Scenario analysis to inform sustainable N management

The model application aimed to verify whether the ambition of the 'Farm-to-Fork Strategy to halve the N surplus, defined as the difference between N input and N output at harvest, can be achieved for winter wheat in the Netherlands. For this purpose, N input, N output, and N surplus were calculated for four different scenarios (Fig. 2, Supplementary Text S14). The baseline scenario considers the wheat yields and N outputs and the N input estimated using Eq. 4 for each field-year combination. Scenario 1 assumes that the efficiency yield gap is closed on each field-year combination, i.e., wheat yield and N output of each field-year combination i are assumed to equal $Y_{\text{WN,i}}$ and $N_{\text{out,WN,i}}$, respectively. Scenario 2 considers N input is reduced to the minimum amount possible without incurring yield losses. Scenario 3 is a combination of Scenarios 1 and 2 and explores the impact of increasing reported wheat yields to 90% of the simulated water-limited yield. Two variations of scenarios 2 and 3 were devised to allow for soil N mining (2a and 3a) and to not allow for soil N mining (2b and 3b) while adjusting and N output and N input in the respective scenarios.

We adopted the definition of NUE from EUNEP (2015) and soil N mining is assumed to occur when NUE, defined as the ratio of N in the grains to the effective amount of N applied, was above 0.9 kg N kg N^{-1}. Although a negative N balance is possible within a single cropping season, soil N depletion over a whole crop rotation is unlikely in the Netherlands, as crop rotations are well fertilized.

The EUNEP framework also set a threshold value of NUE < 0.5 kg N kg N^{-1} as inefficient N use, and a provisional reference for N surplus at 80 kg N ha^{-1} as a maximum allowable N surplus to avoid large environmental impacts (EUNEP, 2015). We adopted these thresholds as well (Fig. 2).

3. Results

3.1. WOFOST calibration on the 1982-1984 growing seasons

3.1.1. Crop dry matter and N uptake

After model calibration (Table 1), WOFOST performed well in simulating the dry matter of leaves (RMSE = 0.3 Mg ha^{-1}), stems (RMSE

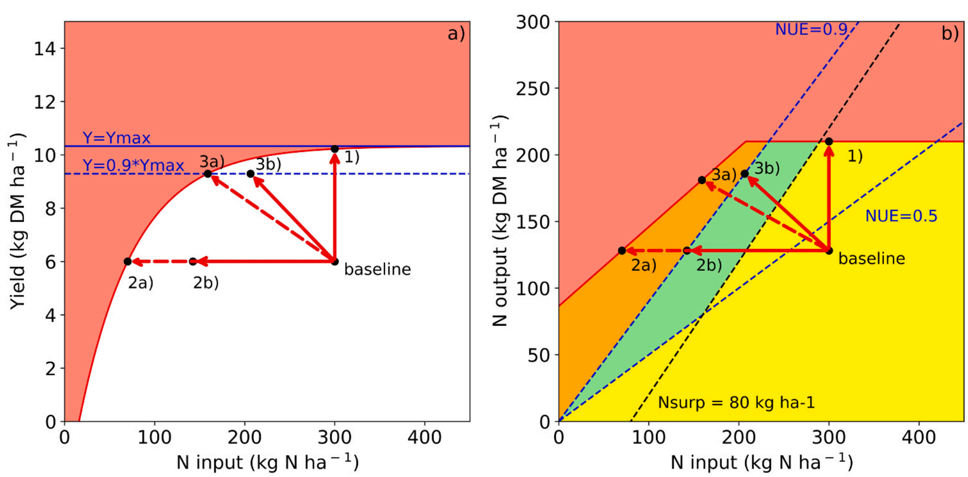

Fig. 2. Schematic representation of the pathways for sustainable N management explored in this study in relation to crop yield (a) and N output (b).The red area represents unattainable input-output combinations as these are above the simulated N limited yield and N output response to N input. The coloured areas represent the input-output combinations for which the N use is either inefficient (yellow), within a desirable range (green), or translates into soil N mining (orange). The black dots represent the yield (a) and N output (b) of a field under the different scenarios explored. The scenarios assume that either the efficiency yield gap is closed (Scenario 1), the N input is reduced to a level where further N input reductions would lead to either yield loss while preventing soil N mining (Scenario 2a) or both yield loss and soil N mining (Scenario 2b), or that 90% of the water-limited yield is reached with soil N mining (Scenario 3a) and without soil N mining (Scenario 3b). In (a), the solid blue line represents the simulated water-limited yield and the dotted blue line the target yield of Scenario 3. In (b), the blue dotted lines represent the N output for a given N input when NUE = 0.5 kg N kg^{-1} N and when NUE = 0.9 kg N kg^{-1} N whereas the black dotted line represents the N output corresponding to a N surplus of 80 kg N ha^{-1}. The NUE and N surplus thresholds were proposed by EUNEP (2015).

= 1.2 Mg ha^{-1}), and grains (RMSE = 0.6 Mg ha^{-1}) in the N3 treatments of both growing seasons (Fig S3, Supplementary Table S8). Consequently, the model performed well in simulating the aboveground dry matter (RMSE = 0.9 Mg ha^{-1}). The leaf area index was well simulated (RMSE = 0.77 m^2 m^{-2}). Lastly, WOFOST simulated the amount of N in the leaves with a RMSE of 23.3 kg ha^{-1}, in the stems with a RMSE of 24.7 kg ha^{-1}, and in grains with a RMSE of 17.1 kg ha^{-1} (Supplementary Fig S4, Supplementary Table S10). The total aboveground N uptake was simulated with a RMSE of 39.1 kg N ha^{-1} and a MBE of 27 kg N ha^{-1} (Fig. 3, Supplementary Table S9). The calibrated model was therefore able to reproduce the field observations of the N3 treatment during the 1982–1983 growing season with a level of precision and accuracy.

WOFOST substantially overestimated the amount of dry matter in stems of the N1 treatments in De Eest in 1982–1983 (MBE = −2.0 Mg ha^{-1}, RMSE = 2.2 Mg ha^{-1}) and in grains (MBE = −0.97, RMSE = 1.4 Mg ha^{-1}; Fig. 4, Supplementary Table S8). These overestimations are also reflected in the model performance to simulate the total aboveground dry matter (MBE = −2.2 Mg ha^{-1}, RMSE = 3.0 Mg ha^{-1}) and total aboveground N uptake (MBE = −48 kg N ha^{-1}, RMSE = 58.1 kg N ha^{-1}). Nevertheless, the overall model performance for the N1 treatments at all other sites and years was considerably better for the dry matter in the stems (MBE = −0.3 Mg ha^{-1}, RMSE = 1.0 Mg ha^{-1}) and in the grains (MBE = −0.3 Mg ha^{-1}, RMSE = 0.6 Mg ha^{-1}), total

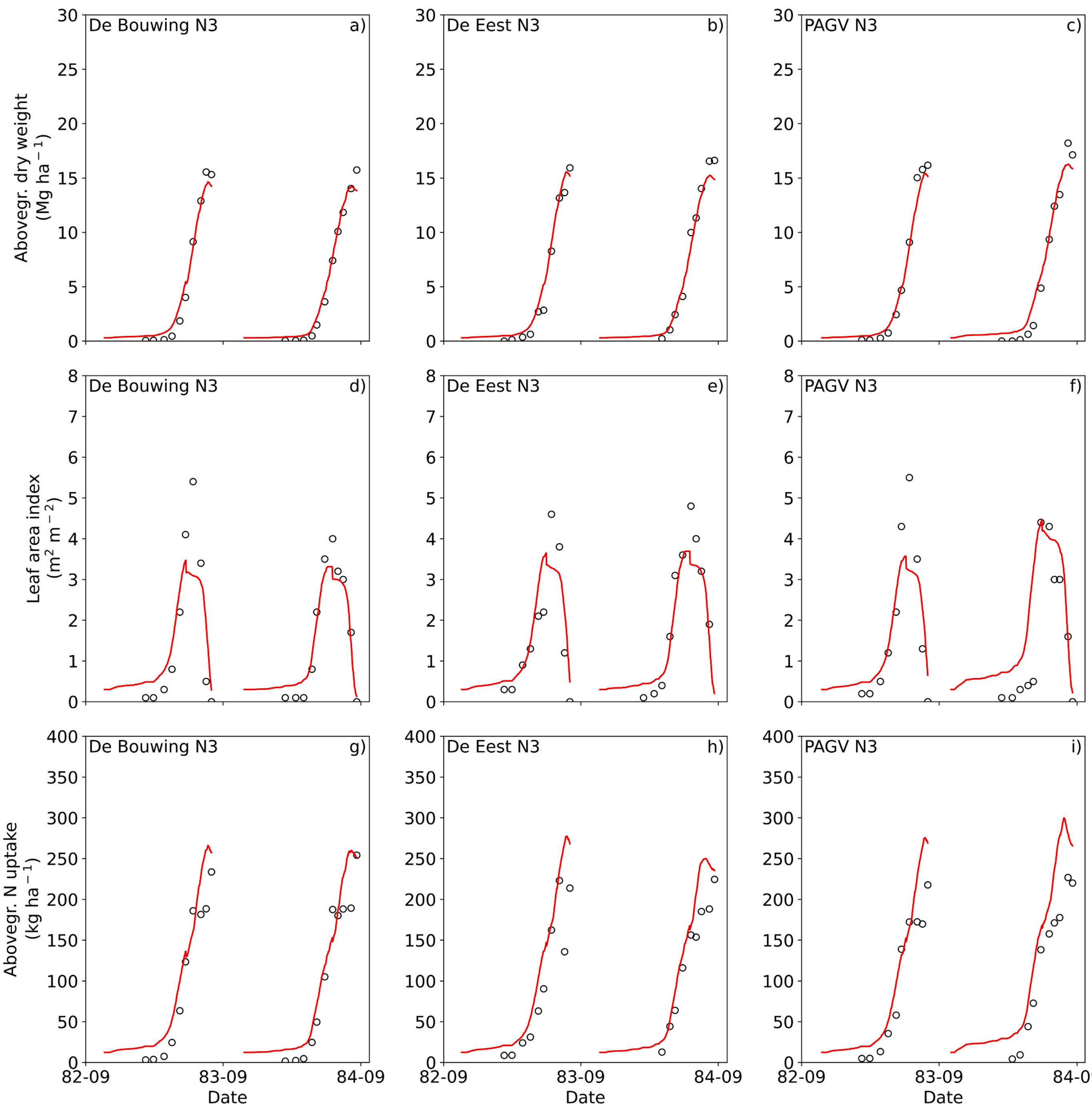

Fig. 3. Measured (dots) and simulated (lines) aboveground dry matter, leaf area index, and aboveground N uptake in aboveground dry matter in the N3 treatment of the calibration data set.

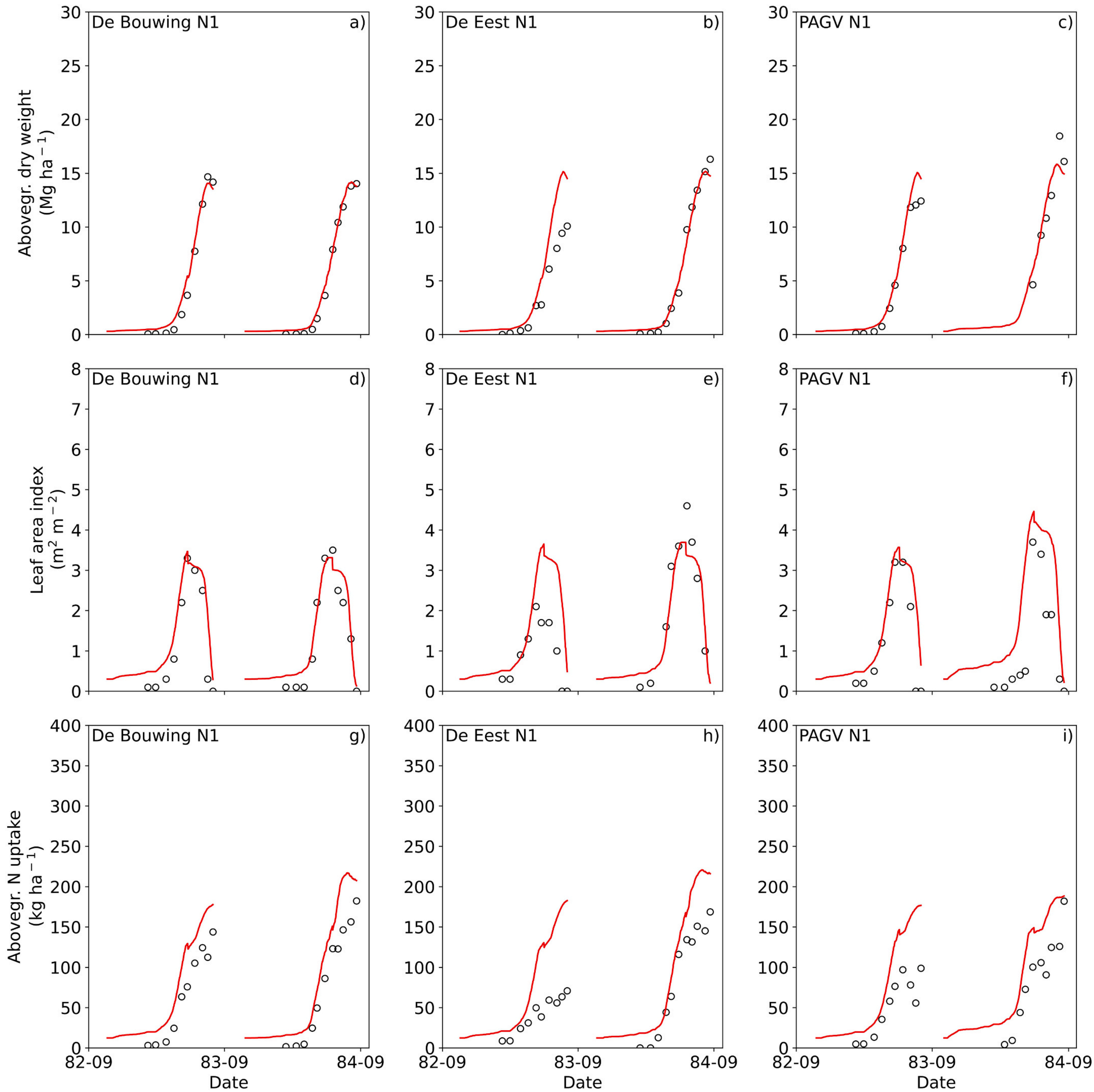

Fig. 4. Measured (dots) and simulated (lines) aboveground dry matter, leaf area index, and aboveground N uptake in aboveground dry matter in the N1 treatment of the calibration data set.

aboveground dry matter (MBE = −0.30 Mg ha^{-1}, RMSE = 1.0 Mg ha^{-1}), and total aboveground N uptake (MBE = −36 kg N ha^{-1}, RMSE = 43 kg N ha^{-1}). In the N2 treatments, WOFOST simulated the dry matter in the leaves, stems and total aboveground dry matter with a RMSE of 0.2, 0.9, and 0.9 Mg ha^{-1}, respectively, comparable to results of model performance in the N3 treatment (Fig. 5, Supplementary Table S8).

3.1.2. Soil water dynamics

WOFOST overestimated the amount of soil water between 0 and 100 cm in 1983–1984 in the N3 treatment at site De Bouwing with MBE of – 54.2 mm (Fig. 6, Supplementary Table S11) and underestimated the amount of water in De Eest during the same growing season (MBE = 72.7 mm). The MBE for the other site and year combinations in the N3 treatment varied considerably less (between −22.7 mm and 22.4 mm). The MBE for all sites combined was low (8.0 mm) and so was the RMSE (46.7 mm). For all sites in the 1982–1983 growing season and in De Bouwing in the 1983–1984 growing season, the observations showed a substantial decline in the amount of water towards the end of the growing season and the model could reproduce this phenomenon. The model explained the variation in the observation at the different sites and years well as the r^2 varied between 0.59 (PAGV, 1983–1984) and 0.84 (De Eest, 1983–1984). The patterns in the N1 (Supplementary Fig S10) and N2 treatments (Supplementary Fig S11) were similar. The soil water amount between 0 and 100 cm was calculated from measured and

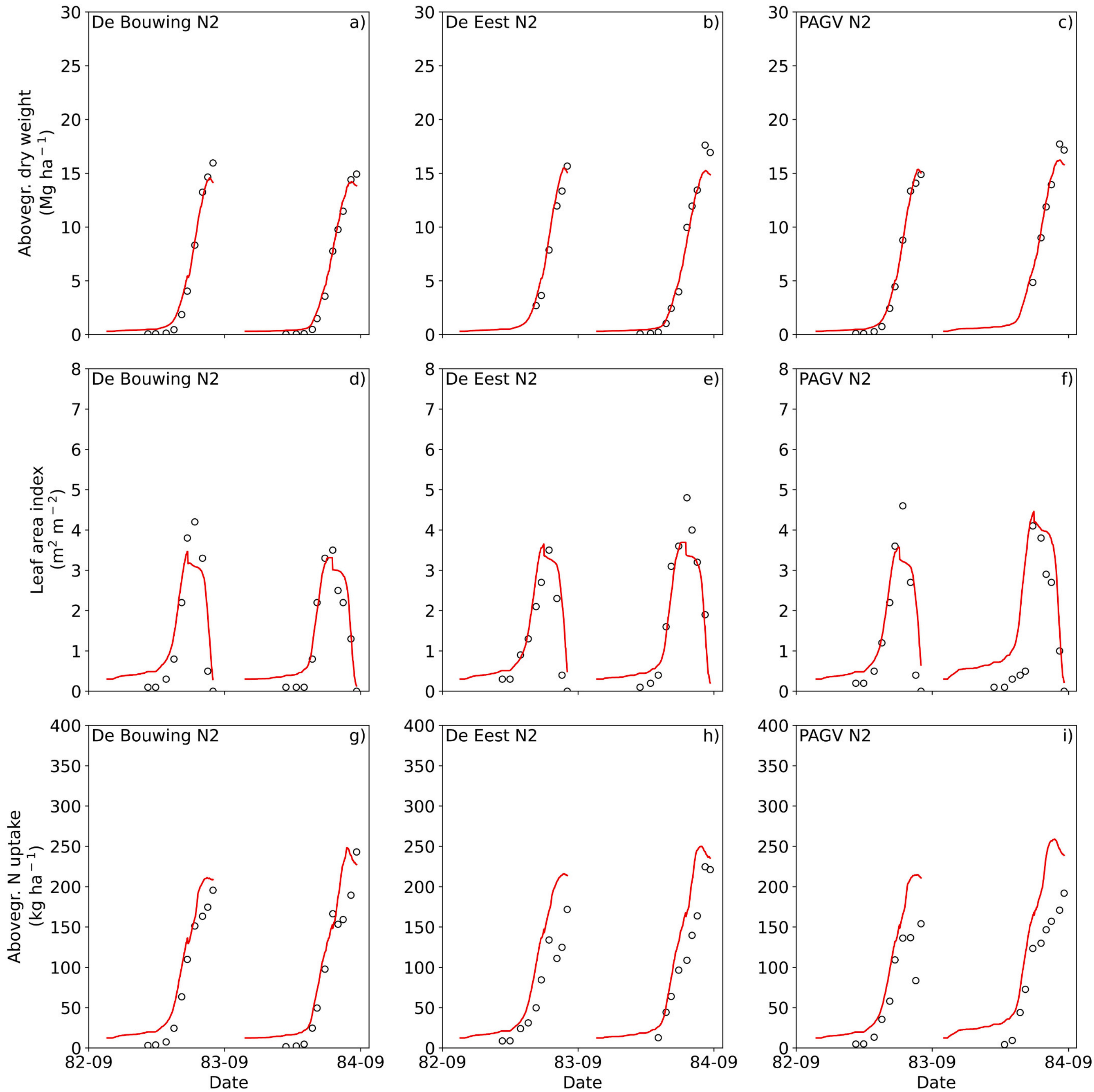

Fig. 5. Measured (dots) and simulated (lines) aboveground dry matter, leaf area index, and aboveground N uptake in aboveground dry matter in the N2 treatment of the calibration data set.

simulated soil moisture contents considering the depths of different soil layers and the results are summarized in Supplementary Figs S14 - S19.

3.1.3. Soil nitrogen dynamics

WOFOST simulated the amount of inorganic N in the first 100 cm of the soil in the N3 treatment with an MBE of 3.4 kg N ha^{-1} and a RMSE of 38.3 kg N ha^{-1} (Fig. 7, Table S11). There was quite some difference between the capability of WOFOST to explain the variation in the soil inorganic N observations, as the r^2 varied between close to nil (PAGV, 1982–1983) and 0.90 (De Eest, 1983–1984). As expected, the model always predicted an increase in the amount of inorganic N after an application event. The combinations of site and year for which the model was capable to explain a substantial amount of variation, i.e., $r^2 \geq 0.35$, have in common that the observations also show a substantial increase in the amount of inorganic N after the first fertilizer application event. The model performed much better in explaining the variation of the N1 and N2 treatments, for which the r^2 varied from 0.79 to 0.88 for the N1 treatment (Supplementary Fig S12) and between 0.64 and 0.86 for the N2 treatment (Supplementary Fig S13). The better model performance for the lower N treatments is likely due to the smaller number of application events and smaller application amounts in these treatments. The inorganic soil N amounts between 0 and 100 cm soil depth were calculated from measured and simulated amounts of inorganic soil N in different layers and results are shown in Supplementary Figs S14 -

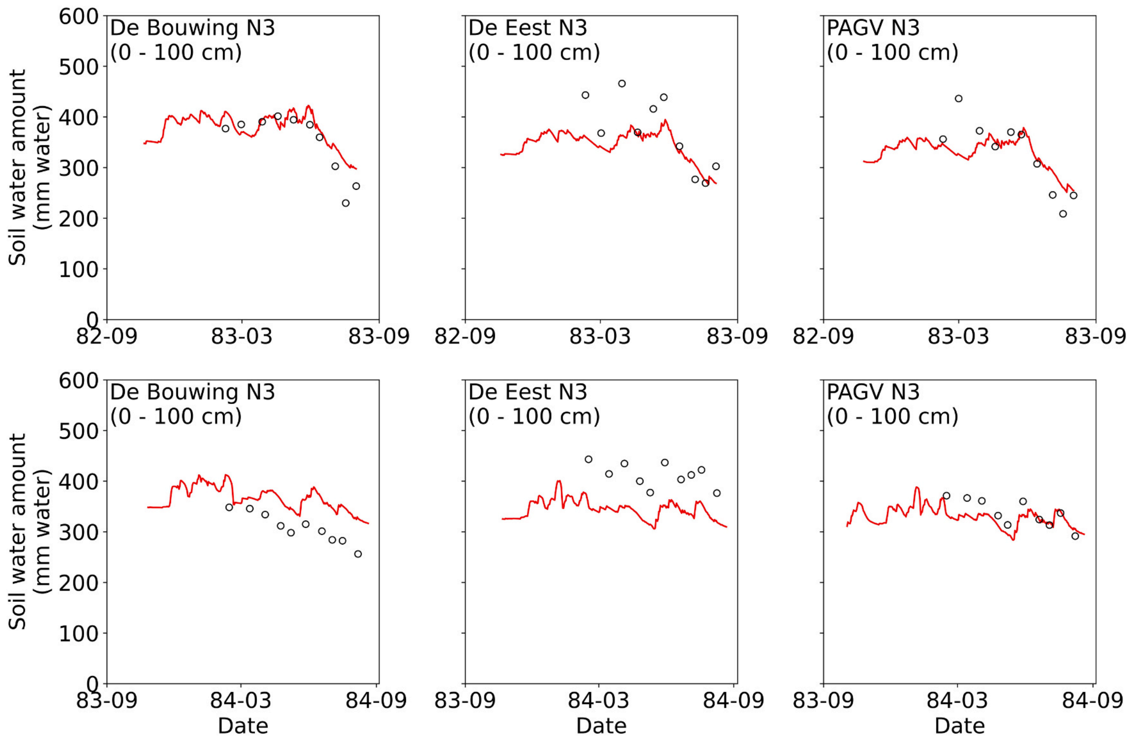

Fig. 6. Measured (dots) and simulated (lines) soil moisture content between 0 and 100 cm depth for the N3 treatment at each location in the calibration data set in the 1982–1983 (top) and 1983–1984 (bottom) growing seasons.

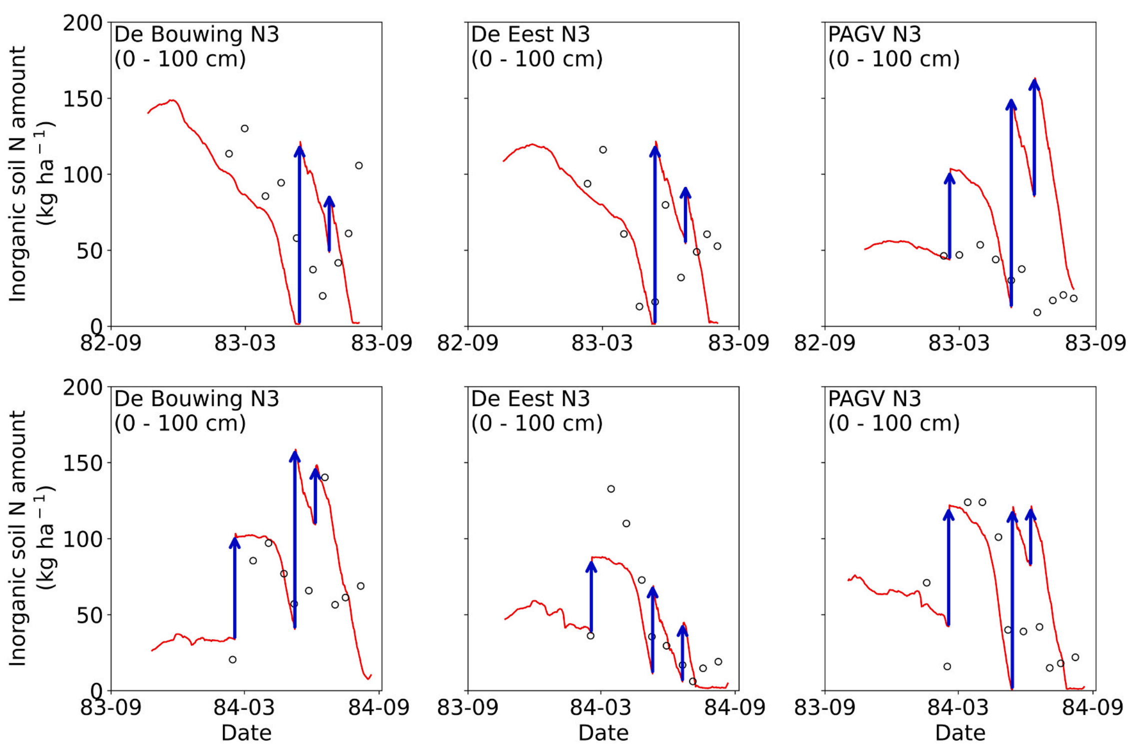

Fig. 7. Measured (dots) and simulated (lines) inorganic N amounts (sum of NO_3^--N and NH_4^+-N amounts) in the soil between 0 and 100 cm depth for the N3 treatment at each location in the calibration data set in the 1982–1983 (top) and 1983–1984 (bottom) growing seasons. The arrows are drawn at dates of N application and the size of the arrow represents the amount applied.

S19.

3.2. WOFOST evaluation on the 2013-2015 growing seasons

The TSUM1 estimated for the evaluation data set was 880 °Cd, a value close to that determined for Arminda (885 °Cd), while, the estimated value of TSUM2 (909 °Cd) was larger than that determined for Arminda (870 °Cd, Table 1).

The differences between the measured yields in the N3 and N1 treatments in the 2013–2014 and 2014–2015 growing seasons were small for the cultivars Julius and Ritmo (between 0.04 Mg ha^{-1} and 0.9 Mg ha^{-1}; Fig. 8, Supplementary Table S12), but substantial for Tabasco (1.5 Mg ha^{-1}). However, this difference was not observed for Tabasco in the 2013–2014 growing season, when there was even a very small negative yield difference between the N3 and the N1 treatment (−0.02 Mg ha^{-1}). This indicates that there was little N stress in either of the treatments. This low N stress was well reproduced by the model, which simulated the amount of dry matter in leaves, stems, and grains similar to the measured values for all treatments (Fig. 8, Supplementary Tables S12-S13; Supplementary Fig S9). The model performed well in reproducing the measured dry matter in the leaves (MBE =- 0.28 Mg ha^{-1}; RMSE = 0.42 Mg ha^{-1}) and stems (MBE = 0.50 Mg ha^{-1}; RMSE = 1.3 Mg ha^{-1}) (Table S12). WOFOST also performed well in simulating the grain dry matter at harvest in the 2013–2014 growing season (MBE = 0.5 Mg ha^{-1}; RMSE = 0.8 Mg ha^{-1}) but underestimated it in the 2014–2015 growing season (MBE = -2.6 Mg ha^{-1}; RMSE = 2.7 Mg ha^{-1}). Given the good model performance in simulating crop dry matter, with the exception of grain dry matter in the 2014–2015 growing season, WOFOST also performed well in simulating the total aboveground dry matter (MBE = 0.6 Mg ha^{-1}, RMSE = 1.4 Mg ha^{-1}). The leaf area index and aboveground N uptake were simulated with RMSEs of 1.25 m^2 m^{-2} and 34.5 kg N ha^{-1}, respectively.

3.3. Pathways for sustainable N management for wheat crops in the Netherlands

Fitting Eq. 5 to the simulated water- and N-limited wheat yields resulted in the estimates $Y_{WN,0} = -3.05$ Mg ha^{-1}, $Y_{WL} = 1.03$ Mg ha^{-1}, and $c_1 = 0.0161$ ha kg^{-1} N (Fig. 9a). Fitting Eq. 6 to the simulated grain N uptake resulted in estimates of $N_{out,0} = 86.41$ kg N ha^{-1}, $N_{out,mx} = 210.0$ kg N ha^{-1}, and $c_2 = 0.595$ ha kg^{-1}N (Fig. 9b). There were 9 out of 141 field-year combinations, 6% of the sample, for which the farm-reported wheat yield was greater than the simulated Y_{WN}. There were only three fields out of 141, in which the farm-reported yield was larger than the simulated water-limited yield Y_{WL}. According to the EUNEP framework, only one field exhibited inefficient N use (NUE < 0.5 kg N kg^{-1} N) whereas 104 fields, or 74% of the sample, exhibited efficient N use (0.5 < NUE < 0.9 kg N kg^{-1} N). The remaining 36 fields, or 26% of the sample, showed potential for soil N mining in the long-term (NUE > 0.9 kg N kg^{-1} N). The average N surplus across all field-year combinations was 41 kg N ha^{-1} and there were 29 field-year combinations, or 21% of the sample, for which N surplus was higher than 80 kg N ha^{-1} (Fig. 10).

The average reported N input was 213 kg N ha^{-1} and N output was 171 kg N ha^{-1}. The average N surplus was 41 kg N ha^{-1} in the baseline scenario. Closing the efficiency yield gap without changing N input (Scenario 1) reduced the average N surplus by 75% to 11 kg N ha^{-1} (Fig. 10; Table S14). Reducing N input without incurring yield losses nor allowing for soil N mining (Scenario 2b) allowed to reduce the N input by 10% to 191 kg N ha^{-1} and N surplus by 54 to 19 kg N ha^{-1}. In Scenario 3b, in which all field-year combinations were assumed to achieve

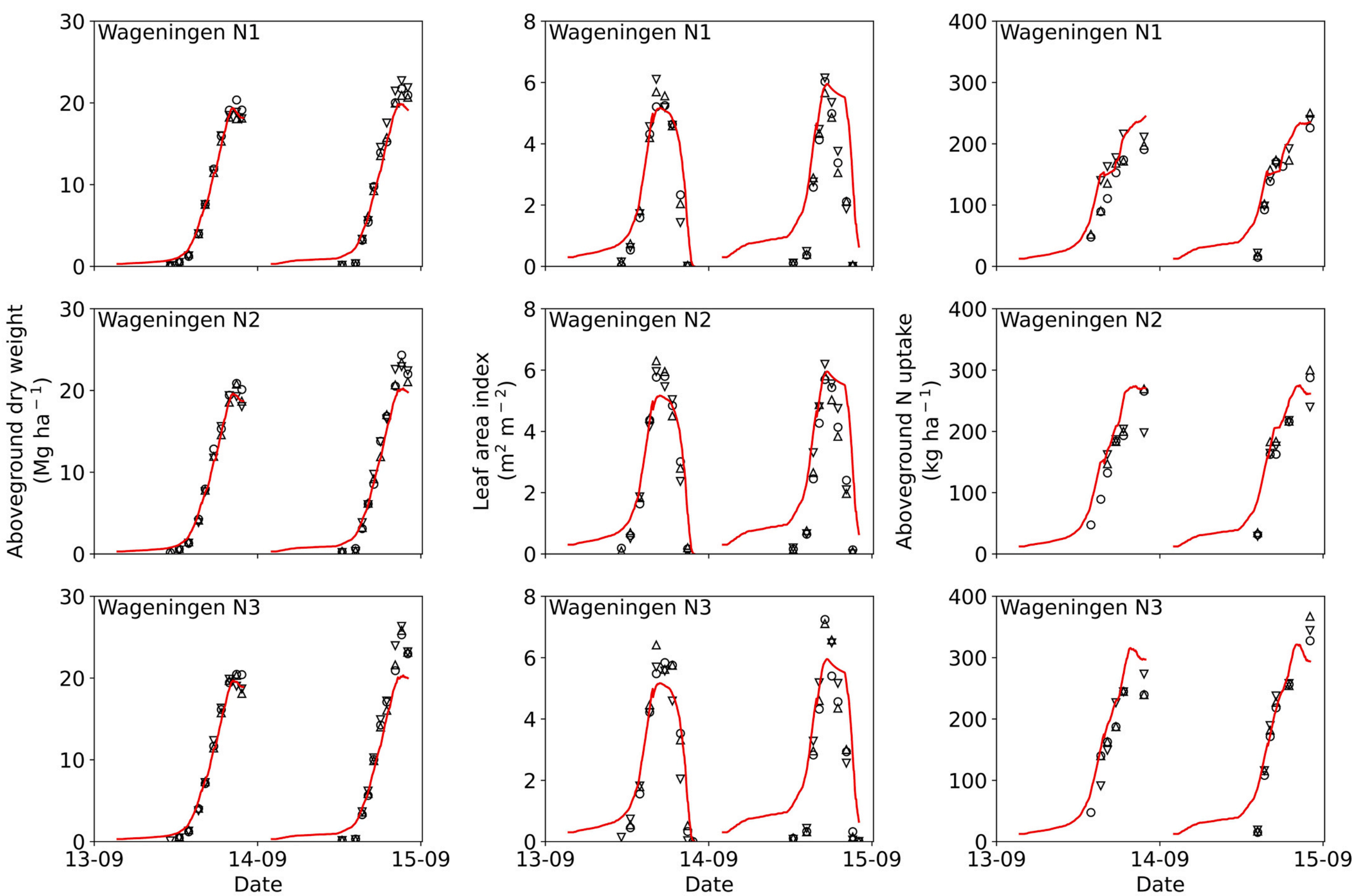

Fig. 8. Measured (squares, triangles, inverted triangles) and simulated (lines) aboveground dry matter, leaf area index, and aboveground N uptake in aboveground dry matter in the N1, N2, and N3 treatments of the evaluation data set. Measurements are presented as squares (cv Julius), triangles (cv Ritmo), and inverted triangles (cv Tabasco). There were no separate simulations for each cultivar.

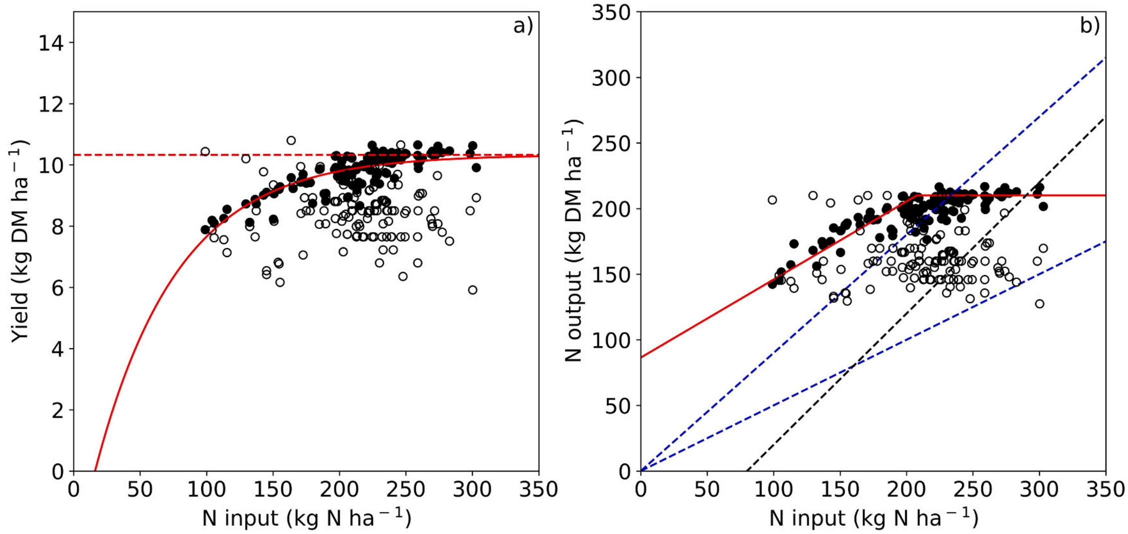

Fig. 9. Relationship between wheat yield (a) and N output (b) and N input. The closed dots refer to the simulated water- and N-limited yield (a) and N output (b) for individual field-year combinations. The open dots are measured farm wheat yield (a) and N output (b) for the same set of field-year combinations. The red solid lines are (a) the minimum of either Eq. 4 and the wheat yield for which NUE > 0.9 kg N kg^{-1} N, or (b) the minimum of Eq. 5 and the N output for which NUE < 0.9 kg N kg^{-1} N. The red dotted line (a) represents the average water limited yield across all field-year combinations. The blue dashed lines in (b) represent the the NUEs of 0.5 and 0.9 kg N kg^{-1} N. The black dotted line represents a N surplus of 80 kg N ha^{-1}.

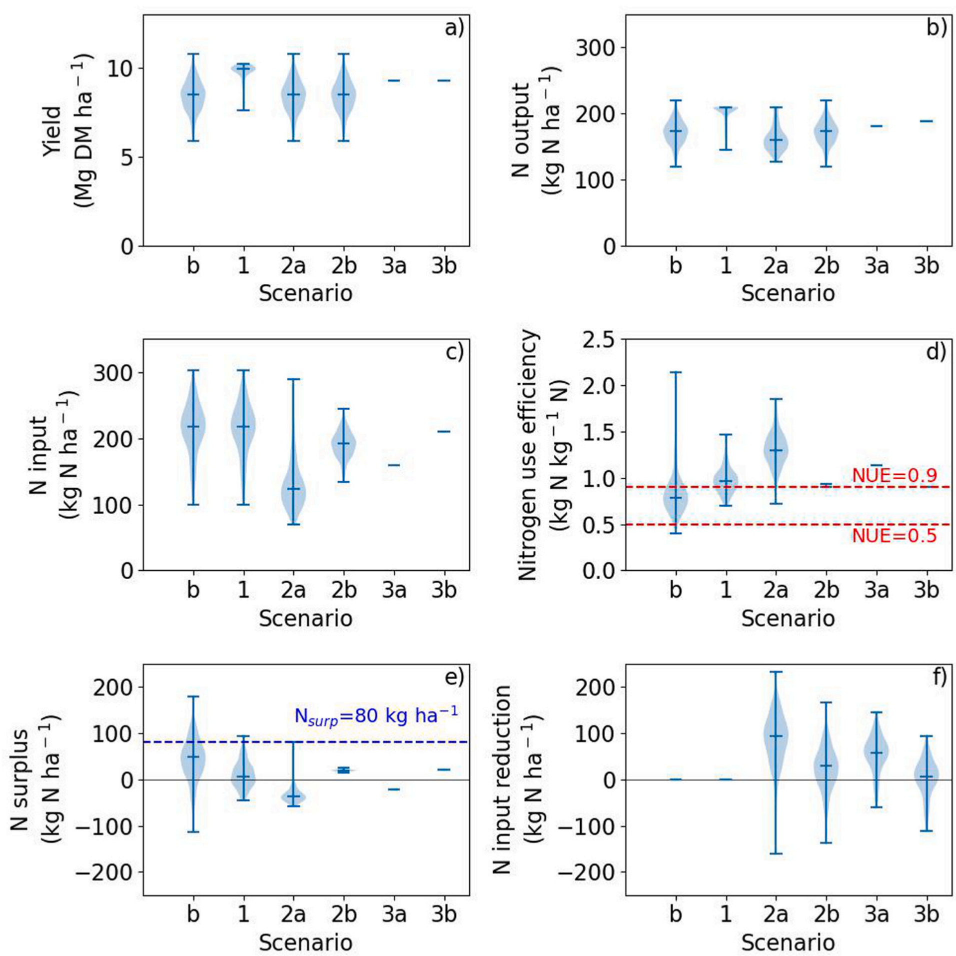

Fig. 10. Distribution of wheat yield (a), N output (b), N input (c), NUE (d), N surplus (e), and N input reduction (f) for different scenarios. The investigated scenarios are the baseline situation (b), the scenario in which the efficiency yield gap is closed (Scenario 1), the N input is reduced to the lowest level without incurring yield losses and allowing for soil N mining (Scenario 2a), or not allowing for soil N mining (Scenario 2b), or actual farm yields of 90% of the water-limited yield while allowing for soil N mining (Scenario 3a) or not allowing for soil N mining (Scenario 3b). The ticks in the violin plots represent the minimum, median, and maximum value of each variable in each scenario.

90% of the simulated water-limited without soil N mining, the average N input reduction is small (3 kg N ha$^{-1)}$, but the average N surplus would also be reduced by 49% to 21 kg N ha^{-1}.

Considering that soil N mining is not a large risk in the Netherlands, larger N reductions in N input and N surplus seem feasible. Reducing N input without incurring yield losses and allowing for soil N mining (Scenario 2a) reduced the average N input to 129 kg N ha^{-1} (39% reduction) and resulted in a negative N surplus (−34 kg N ha^{-1}). Aiming for 90% of the simulated water-limited while accepting soil N mining (Scenario 3a) allowed an average N input reduction of 159 kg N ha^{-1} (25%) and resulted in a negative N surplus of -22 kg N ha^{-1}.

In Scenario 1, N input was not reduced relative to the baseline scenario because this scenario assumes that the water- and N-limited yield can be achieved with the same N input as in the baseline scenario by overcoming yield constraints other than water and N. The N input reductions were smaller for Scenarios 2b and 3b, in which soil N mining is prevented than in Scenarios 2a and 3a, in which soil N mining is allowed. While the N input reductions in Scenario 2a and 3a were 84.0 kg N ha^{-1} and 53.8 kg N ha^{-1}, the N input reductions in Scenarios 2b and 3b were considerably smaller, 22.3 kg N ha^{-1} and 2.6 kg N ha^{-1}, respectively. Our results thus indicate that reductions in N surplus are best achieved through N input reductions to a level below which yield losses would be expected (Scenarios 2a and 3a). Yet, this would also lead to NUEs (Scenario 2a: 1.31 kg N kg N^{-1}, Scenario 3a: 1.14 kg N kg N^{-1}) considerable higher than the NUE threshold of 0.9 kg N kg^{-1} N proposed by EUNEP above which soil N mining is expected to occur.

There was considerable variation in the reported N input, ranging between 99 and 303 kg N ha^{-1}, and N output, ranging between 120 and 220 kg N ha^{-1} (Fig. 10, Supplementary Tables S16-S17). This variability translated in a large variability of N surplus (−113 to 180 kg N ha^{-1}) and NUE (0.40 - 2.1 kg N kg^{-1} N). In all scenarios, the average N surplus was below the 80 kg N ha^{-1} threshold proposed by EUNEP (2015) and hence below the national threshold for clay soils. In Scenario 1, N surplus varied considerably (between −46 kg N ha^{-1} and 93 kg N ha^{-1}). In only one field, N surplus was above the EUNEP threshold of 80 kg N ha^{-1}. In Scenario 2a, N surplus varied between -46 and -36 kg N ha^{-1}. In Scenario 2b, there was hardly any variation in N surplus: in 139 out of 141 fields, N surplus was 19.0 kg N ha^{-1}. The achieved reduction of N input varied considerably between fields in Scenarios 2a (−160 to 231 kg N ha^{-1}), 2b (−137 to 166 kg N ha^{-1}), 3a (−60 to 144 kg N ha^{-1}), and 3b (−111 to 92 kg N ha^{-1}). So, despite N input reductions in Scenarios 2a (84 kg N ha^{-1}), 2b (22 kg N ha^{-1}), 3a (54 kg N ha^{-1}), and 3b (2.6 kg N ha^{-1}), the field-specific N input reduction in these scenarios differed strongly per field to a point that N input was estimated to increase in 41 and 62 field-year combinations in Scenarios 2b and 3b.

4. Discussion

4.1. Model improvement

4.1.1. CO_2 assimilation module

One of the extensions of WOFOST presented in this study was the possibility to calculate the maximum gross reference CO_2 assimilation rate, $A_{mx,rf}$, from the specific leaf N content (Supplementary Text S4). This was done using a generic linear relationship (Peng et al., 1995; Van Keulen and Seligman, 1987). More complex functional forms of the response curve for $A_{mx,rf}$ to the specific leaf N content have been proposed though. Examples are a curvilinear relationship (Sinclair and Horie, 1989) or a piece-wise linear relationship (Bouman et al., 2001). These functional forms may perform better in describing crop-species specific $A_{mx,rf}$ responses to the specific leaf N content. Nevertheless, we opted for the linear relationship from Peng et al. (1995) because it is generic for C_3 species and determining more complex relationships requires coupled observations of the specific leaf N content and gross leaf CO_2 assimilation rates that are often not available.

Since various previous studies (Ågren, 1985; Greenwood et al., 1991; Justes et al., 1994) observed that total dry matter production does not increase once a critical N concentration is reached, the maximum gross reference CO_2 assimilation rate cannot exceed a maximum value represented by $A_{mx,rf,mx}$ (Equation S4.5). It should be noted that the value of this parameter is likely species specific, as the estimates of the maximum gross CO_2 reference assimilation rate in the previous versions of WOFOST at early development states are different for different crop species (Boons-Prins et al., 1993). Also, it should be mentioned that the linear relationship between the specific leaf N content and maximum gross photosynthesis rate that we adopted from Peng et al. (1995) was only determined for C_3 species. So it is likely not valid for C_4 species, for which the slope is higher (Wang et al., 2022). Future research is required to determine appropriate values of $A_{mx,rf,mx}$ for other crops and to formulate an alternative relationship between the net CO_2 assimilation rate and the specific leaf N content for C_4 species.

4.1.2. Crop N module

An important parameter for the calculation of the actual gross CO_2 assimilation rate and, therefore, the total dry matter production rate, is the development state dependent tabular function of maximum leaf N concentration, NMAXLV_TB. We adopted values for NMAXLV_TB from the LINTUL-4 model (Wolf, 2012). WOFOST performed relatively well in calculating the amount of N in leaves during the growing season (Supplementary Figs S4-S6) and the total aboveground dry matter production (Figs. 3–5, 8). This suggests that NMAXLV_TB has appropriate values for winter wheat. Nevertheless, NMAXLV_TB is likely not generic for other crops. NMAXLV_TB thus needs to be calibrated for crops other than wheat. Suitable values may be, for instance, found in the crop parameters for LINTUL-4 (Wolf, 2012) which has example values for NMAXLV_TB for 24 crop species.

4.1.3. Soil N and water modules

The addition of the soil N module SNOMIN (Supplementary Text S1, S2, Fig. 1) was necessary to determine how much N was daily available for root uptake throughout the growing season. In contrast to many other models, SNOMIN defines separate state variables for the amount of organic matter, C, and N in each amendment and soil layer (Fig. 1) from the moment they are applied. The types of amendments differ in their initial apparent age. The latter parameter can be estimated from measured time series for the decomposition of organic material in that amendment and this has been done for various type of materials that contain organic matter (Groenendijk et al., 2016; Janssen, 1984; Yang and Janssen, 2000; Janssen, 1986). This approach has been applied in the 2-layered soil model NDICEA (Van der Burgt et al., 2006) and tested worldwide (Nascimento et al., 2011; Rietberg and Van der Burgt, 2012; Smith et al., 2016; Van der Burgt et al., 2006). In this study, we used the same approach and made it more flexible than NDICEA by allowing any number of soil layers with user-defined depths. We also made it more widely applicable by embedding it in the publicly available PCSE modelling framework. In order to make it possible to simulate the interaction of soil N with the amounts and flows of soil water, we also replaced the soil water module from De Wit (2021), with the multi-layered soil water module WATFDG (Rappoldt et al., 2012) to provide soil moisture contents and fluxes between the layers to the layered soil N module.

The parameters initial age of organic matter and the C:N ratio of the microbial biomass in SNOMIN are also used in the MINIP-C, MINP-N (Heinen and De Willigen, 2005) and NDICEA (Van der Burgt et al., 2006) models to simulate mineralization rates. SNOMIN adopted the value for the C:N ratio of the soil microbial biomass from MINIP-N and of the initial age of organic matter from NDICEA (Van der Burgt et al., 2006). Yet, these parameters are likely soil specific (Van der Burgt et al., 2006). Default values from these models were used in this study due to lack of field observations, but we recommend future studies to derive such parameters from direct measurements. The initial age of organic matter lumps the effects of decomposition of amendments applied during recent growing seasons and we recommend in future simulation studies to initialize the model several growing seasons before the growing season of interest to calculate the amounts of organic matter, apparent age, and the C:N ratios of previously added amendments. Yet, this approach requires that the date of application and the types and amounts of fertilizers applied during past growing seasons are known, which was neither the case in the calibration nor in the evaluation data set. Future experiments aiming to calibrate crop models for N-limited growth should thus measure the C:N ratio of the microbial biomass (Luo et al., 2022) and document the fertilization history of the field during past growing seasons.

4.2. Performance of the improved WOFOST model

The soil water module added in this study (WATFDGW) was previously evaluated (Rappoldt et al., 2012) against the output generated by the more complex SWAP model (Kroes et al., 2017). Our study is the first study in which WATFDGW has been tested against measured data and the results were mostly satisfactory (Fig. 6, Supplementary Figs S10-S11). The initial input values for WATFDGW were derived from data in the BOFEK soil map (Heinen et al., 2021). While this parametrization mostly resulted in adequate simulations, the bottom soil layer in Wageningen had, unlike the upper soil layers, a very low bulk density and consisted of low percentages of clay and silt (Supplementary Table S2). Initial simulations showed that the use of the original soil profile to parametrize the soil water module resulted in strong drought stress towards the end of the growing season and strong underestimations of the final yield in both growing seasons for all N treatments. To solve this issue, we had to assume that the bottom soil layer had the same properties as the layer above (Supplementary Text S12). Model inputs for the soil N module were partially obtained from the BOFEK soil map. Also here, there was an issue with soil map data for one site. The bottom soil layer of De Eest contained an organic matter mass percentage of 65%. Such a high percentage is unlikely for this marine clay soil and also was also not confirmed by soil textural measurements conducted in De Eest (Groot and Verberne, 1991). Initial simulations showed that the use of this value would result in very high release of inorganic N in this layer, which was not reflected in the inorganic N or N uptake observations. Therefore, we assumed that the bottom soil layer had the same soil textural properties as the layer above. Another issue was that WOFOST was not able to explain why measured amounts of inorganic N in the 1982–1983 growing season did not increase after the first N application event in the N3 treatment. The same issue was reported in three other studies that used this data set to calibrate and evaluate crop and soil models (Addiscott et al., 1991; Asseng et al., 2000; Grant, 1991). To the best of our knowledge, there is no modelling study available that can explain this issue. Since the model was able to explain more than half of the variation in most other treatments and that the overall MBE for these other treatments was low (14.3 kg N ha^{-1}), we conclude that the model can be used to simulate the amount of inorganic N in the soil.

We compared the performance of WOFOST in reproducing the calibration and evaluation data sets with the performance of other models that were also evaluated on either of these data sets. In a previous study (Berghuijs et al., 2023), PCSE-LINTUL3 was evaluated on the N3 treatments of the evaluation data set. The WOFOST model, as parametrized in this study, performed considerably better in reproducing the total aboveground dry matter (MBE = 0.71 Mg ha^{-1}, RMSE = 1.77 Mg ha^{-1}) than the PCSE LINTUL-3 model (MBE = 0.92 Mg ha^{-1}, RMSE = 2.12 Mg ha^{-1}) on this data set, hence improving our ability to simulate wheat growth and development. Data from the calibration set were used for crop growth modelling in several studies, including a model comparison exercise of 14 crop models (De Willigen, 1991). However, direct comparisons with our results are not straight forward as these studies either used different indicators to quantify model performance or they did not use any indicator. Also, most of these 14 models were only tested for a subset of all combinations of locations, treatments, and years within the calibration data set. Furthermore, it was remarkable that most of the 14 crop models (Bergström et al., 1991; Grant, 1991; Lafolie, 1991; Kersebaum and Richter, 1991; Whitmore et al., 1991; Addiscott et al., 1991; Mirschel et al., 1991; Eckersten and Jansson, 1991) were initialized between January and March of the harvest year rather than at the actual sowing date (November of the sowing year). Therefore, these studies provide no evidence on model performance at early development stages and how early crop growth development is affected by vernalization and daylength, which is particularly relevant for winter wheat (Ceglar et al., 2019; Olesen et al., 2012; Van Bussel et al., 2015). The initialization of our soil N module SNOMIN was a major challenge in our study as well. Even though SNOMIN was initialized at the sowing dates, preliminary simulations had to be done to estimate the amounts of NO_3^--N and NH_4^+-N in the various soil layers at the sowing dates. We recommend future studies to conduct soil water and N measurements around the sowing date to make it possible to properly initialize crop and soil models. Unlike most of the aforementioned 14 models in the model comparison exercise (De Willigen, 1991), two other studies (Asseng et al., 2000; Yin et al., 2001) did simulate all treatments in the calibration data set and managed to start the simulation at the sowing date with. They used the APSIM-NWHEAT (Keating et al., 2001) and the MAGEC models (Yin et al., 2001). MAGEC simulated the total aboveground dry matter, grain matter, and aboveground N uptake with r^2 values of 0.17, 0.31, and 0.66, whereas APSIM-NWHEAT reproduced the same variables with r^2 values of 0.97, 0.90 and 0.82. WOFOST reproduced these variables with r^2 values of 0.98, 0.97, and 0.88. Additionally, APSIM-NWHEAT reproduced the amounts of soil mineral N per soil layer with RMSEs of 9 kg N ha^{-1} and a r^2 value of 0.46. WOFOST reproduced this variable with a RMSE of 11 kg N ha^{-1} and a r^2 value of 0.44. We conclude that WOFOST had a similar performance as APSIM-NWHEAT to reproduce the calibration data set and performed considerably better than MAGEC. In addition, we note that, even though a direct comparison is not possible, the current study and modified model performs reasonable or better compared to other recent studies (Yin et al., 2020).

4.3. Pathways for sustainable N use with crop models

WOFOST was used to simulate the water- and N-limited yield for farmers' wheat fields in the Netherlands. In only 9 out of 141 simulated field-year combinations, the farm-reported yields were greater than simulated yields for the N management reported for each field (Fig. 5a) and there were only 3 fields in which the simulated water-limited yield was exceeded by the reported yield. WOFOST can thus be used to delineate upper boundaries for crop yield response to N, and hence to explore options for sustainable N management under on-farm conditions.

Three scenarios and two sub-scenarios (Fig. 2) were devised to explore pathways for sustainable N management of wheat crops in the Netherland in relation to the baseline situation considering the actual yield and N management practices reported on-farm. Overcoming yield constraints other than water and N through narrowing efficiency yield gaps (Scenario 1; Silva et al., 2017) increased wheat yield by 10% relative to the baseline situation (8.4 to 9.8 Mg ha^{-1} on average) and reduced N surplus by 75% (Fig. 10). This is an attractive option for farmers as it combines the double-edged goals of productivity on one hand and economic and environmental sustainability on the other (Silva et al., 2021). Achieving this requires more attention to fine-tuning current management practices, particularly in relation to disease management, and to optimize crop rotations for wheat productivity (Silva et al., 2017). The feasibility of the latter is questionable though as farmers tend to prioritize high value root and tuber crops over low value cereal crops.

Another pathway for sustainable N management is to reduce N input without incurring yield losses (Scenarios 2a and 2b). Although the average N surplus can be negative when N input is reduced to a level below which yield loss occurs (Scenario 2a), this practice would result in a rather high average NUE of 1.31 kg N kg^{-1} N, exceeding the threshold of 0.9 kg N kg^{-1} N proposed by EUNEP (2015) above which soil N mining may occur in the long term. N input reductions to levels at which neither yield loss nor soil N mining are expected (Scenario 2b) would reduce N surplus by 54% compared to the baseline situation (Fig. 10). Combining yield increases with N input reductions would reduce N surplus by 49% over the baseline situation when respecting a maximum NUE of 0.9 kg N kg^{-1} N (Scenario 3b) and would result in a negative N surplus when soil N mining would be allowed (Scenario 3a). Fully exploiting Scenarios 2a, 2b, 3a, and 3b may not be attractive for farmers as they entail risks of N limitation on crop yield and do not optimize the use of organic manures available in the Netherlands. In addition, when wheat is cultivated for bread wheat, a minimum N concentration is required (Osman et al., 2012). Yet, N input reductions are possible while maintaining yield. The results thus suggest that it is indeed possible to fulfil the ambition of the European Commission of reducing the area-based average N surplus by 50% (European Commission, 2020) for winter wheat crops in the Netherlands with Scenarios 1, 2a, 2b, and 3a, and to some extent Scenario 3b. From a nitrate leaching perspective this may not be most urgent on the clay soils in Flevoland investigated here, but relationships are similar on sandy soils (Silva et al., 2021), where the national threshold for N surplus is much lower with 50 kg N ha^{-1} (Ros et al., 2023). Future research is required at crop rotation level to explicitly consider how to optimize N management for multiple crops and soil types, which requires the evaluation and application of WOFOST to simulate N dynamics over entire crop rotations at different locations.

Our study unravelled large differences between the required N input reduction to achieve Scenarios 2a, 2b, 3a and 3b. In a considerable number of field-year combinations in these scenarios, the negative N input reductions (Fig. 6) indicate that it is often necessary to *increase* N input to prevent yield losses and, for Scenarios 2b and 3b, also to prevent soil N mining. This finding underlines that recommendations to reduce N input reductions should be field-specific to the extent possible, instead of imposing the same recommendations on all fields. It also demonstrates that WOFOST can potentially be used as a decision support system to obtain N recommendations for individual fields.

5. Conclusions

WOFOST was extended with N-limited growth through improvements in the CO_2 assimilation module, and the addition of crop and soil N dynamics modules. A new soil N module, abbreviated as SNOMIN (Soil Nitrogen for Organic and Mineral Nitrogen module) was developed. This new soil module also required the replacement of the single-layered with a multi-layered soil water module. These improvements allowed to calculate the maximum reference net rate of gross CO_2 assimilation from a specific leaf N concentration instead of specifying a tabular function linking the maximum reference gross CO_2 assimilation rate (AMAXTB) to the development stage, as used in all previous versions of WOFOST. Simulations for potential and water-limited production now require a tabular function, NMAXLV_TB, with the maximum leaf N concentration as a function of development stage. The biomass partitioning module was also modified. The improved WOFOST model was able to simulate crop growth, biomass partitioning, and N partitioning of winter wheat crops field experiments conducted in Netherlands for different cultivars, locations, and time periods.

The improved WOFOST model was further used to investigate pathways for sustainable N management for farmers' winter wheat fields in the Netherlands. Scenario 1 assumed that the efficiency yield gap was closed, while maintaining the same N input, which reduced the average N surplus by 74% from 41 kg N ha^{-1} to 11 kg N ha^{-1}. Scenario 2b considered a reduction of N input without incurring yield losses but preventing soil N mining and resulted in an average N surplus reduction of 54% to 19 kg N ha^{-1}. Scenario 3b assumed on-farm yields of 90% of the water-limited yield, while preventing soil N mining and resulted in a N surplus reduction of 49% to 21 kg N ha^{-1}. These scenarios indicate that the Farm-to-Fork target of 50% reduction in N surplus can be reached without incurring yield losses and soil N mining for winter wheat grown in the Netherlands. Yet, as soil mining is not a large risk in the Netherlands, N surplus may be further reduced to -34 kg N ha^{-1} while maintaining yield (Scenario 2a) or to -22 kg N ha^{-1} while increasing actual yield to 90% of the water-limited yield (Scenario 3a). Scenarios 1, 2a, 2b, 3a and 3b allowed N input reductions of 0%, 39%, 10%, 25%, and 1%, respectively. However, there was considerable variation in the scope to reduce N input across fields, pointing the importance of site-specific nutrient management for high-yielding cropping systems.

We recommend future model improvements to focus on 1) calibrating the maximum leaf N concentration for crops other than wheat, 2) refining the relationship between leaf N concentration and maximum reference gross CO_2 assimilation rate for C_4 crops, 3) test for more fields whether the soil texture data from soil maps are adequate to simulate crop growth with WOFOST, and 4) evaluate model performance of simulations of crop yield and resource-use efficiency at cropping systems level. This will allow to further evaluate sustainable N use in a cropping systems context and in the long-term.

CRediT authorship contribution statement

De Wit Allard: Writing – review & editing, Supervision, Software, Methodology, Formal analysis, Conceptualization. **Reidsma Pytrik:** Writing – review & editing, Supervision, Project administration, Methodology, Funding acquisition. **Silva João:** Writing – review & editing, Methodology, Investigation, Data curation. **Berghuijs Herman:** Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

The datasets for model calibration and evaluation can be shared on request and are also available online. The commercial field data are confidential.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.eja.2024.127099.

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