Nitrogen dynamics in flooded soil systems: An overview on concepts and performance of models

Running title: *Model concepts of nitrogen dynamics in flooded soils*

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ABSTRACT

Extensive modelling studies on nitrogen (N) dynamics in flooded soil systems have been published. Consequently, many N dynamics models are available for users to select from. With the current research trend, inclined towards multi-disciplinary

research, and with substantial progress in understanding of N dynamics in flooded soil systems, the objective of this paper is to provide an overview of the modelling concepts and performance of 14 models developed to simulate N dynamics in flooded soil systems. This overview provides breadth of knowledge on the models, and, therefore, is valuable as a first step in the selection of an appropriate model for a specific application.

Keywords: Nitrogen, dynamic model, flooded soil, flooded rice

INTRODUCTION

Nitrogen (N) fertiliser is applied in flooded rice systems to increase grain production, but not all applied N will be absorbed by the rice crop.[1] The total N loss in fertilised and flooded rice systems can reach up to 50 % of the total N applied, and may occur through several pathways such as ammonia (NH_3) volatilisation, nitrogen oxides (NO_x) emissions from simultaneous nitrification and denitrification, and N leaching.[2-5] Although our aim is to increase grain production, it is also equally important to minimise total N loss from fertilised and flooded rice systems to reduce production costs and negative environmental outcomes.[6, 7]

As an alternative to a conventional experimental approach, many semi-physical N dynamics models for simulating N dynamics in flooded soil systems have been developed over the last 30 years.[5, 8-16] Simulations of system behaviour by these models under different conditions provide insights into the underlying mechanisms, and are useful in evaluating management practices to reduce N losses and increase grain production. However, the interactive, non-linear and time-varying N processes in flooded soil systems have resulted in models of different complexities. Consequently, model selection for a specific research application is challenging.

Jayaweera and Mikkelsen[17] reviewed the concepts and performance of physically-based models developed for the estimation of NH_3 volatilisation in flooded soil systems without a rice crop and in the absence of other N processes, e.g., models of Bouwmeester and Vlek,[18] Moeller and Vlek,[19] and Jayaweera and Mikkelsen.[9] Benbi and Richter[20] reviewed the objectives and capabilities of about 20 soil N dynamics models, but the reviewed models were not applied to simulate N dynamics in flooded rice systems. Nieder and Benbi[21] reviewed models of carbon (C) and N dynamics in a soil-plant-atmosphere system, but few models were selected to illustrate different modelling concepts. Giltrap et al.[22] and Gilhespy et al.[23] specifically reviewed the development and performances of DeNitrification-DeComposition (DNDC) variants, while Keating et al.[24] provided an overview on the Agricultural Production Systems Simulator (APSIM).

To the best of our knowledge, current reviews either focus on N dynamics models not specific for simulating behaviour of flooded soil systems, dedicated in understanding only one specific N process, or focus on demonstrating the capability of only one model, and, therefore, do not include comparison with alternative models.

The objective of this paper is, therefore, to provide an overview of modelling concepts and performance of 14 models developed to simulate N dynamics in flooded soil systems. The 14 models are NFLOOD v.1,[8] NFLOOD v.2,[10] J-M's,[9] S-K's,[25] CERES-Rice,[11] Chowdary's,[5] Nakasone's,[26] Yoshinaga's,[27] DNDC-Rice,[12] K-K's,[28] Liang's,[13] RIWER,[15] RICEWNB,[14] and APSIM-Oryza.[16, 29] With substantial progress in modelling of N dynamics in flooded soil systems since previously published multi-model reviews, this overview provides breadth of knowledge on available models for simulating N dynamics in flooded soil systems, and, therefore, is valuable as a first step in the selection of an appropriate model for a specific application.

Some of these N dynamics models were integrated with a rice plant growth and development model, and a water balance model.[11, 12, 16] However, the conceptualisation of the rice plant growth and development models is not detailed in this paper, as that would require an extensive review on its own.

In the following sections, backgrounds of the 14 models are given, followed by an overview of the key modelling concepts on N processes in flooded soil systems and the performance of the models. The paper concludes with a discussion and conclusions section.

BACKGROUND OF THE MODELS

General information on the 14 models is provided in Table S1. DNDC,[30] CERES,[31] and APSIM[32] were originally developed to simulate N dynamics in upland agro-ecosystems. They were eventually adapted to simulate N dynamics in rice systems and are referred to as DNDC-Rice,[12] CERES-Rice,[11] and APSIM-Oryza.[16, 29] The DNDC-Rice is a modification of DNDC v. 8.5, and the chronological development of the DNDC is given in Gilhepsy et al.[23] and Zhang et al.[33] CERES-Rice is now incorporated into the DSSAT model.[34, 35] RIWER[15] was developed to simulate N dynamics for rice-wheat cropping systems, but only components relevant to the rice system are discussed in this paper. The remaining models presented in this paper were developed specifically for flooded soil systems. The user input required to run the models is summarised in Table S2. Additional inputs are needed to simulate rice crop growth and development with respect to N uptake, but detailing of this information is not within the scope of this paper. The N transport and transformations conceptualised in all 14 models are summarised in Table S3.

COMPARTMENTAL MODELLING

A compartmental modelling approach is typically used to approximate a floodwater-soil continuum in a flooded rice field. In simpler models such as Chowdary's, Liang's, and RICEWNB, the floodwater-soil continuum is divided only into two compartments, which are a floodwater compartment and a bulk reduced soil compartment. In these models, both compartments are assumed homogeneous, and the thin aerobic soil layer at the floodwater-soil interface is neglected (see also Table S1).

In more complex models such as NFLOOD v.1 and v.2, S-K's, CERES-Rice, and APSIM-Oryza, the soil compartment is also conceptually segmented vertically into several smaller compartments. In these models, each segmented soil compartment is assumed to be ideally mixed .

Under flood conditions, NFLOOD v.1 and v.2, and CERES-Rice assume a thin aerobic layer at the floodwater-soil interface. In CERES-Rice, the thickness of the aerobic soil is calculated based on organic carbon content of the soil surface and percolation rate.[36] Meanwhile, APSIM-Oryza assumes there is no thin aerobic soil layer under flooded conditions, for simplification[29] Alternatively, DNDC-Rice simulates the volume of aerobic and anaerobic microsites within each segmented soil compartment based on the soil redox potential, which is calculated using the Nernst equation on the basis of dominant oxidant and reductant concentrations in the soil.[12] The floodwater is typically treated as a homogeneous compartment in all models discussed in this paper.

SOURCES OF NITROGEN IN FLOODED SOIL SYSTEMS WITH RICE CROP

NO_3^- based fertilisers are not recommended in flooded rice systems due to potential N loss through denitrification in the anaerobic plough layer.[37] In flooded rice systems, urea continues to be the primary source of synthetic N. Hydrolysis of urea is most often described by first-order kinetics, either with a constant rate coefficient (i.e., Chowdary's, Liang's, RIWER), or a time-varying rate coefficient that is governed by sub-daily pH and temperature (i.e., CERES-Rice, APSIM-Oryza). Urea is either conceptualised to be fully hydrolysed in the floodwater (i.e., Chowdary's, Liang's, CERES-Rice, APSIM-Oryza), or to be incorporated directly into the soil (i.e., CERES-Rice, APSIM-Oryza) (Table S4).

Vlek and Craswell[38] reported that, unless deep placement of urea is undertaken, 50 % to 60 % of applied urea still enters the floodwater, despite incorporation into the soil. Thus, model simulations may substantially deviate from reality if the model assumes that all urea incorporated into the soil does not diffuse into the floodwater.

The amounts of additional N supply from biological N_2 fixation, rainfall or irrigation water are site specific. Biological N_2 fixation, however, was considered only in only two models:- DNDC-Rice, as a rate constant that was estimated from experiments, and APSIM-Oryza in simulating the growth of photosynthetic aquatic biomass (PAB, i.e., algae). CERES-Rice calculates an 'algal activity factor' which impacts pond water pH and hence potential for ammonia volatilisation, however doesn't carry this through to simulate an actual algal biomass pool with associated N inputs from fixation.

In APSIM-Oryza, the dead PAB at the end of a rice crop was conceptualised as a source of C and N for the next cropping season. PAB can also senesce during the course of a rice crop and enter the soil pools as fresh organic matter. It was demonstrated that this conceptualisation was essential in simulating the performance of multi-season rice cropping, and allows APSIM-Oryza to self-initialise the values of C and N at the beginning of each cropping season during long-term simulations.[16, 29] In order to estimate N obtained from dead PAB, growth of the PAB needs to be estimated. Currently, there are only two mathematical models that approximate the growth of PAB in fertilised and flooded rice systems.[16, 39]

INORGANIC NITROGEN TRANSPORT

Transport of dissolved inorganic N (NH_4^+, NO_3^-, and urea) across the floodwater and soil compartments occurs via N percolation and/or N diffusion. In this paper, N percolation refers to movement of dissolved N along with the soil water flow. As a result of compartmental modelling, the N percolates out from one compartment into the compartment below. Diffusion, on the other hand, is driven by concentration gradients of dissolved inorganic N, which is described by Fick's law, and can be either in the upward or downward direction.

See Table S3 for the mechanisms of N transport conceptualised in all 14 models. In most models, only NH_4^+ and/or NO_3^- are transported (via mass flow or diffusion) between the floodwater and soil, or throughout the segmented soil compartment. However, in S-K's, CERES-Rice, and APSIM-Oryza, urea can also be transported between the floodwater and soil, and throughout the segmented soil compartment.[11, 25, 29]

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AMMONIA VOLATILISATION FROM FLOODWATER SURFACE

NH_3 in the floodwater is susceptible to volatilisation, and the partitioning between NH_4^+ and NH_3 is regulated by the floodwater properties, such as pH and temperature.[40] However, in Chowdary's, Liang's, and RICEWNB, the NH_3 volatilisation is described in terms of first-order kinetics with a constant rate coefficient, independent of the floodwater properties. In NFLOOD v.1, the NH_3 volatilisation is also described in terms of first-order kinetics, but the partitioning between NH_4^+ and NH_3 is approximated by a function of total ammoniacal-N concentration and floodwater pH.

In J-M's, the NH_3 volatilisation is also described in terms of first-order kinetics, but the volatilisation rate coefficient is expressed as the ratio of an overall mass transfer coefficient and floodwater depth. A function of the overall mass transfer coefficient is further derived on the basis of the two-film theory (i.e., a thin gas film and a thin liquid film), where the movement of NH_3 through the thin films is assumed to occur via molecular diffusion. Consequently, the volatilisation rate coefficient is a function of floodwater depth and temperature, and wind speed.[9] In the J-M's, the partitioning between NH_4^+ and NH_3 is approximated by total ammoniacal-N concentration, and floodwater pH and temperature. In J-M's, the floodwater depth has a two-fold effect, one through the dilution of floodwater NH_4^+-N concentration, and the other directly through the volatilisation rate coefficient.[17]

In CERES-Rice and APSIM-Oryza, NH_3 volatilisation is described by empirical equations which are functions of partial pressure of NH_3 in floodwater, floodwater depth, and wind speed effect. The partial pressure of NH_3 in floodwater is described as a function of NH_3 concentration in the floodwater and floodwater temperature.[41] Due to lack of measured wind speed, in CERES-Rice the wind speed effect is related to pan evaporation rate and leaf area index,[36] whereas in APSIM-Oryza, the wind speed effect is represented by a calibrated rate coefficient and pan evaporation rate.[16]

In DNDC-Rice, the floodwater N dynamics is not conceptualised (Fumoto T, pers. comm.). Instead, NH_3 volatilisation is described as a function of the NH_3 concentration in the soil water, soil temperature and soil water content.[42] The NH_3 volatilisation from the floodwater surface was not conceptualised in RIWER.

Floodwater pH

Floodwater pH is one of the key regulators of NH_3 volatilisation from the floodwater surface.[40] The diurnal trend of floodwater pH, where the floodwater pH typically peaks at about mid-day, was observed by Fillery et al.[2] The trend was hypothesised to be a result of consumption of CO_2 through PAB photosynthesis during the day, and release of CO_2 during respiration during the night. This phenomenon is conceptualised in S-K's, CERES-Rice, and APSIM-Oryza to estimate the sub-daily floodwater pH value.

In CERES-Rice and APSIM-Oryza, the floodwater pH is approximated by a function that follows an absolute sine curve, and the pH magnitude is driven by PAB activity.[11, 16] The sub-daily PAB activity is defined by the most limiting among four factors: available light as a function of solar radiation and rice leaf area index (shading of floodwater), floodwater temperature, and inorganic N concentration and P presence in the floodwater. Each of these factors ranges from zero (no activity) to unity (most active). Additionally, the effect of urea hydrolysis on floodwater pH is included.[16] The ranges of floodwater pH simulated with CERES-Rice and APSIM-Oryza are between pH 7.0 and 9.5.[16]

In S-K's, the sub-daily floodwater pH was calculated from the number of protons added or consumed when there was a net change of HCO_3^- or NH_4^+, due to processes like urea hydrolysis, NH_3 and CO_2 volatilisation, CO_2 consumption by PAB, soil CO_2 production, and transfer of protons between soil and floodwater.[25]

MINERALISATION AND IMMOBILISATION OF NITROGEN

During decomposition of organic matter, inorganic N is released (mineralisation), and simultaneously a fraction of the available inorganic N is used for growth of microbial biomass (immobilisation).

In simpler models, like NFLOOD v.1 and v.2, Yoshinaga's, Chowdary's, Liang's, and RICEWNB, the net mineralisation and immobilisation of N are described by first-order kinetics and are assumed to be one-step processes. In these models, the decomposition of organic matter was not detailed.

However, in DNDC-Rice, CERES-Rice, RIWER, and APSIM-Oryza, the main assumption is that not all of the fresh organic matter is prone to decomposition, and, therefore, the fresh organic matter is, in general, categorised into three pools. Additionally, CERES-Rice may also implement the CENTURY organic matter module[43], but the fresh organic matter is categorised into two pools. Decomposition of each fresh organic matter pool occurs at a different rate, and results in formation of multiple soil organic matter pools with different decomposition rates (active, slow or stable). The active pool may decompose further into a stable pool. The formation of microbial biomass, which creates the N immobilisation demand, is usually accounted by the active pool.[29, 30] Typically, slower potential rates of decomposition are defined under flooded soil systems compared to non-flooded soil systems.[15, 29]

Details and flow diagram of the concepts for DNDC-Rice are given in Li et al.,[30] for RIWER in Jing et al.,[15] for CERES-Rice in Godwin and Singh [11] or in Parton et al.[43], and for APSIM in Probert et al.[44] and Gaydon et al.[16] The net N mineralised or immobilised is calculated from the mass balance of N that resulted from the decomposition. Factors that regulate the rate of decomposition in these models are summarised in Table S5.

The decomposition of organic matter is assumed to take place below ground surface in DNDC-Rice,[12] and RIWER.[15] Alternatively, CERES-Rice (with CENTURY organic matter module)[43] and APSIM-Oryza[16, 29] conceptualised decomposition of fresh organic materials either on the soil surface, and if the fresh organic materials are subsequently tilled into the soil, the materials decompose below ground surface.

The concepts used in the CERES group of models for simulating mineralisation and immobilisation of N, were adapted in APSIM.[24] The immobilisation N demand is satisfied from inorganic N pool below ground surface under aerobic conditions, which is similar to the approach in CERES-Rice, or from inorganic N in the floodwater (simulated by APSIM-Pond module) under flooding conditions.[16, 29, 44]

SIMULTANEOUS NITRIFICATION AND DENITRIFICATION

Nitrification and denitrification are described by first-order or Michaelis-Menten based kinetics. The rate coefficients of the kinetics can be constant or regulated by additional factors in some of the models (Table S6). For simplification, the limiting factors in RIWER, CERES-Rice and APSIM-Oryza are described by index-factors, ranging between zero (no activity) and unity (most active). In APSIM-Oryza, under flooded conditions, nitrification is halted under the assumption that O_2 is immediately lost from the soil profile, but denitrification continues.[29] CERES-Rice conceptualises a lag phase to represent the growth and death of nitrifiers, rather than assuming a simplified immediate change like APSIM.

In the different models, nitrification and denitrification are assumed to occur at different locations in the floodwater-soil profile (Table S6). Chowdary's assumed that the thin aerobic layer is insignificant, and therefore, they conceptualised the nitrification in the floodwater. In Yoshinaga's, denitrification is conceptualised to occur at the floodwater-soil interface. This contradicts with the common perception that denitrification does not occur at the floodwater-soil interface, where typically an aerobic layer at the floodwater-soil interface may form. The influence of rhizosphere on nitrification is excluded from all of the presented models, except in K-K's.

AMMONIUM ADSORPTION AND DESORPTION IN SOIL

The NH_4^+ may reside in soil solution or be adsorbed to clay particles. Several models conceptualised this adsorption and desorption (Table S3). The NH_4^+ adsorption and desorption are complex and site-specific processes, and measurement method to discriminate between native (non-available) and recently adsorbed (plant-available) NH_4^+ needs further research.[45] Detailing NH_4^+ adsorption and desorption in a field-scale model that already has many parameters (calibrated rate coefficients) will most likely lead to unidentifiable parameters.[46] From a systems theory point of view, an unidentifiable parameter does not have a unique value in a parameter estimation (calibration) step, and thus cannot be estimated uniquely.

NITROGEN UPTAKE BY RICE CROP

Inorganic N uptake by rice is conceptualised in all models discussed in this paper, except in NFLOOD v.1 and v.2, J-M's, Nakasone's, and Yoshinaga's (Table S3).

Models that were developed to estimate grain production are coupled to a comprehensive rice plant growth and development model. For instance, DNDC-Rice is coupled to a generic crop growth and development model, MACROS,[12] whereas RIWER and APSIM-Oryza are coupled to a crop growth and development model specific for rice, ORYZA2000.[15, 16] CERES-Rice incorporates its own rice production model.[34] The rice crop growth and development models are complex, but these models allow scenario studies of different management schemes on the daily crop growth (leaf area index, biomass of plant organs) and grain production. Simulation of these models requires additional data beyond those listed in Table S2. Details of these integrated models are beyond the scope of this paper. Readers are referred to Penning De Vries et al.[47] and Bouman et al.[48] for details of MACROS and ORYZA2000, respectively.

Models that were developed to estimate the overall N balances used a simpler approximation of N uptake by the rice crop. For instance, the N uptake by rice in Chowdary's and Liang's is described as a function of established rice crop coefficient and daily evapotranspiration. In RICEWNB and K-K's, the N uptake is described by Michaelis-Menten kinetics. In RICEWNB, the maximum rate of N uptake is limited by leaf area index, root distribution, and temperature, where each of these limiting factors is expressed as an index-factor.

PERFORMANCE OF NITROGEN DYNAMICS MODEL

In this section, an overview of performance of each model with respect to measurements shown in Table S7 is given. Only data sets relevant to N dynamics in flooded soil systems that are either continuously flooded or flooded during at least part of the rice cropping period are listed in Table S7.

Chowdary's, Liang's, and RICEWNB are appealing due to their simplicity where all of the N processes in these models, except for N uptake by the rice crop, are described by first-order kinetics, each with a constant rate coefficient. Models with such concepts seem appropriate for estimating N balances in fertilised and flooded rice systems at the end of a cropping season, such as seasonal N uptake by rice crop, NH_3 volatilisation, denitrification, mineralisation, immobilisation, or NO_3^- leaching (Table S7). In these models, the estimates of seasonal N balances are largely determined by the calibrated constant rate coefficients which may change over time. Differences in the modelling concepts in each of these models must be evaluated for the conditions at a study site (Table S3). For instance, mineralisation and immobilisation are included in Chowdary's, but not in Liang's. N loss via surface runoff and horizontal seepage is conceptualised in Liang's, but not in Chowdary's.

The J-M's has been evaluated for estimating temporal NH_3 volatilisation from ammoniacal-N solutions (Table S7). Key regulating factors of NH_3 volatilisation were conceptualised in the J-M's, and, therefore, the model is appropriate for studying mechanism of NH_3 volatilisation from the floodwater surface of a flooded soil system. The trade-off, however, is that the operation of the model requires several measured input data such as sub-daily concentrations of total ammoniacal-N in the floodwater, wind speed, floodwater pH, temperature, and depth. A significant assumption underlying this model is that the rate of NH_3 volatilisation equates to the change in total ammoniacal-N in the floodwater. Consequently, estimation of NH_3 volatilisation from the floodwater using this model is currently limited to flooded soil systems without a rice crop.

CERES-Rice, RIWER, and APSIM-Oryza offer estimation of temporal N content in the floodwater and soil, temporal N uptake by a rice crop, and the crop biomass (root, stem, leaf, grain). In order to operate these models, detailed input on rice varietal crop stages (phenology) is required. CERES-Rice and APSIM-Oryza have been rigorously evaluated for grain production (Table S7).

In addition to Table S7, a comprehensive review on the performance of CERES-Rice is already provided by Basso et al.[49] The review reported that CERES-Rice has been evaluated for grain production in over 20 studies, and the prediction RMSEs for grain production mostly ranged from 200 to 1672 kg ha^{-1}. Although several poor fits between simulations and observations were reported, the studies covered a diverse combinations of planting/sowing dates, plant densities, nitrogen treatments and water managements. CERES-Rice has also been evaluated for crop phenology (21 studies) and aboveground biomass (5 studies). Basso et al.[49] further revealed that soil nitrogen prediction validation has not been done for CERES-Rice. Similarly, APSIM has recently been comprehensively evaluated for its performance in cropping systems of Asia,[50] from the perspectives of grain production, rotational effects, and soil dynamics.

Of the three models, APSIM-Oryza can self-initialise the soil C and N values due to accounting for C and N inputs from PAB, and, therefore, the model can continuously simulate the N dynamics and the crop biomass for several cropping seasons without reset.[16, 50] Unlike CERES-Rice and APSIM-Oryza, application of RIWER is currently limited to conditions where NH_3 volatilisation is negligible.

DNDC-Rice (deduced from DNDC v. 8.5) was developed mainly to estimate emission of greenhouse gases (N_2O and NO), and NH_3 loss in fertilised and flooded rice systems. In comparison with the other models, DNDC-Rice has been rigorously evaluated with N_2O emissions from fertilised and flooded rice systems (Table S7), but not for NH_3 volatilisation. Note that the NH_3 volatilisation was conceptualised to occur from the soil. Overall, DNDC-Rice is able to produce good estimates of seasonal N_2O emissions, but at times, poor performance in simulating the temporal trends of N_2O was observed (Table S7). Additionally, the DNDC-Crop (deduced from DNDC v. 8.0), and the latest DNDC v.9.5 have also been used to simulate the N dynamics in rice systems.[51-54] These additional DNDC variants have fundamentals that are different from those of DNDC-Rice, but a detailed discussion on these variants is beyond the scope of this paper.

The NFLOOD v.1, NFLOOD v.2, and S-K's, were developed to simulate temporal N dynamics in both the floodwater and soil. NFLOOD v.2 was evaluated with temporal concentrations of NH_4^+ in the soil profile (Table S7), but the NFLOOD v.2 did not include NH_3 volatilisation unlike NFLOOD v.1 (Table S3). S-K's has not been evaluated with measurements, but an advantage of the S-K's model compared to all models is its ability to simulate the diurnal floodwater pH based on the total ammoniacal-N and organic C balances in the floodwater and soil.

Nakasone's and Yoshinaga's are limited to simulating temporal concentrations of inorganic N in the soil and floodwater, respectively (Table S7). Although the total N uptake by the rice crop was not conceptualised in Yoshinaga's, simulation of the model for flooded soil systems with young rice crops resulted in a good fit between measured and simulated inorganic N concentration in the floodwater. It is most plausible that the conceptualised phytoplankton N uptake from the floodwater compensated for the absence of rice crop N uptake.

Initially, ORYZA2000 v.2 extensively modelled rice crop growth and development, but the model does not include soil N transformations.[55] Therefore, ORYZA2000 v.2 was not included in this overview. Recently, subsequent to the analysis presented in this manuscript, ORYZA (v3) was released as the next generation of ORYZA2000, in which Li et al.[56] conceptualised the root growth, soil temperature, and soil N transformations, i.e., mineralisation, nitrification, and denitrification. ORYZA (v3) has been evaluated for grain production, leaf area index, leaf N content, biomasses of dead and green leaves, stem, and panicle that were observed at four locations, but not against soil N data or N gaseous flux such as NH_3 and N_2O.[56]

DISCUSSION AND CONCLUSIONS

Detailed modelling of soil N dynamics easily results in complex models, but the model component related to the soil N dynamics is also the component least evaluated against measurement. Table S7 shows that, except for NFLOOD v.2, RICEWNB, and RIWER, the temporal soil inorganic N simulated by other models are not evaluated with measured soil N data, mainly due to scarcity of data. Notice also from Table S7 that for the evaluation of RICEWNB, the measured soil N data set is small; only three measurements of soil total inorganic N were recorded after the first N fertiliser application, and another three measurements following the second application.

Detailed spatial and temporal soil inorganic N variation in fertilised and flooded rice systems was reported in two papers.[57, 58] In Dobermann et al.,[58] the experimental plot received a total of 200 kg N ha^{-1}; 80 kg N ha^{-1} was incorporated into the soil for basal application and 120 kg N ha^{-1} was broadcasted into the floodwater in three equal splits. Dobermann et al.[58] observed low concentration of NH_4^+-N, ranging from 0 mg N L^{-1} to 3 mg N L^{-1}, in soil solutions that were extracted using three techniques: soil solution extracted using a rhizon soil solution sampler (diameter of 2.3 mm and a pore size of 0.1 µm), soil solution extracted by centrifuging field-moist soil (9000 rpm for 15 minutes), and solution obtained with a standard cation displacement technique (3 g of field moist soil in 30 mL of 2 M KCl). Similarly, low concentrations of NH_4^+-N, ranging from 0 mg N L^{-1} to 3 mg N L^{-1}, were observed by Makarim et al.[57]

At low concentrations of NH_4^+-N, the temporal dynamics may be masked by the spatial variation.[58] Based on this setback, in combination with interactive soil N processes (e.g., mineralisation, immobilisation, nitrification, denitrification, and NH_4^+ adsorption and desorption), we infer that the validation of field-scale models for simulating N dynamics in fertilised and flooded rice systems against measured temporal inorganic soil N content may not be informative with respect to the model structure adequacy. It is noted that other N processes such as anaerobic ammonium oxidation[59] and dissimilatory reduction of NO_3^- were as yet not conceptualised in any of the 14 models. Regardless of this, some of the outputs of the models have been satisfactorily validated against some measurements.

On the one hand, although soil N processes contribute to the overall N dynamics in the systems, detailing of soil N processes would lead to an increase in the number of parameters that may not be accurately estimated from limited soil N measurements. It was suggested by Cassman et al.[60] that a realistic prediction of soil N dynamics using models is difficult due to the complexity of the interactive soil N processes. On the other hand, conceptualisations of soil N processes in models are necessary for estimating N losses that may occur through simultaneous nitrification and denitrification, leaching, anaerobic ammonium oxidation, or immobilisation.

Furthermore, measurements always contain errors. Ideally, only reliable measurements must be used, but for field-scale agricultural systems, quality of the measurements is an issue. For instance, time series of measurements are often sparse, and not all process variables will be simultaneously measured as the procedures are laborious and costly. Moreover, different measurement methods may yield different values. Measurements of gaseous flux, for instance, are affected by the method of measurement - the micrometeorological methods are claimed to be more representative of the net gas loss than the chamber methods.[6, 61] In the previous section, inconsistency in the accuracy of prediction by an individual model was observed at different sites. Although this inconsistency may be caused by model science, it is also possible that this inconsistency is due to errors in the measurements.

Therefore, parameter estimation approaches that take into account the errors in the model science, measurements, and parameters, are useful. See examples of parameter estimation approaches demonstrated by Confalonieri et al.[62] where multiple trajectories of outputs were generated and used to estimate the parameters in order to account for the errors in the measurements, or Nurulhuda et al.[63] where the errors in the model structure, measurements, and parameters, were all simultaneously accounted for via a set-membership parameter estimation approach. Additionally, researchers should consider collecting new measurements if new and more reliable measurement techniques are made possible with current advances in technology.

Confalonieri et al.[64] showed that differences in model structure could result in similar prediction, while similar structures could lead to large differences in model outputs. Meanwhile, Li et al.[65] compared DNDC-Rice, CERES-Rice and APSIM-Oryza with respect to their common output (i.e., rice grain production) along with another 10 crop growth and development models (both generic and specific for rice crop), and found that none of these models consistently provided reliable predictions of rice grain production across four sites with different climatic conditions, management practices, rice cultivars and years.

Indeed, all models are approximations of the actual systems. All models have defined working ranges, thus are bound to produce unreliable estimates under some specific conditions, which especially holds for complex biological systems with various interactive feedbacks. Thus, it can be inferred that validation of a single model against limited measurements is not enough to properly evaluate that model. Clearly defining the working range of a model (making limitations explicit) is, therefore, as important as validation of the model.

In the case of predicting rice grain production, Li et al.[65] demonstrated that the average value resulting from simulations with multiple models led to a prediction value closer to the observed value, compared to the prediction value by an individual model. Therefore, when evaluation of models is hindered, either due to lack of measurements as in the case of estimation of soil N processes, or uncertainty in the measurements (as in the case of estimation of N gaseous loss), the model ensembles approach as shown by Li et al.[65] may reduce the uncertainty in prediction.

There is still a lack of co-validation studies among the 14 models presented in this overview with respect to their performance in predicting N losses (Table S7). In flooded rice systems, the total N loss accounts for a significant amount, where the recovery efficiency of N is only about 50 %.[1] Therefore, comparison of the performance of these models against benchmark comparative datasets can be done to characterise performance of models, and to define limitations of each model, in predicting N losses in flooded soil systems, preferably under a range of site conditions.

Given the set of N dynamics models considered with their different concepts, it is challenging for the researcher to choose a model for evaluating static and dynamic management strategies in rice farming to support farmers, producers and researchers, in their decision making. In this paper, however, we have provided a basis to assist the researcher in pre-selection of models based on the main process of focus.

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SUPPORTING INFORMATION

Supporting information may be found in the online version of this article.

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