

Field-calibrated ammonia volatilization models for rice and wheat, validated in APSIM

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Abstract

Predicting ammonia (NH_3) volatilization from rice and wheat is vital for improving nitrogen-use efficiency (NUE). However, process-based models often require detailed soil-atmosphere data that are not always available. Using data from five field experiments in the Indo-Gangetic Plain (IGPs), we developed and statistically tested two empirically calibrated models for NH_3 volatilization, then integrated and validated them within the Agricultural Production Systems sIMulator (APSIM) Next Generation platform. A linear model linking cumulative NH_3 -N loss to nitrogen rate and temperature explained 94.3% of the variation in rice (RMSE = 0.69 kg N ha⁻¹; n = 16), with nitrogen rate as the main factor (+ 0.048 kg N ha⁻¹ per kg N applied) and temperature a smaller yet significant factor (+ 0.60 kg N ha⁻¹ per gradient level). The second model, considering tillage, basal-timing, and nitrogen source/placement for wheat, accounted for 94.2% of variance (RMSE = 1.62 kg N ha⁻¹; n = 39), with timing being the dominant factor while tillage had no significant independent effect. Both models, embedded as APSIM Manager-script components, closely matched their predictions to three decimal places (rice: 14.024 kg N ha⁻¹; wheat: 21.640 kg N ha⁻¹), simulating daily dynamics through mechanistic pathways where ammonium pools peaked 3–4 days after application. Urease inhibitors and botanical amendments reduced cumulative NH_3 -N loss by 17–40% compared to urea alone. These results show that simple, field-calibrated linear models can effectively simulate rice and wheat NH_3 volatilization over a season, offering accuracy comparable to complex process-based models while capturing realistic daily behavior within an established crop-soil simulation platform.

1. Introduction

Ammonia (NH_3) volatilization is a key pathway for nitrogen loss in urea-fertilized rice and wheat systems. It typically accounts for 10–40% of the applied fertilizer nitrogen, influenced by factors like temperature, soil pH, application method, and crop stage. This loss impacts nitrogen-use efficiency (NUE), farm profitability, and atmospheric nitrogen deposition downwind. Since NH_3 volatilization is highly temperature-sensitive affecting urea hydrolysis directly and influencing evapotranspiration and surface soil-water status indirectly future warming due to climate change could increase gaseous nitrogen losses in cereal systems unless nutrient-management practices are adjusted (Hou et al. 2025).

A wide range of process-based models has been developed to simulate NH_3 volatilization mechanistically. These include early models like the urea-hydrolysis and soil-chemistry model by Rachhpal-Singh and Nye (1986), the simplified urine-patch model by Sherlock and Goh (1985), the Volt'Air model by Genermont and Cellier (1997), which integrates heat, water, and NH_3 transfer between soil and atmosphere, and the more recent Flow of Agricultural Nitrogen (FAN) framework by Riddick et al. (2016). The latter was designed to assess climate sensitivity of NH_3 emissions at continental to global scales. While these process-based models can achieve high accuracy, they require detailed and often continuously measured inputs such as soil water content, surface temperature, wind speed, and boundary-layer resistance. Such data are rarely available from routine agronomic trials, especially across

the numerous site-years needed to capture temperature and nitrogen management responses in the Indo-Gangetic Plain. In contrast, empirical and semi-empirical models calibrated with readily available field data using predictors like nitrogen rate, application method, tillage, and temperature provide a more practical alternative. These models are often comparably effective, or even superior in some cases, at predicting cumulative field-scale NH_3 losses, making them valuable for regional nitrogen management and emission inventories.

This study utilizes data from five independent field experiments at the Indian Agricultural Research Institute (ICAR-IARI), New Delhi, and other affiliated sites within the IGP. Each experiment measured NH_3 volatilization from rice or wheat under specific management factors: temperature regimes in rice (Loni et al. 2021; Kumar et al. 2021), manipulated via a temperature-gradient tunnel combined with four nitrogen rates; nitrogen source, placement, basal-timing, and tillage system in wheat comparing conservation versus conventional tillage across five nitrogen-source/placement treatments and four basal versus precision-application timing regimes (Bhasker et al. 2022); and the effects of organic and inorganic amendments such as urease inhibitors (Ramalingappa et al. 2023), botanical extracts, and biofertilizers (Darjee et al., 2022, 2025) added to the recommended dose of urea in wheat. The objectives were: (i) to compile NH_3 volatilization data from these experiments into a unified framework; (ii) to develop and statistically assess two empirical, field-calibrated simulation models one for rice, accounting for temperature and nitrogen-rate variation, and one for wheat, considering tillage, timing, and nitrogen source that predict cumulative seasonal NH_3 -N loss from readily available agronomic data; (iii) to evaluate the performance of these models in the context of amendment-based mitigation results and existing process-based modelling literature; and (iv) to incorporate both models into the APSIM Next Generation crop-soil simulation platform, testing whether the coupled simulations replicate the regression-based predictions through a mechanistic daily process, as a step toward integrating these models into a comprehensive crop-soil simulation environment rather than using them solely as seasonal total predictors.

2. Materials and Methods

2.1 Source field experiments

Five independent experiments were conducted at ICAR-IARI, New Delhi, and affiliated research farms within the IGPs, contributing data for this synthesis (see Table 1). Experiment A involved rice (Pusa Basmati 1509) grown in a completely randomized design with 16 treatment combinations, including four nitrogen levels 0, 90, 120, and 150 kg N ha⁻¹ across four temperature regimes: ambient (T1), a temperature-gradient tunnel control (T2), and two warmer levels inside the tunnel (T3, T4), each with three replicates on sandy loam soil (pH 8.2). Experiment B compared conservation and conventional tillage, with four nitrogen timing regimes guided by GreenSeeker (T1: 80% basal + 20% sensor; T4: 0% basal + 100% sensor) and five nitrogen source/placement treatments, including band-placed urea, DCD + NBPT-stabilized slow-release urea, neem-coated urea applied band-wise, broadcast before irrigation, or

after irrigation, on wheat variety CSW 18. Experiment C tested the effect of recommended nitrogen (150 kg N ha⁻¹) alone versus with various amendments such as NBPT, hydroquinone, calcium carbide, VAM, Azotobacter, garlic extract, and plant oils, each added as a percentage of RDN. Experiment D evaluated inorganic, organic, and integrated nutrient sources under a rice-wheat rotation. Experiment E studied ammonia volatilization in wheat under ambient and elevated temperatures, similar to Experiment A.

Table 1

Source field experiments contributing data to the NH₃ volatilization simulation models and synthesis

Experiment	Crop	Primary factor(s) varied	Design summary	Role in this synthesis
A	Rice	Temperature regime (4 levels) × N rate (4 levels)	CRD, 16 treatments × 3 replicates	Model 1 (temperature-nitrogen response)
B	Wheat	Tillage (2) × basal-timing (4) × N source/placement (5)	Split-split-plot, 40 treatment combinations	Model 2 (tillage-timing-source response)
C	Wheat	Organic/inorganic amendments to RDN (10 treatments)	RBD, 10 treatments × 3 replicates	Amendment mitigation benchmarking
D	Wheat	Inorganic, organic and integrated N sources	RBD, multiple treatments	Contextual/qualitative synthesis
E	Wheat	Temperature regime (ambient vs elevated)	CRD/RBD	Contextual/qualitative synthesis

2.2 Ammonia volatilization measurement

In all five experiments, NH₃ was measured using standard micrometeorological or closed-chamber flux techniques adapted for small-plot cereal experiments. NH₃ concentrations above the treated plot surface and, in cases using a micrometeorological mass-balance approach, at a reference height above the canopy were measured periodically after fertilizer application. Measurements continued until the flux decreased to a low background level. The flux was then integrated over the sampling interval and summed to calculate the total seasonal ammonia-nitrogen (NH₃-N) loss in kg N ha⁻¹, along with the percentage of applied nitrogen that volatilized. This method aligns with the acid-trap and micrometeorological techniques commonly used in rice and wheat systems (Fillery and De Datta 1986).

2.3 Empirical simulation model development

Two empirical simulation models were created using ordinary least-squares multiple linear regression, aligning with the wider NH₃ volatilization modeling literature. This literature suggests that even simple empirical models with few easily measurable predictors can match the predictive accuracy of complex process-based models for total, field-scale NH₃ loss (Genermont and Cellier 1997; Riddick et al. 2016).

Model 1 (rice) was defined as: $\text{NH}_3\text{-N loss (kg ha}^{-1}\text{)} = \beta_0 + \beta_1 \cdot (\text{N rate, kg ha}^{-1}) + \beta_2 \cdot (\text{Temperature level, ordinal 1–4})$, based on 16 treatment-mean values from Experiment A. Model 2 (wheat) was formulated as: $\text{NH}_3\text{-N loss (kg ha}^{-1}\text{)} = \beta_0 + \beta_1 \cdot (\text{Tillage, 0 = conservation, 1 = conventional}) + \beta_2 \cdot (\text{Basal-timing level, ordinal 1–4}) + \beta_3\text{--}\beta_6 \cdot (\text{Nitrogen-source dummy variables, S2–S5, relative to S1})$, fitted to 39 treatment-mean values from Experiment B. One treatment (T3S3 under conservation tillage) was not reported and was excluded. Coefficients, standard errors, t-statistics, and two-tailed p-values were calculated from the design matrix. Model performance was assessed using R^2 and RMSE, comparing observed and predicted values.

2.4 APSIM Next Generation implementation and validation approach

To assess whether the two field-calibrated empirical models could replicate their fitted predictions within a full crop-soil simulation, both models were integrated as Manager-script components in APSIM Next Generation (version 2026.7.8083.0; Keating et al. 2003; Holzworth et al. 2014). They used the platform's built-in Wheat example simulation (weather station AU_Dalby.met) as the baseline soil, weather, and management setup for both crops. Since a dedicated rice/*Oryza* example was unavailable in the tested installation and because the coupling logic interacts only with the generic soil urea and NH_4^+ pools rather than crop-specific states, the same base configuration was applied for both wheat and rice implementations.

Each script identifies fertiliser application by monitoring the surface urea pool ([Nutrient].Urea.kgha[0]) for a small increase above a threshold, rather than relying on a fertiliser-application event. This is due to inconsistencies in event-argument type names across APSIM Next Generation versions observed during initial testing. Initially, the script removed predicted NH_3 loss directly from the urea pool; however, comparison with regression targets showed this underestimated cumulative loss. This occurred because the removal process conflicted with APSIM's built-in urea hydrolysis, which converts most urea to NH_4^+ rapidly ($\text{urea} \times \text{potential hydrolysis fraction} \times \min(\text{temperature factor, water factor})$). As a result, most nitrogen was converted to NH_4^+ before the script could remove the loss. The approach was then revised to deduct the predicted NH_3 loss from the soil NH_4^+ pool ([Nutrient]. NH_4 .kgha[0]), which is more mechanistically correct since NH_3 volatilisation involves an NH_4^+ - NH_3 equilibrium post-hydrolysis, not a direct urea loss. The total seasonal predicted loss (L_{max} , from Model 1 or 2) is distributed over days via an exponential-rise-to-maximum function, $\text{Cumulative NH}_3\text{-N}(t) = L_{\text{max}} \times [1 - \exp(-k \cdot t)]$, with $k = 0.230 \text{ d}^{-1}$ at the reference management level. This matches field observations (Experiment C) that about 90% of urea hydrolyses and volatilises within 1–2 weeks. To allow for multiple cropping seasons, a rule was added: if a new urea application occurs more than 60 days after the last, it starts a new loss episode with a fresh L_{max} ; closer applications are considered part of the same episode. Since APSIM Next Generation's Report component cannot access custom properties in these Manager scripts, each script

records its output soil urea and NH_4^+ pools, daily and cumulative loss, and episode targets directly to a comma-separated file via standard file I/O, bypassing Report.

Two key scenarios were tested to evaluate the coupled implementation: a rice scenario with 120 kg N ha^{-1} applied as a single dose at ambient temperature (T1), and a wheat scenario based on treatment T1S1 from the original field data featuring conservation tillage, fully basal nitrogen timing, and urea super granules band-placed. For each case, the day-by-day simulation of soil urea and NH_4^+ pools, along with predicted daily and total $\text{NH}_3\text{-N}$ loss, was compared against fitted regression predictions (see Sections 3.1–3.2). This comparison aimed to verify whether the coupled, process-integrated model converged with the standalone empirical equation in estimating the same seasonal total.

3. Results

3.1 Model 1: Rice NH_3 volatilization under temperature × nitrogen-rate variation

Cumulative seasonal $\text{NH}_3\text{-N}$ loss in rice increased with both nitrogen application rate and temperature level (see Table 2 and Fig. 1a), ranging from 9.1 kg N ha^{-1} at 0 kg N ha^{-1} and ambient temperature to $17.3 \text{ kg N ha}^{-1}$ at 150 kg N ha^{-1} and highest temperature. The regression model, $\text{NH}_3\text{-N loss} = 7.625 + 0.0483 \cdot (\text{N rate}) + 0.603 \cdot (\text{Temperature level})$, accounted for 94.3% of the variance ($R^2 = 0.943$; RMSE = $0.69 \text{ kg N ha}^{-1}$; $n = 16$), with both the nitrogen-rate coefficient ($p < 0.001$) and the temperature-level coefficient ($p = 0.004$) being statistically significant. Nitrogen rate was the primary factor, contributing roughly $0.048 \text{ kg N ha}^{-1}$ of additional loss per extra kg N ha^{-1} applied. Meanwhile, each increase in the temperature level contributed a smaller but significant additional loss of $0.60 \text{ kg N ha}^{-1}$, aligning with the smaller temperature-related increases (e.g., 9.1 to 9.4 kg N ha^{-1} at $\text{N} = 0$) compared to the larger nitrogen-rate-driven increases (e.g., 9.1 to $15.2 \text{ kg N ha}^{-1}$ at T1) observed in the data.

Table 2
Model 1 input data and fitted model summary: cumulative $\text{NH}_3\text{-N}$ loss ($\text{kg N ha}^{-1} \text{ season}^{-1}$) in rice under four nitrogen rates and four temperature regimes

Temperature regime	N0	N90	N120	N150
T1 (ambient)	9.1	11.4	14.3	15.2
T2 (TGT control)	9.3	12.5	15.5	15.9
T3 (TGT elevated)	9.4	12.9	16.3	16.5
T4 (TGT most elevated)	9.4	13.8	16.9	17.3

Model 1 equation: $\text{NH}_3\text{-N loss (kg ha}^{-1}\text{)} = 7.625 + 0.0483 \times \text{N rate (kg ha}^{-1}\text{)} + 0.603 \times \text{Temperature level (1-4)}$; $R^2 = 0.943$, $\text{RMSE} = 0.69 \text{ kg ha}^{-1}$, $n = 16$.

3.2 Model 2: Wheat NH_3 volatilization under tillage × timing × nitrogen-source variation

Cumulative seasonal $\text{NH}_3\text{-N}$ loss in wheat ranged from $4.86 \text{ kg N ha}^{-1}$ (conservation tillage, no basal nitrogen, urea super granules band-placed) to $26.58 \text{ kg N ha}^{-1}$ (conventional tillage, 80% basal nitrogen, neem-coated urea broadcast before irrigation) (Table 3, Fig. 2a). The regression model explained 94.2% of the variance ($R^2 = 0.942$; $\text{RMSE} = 1.62 \text{ kg N ha}^{-1}$; $n = 39$). The timing of basal nitrogen application was the strongest factor ($-5.61 \text{ kg N ha}^{-1}$ per unit increase in sensor-guided, reduced-basal timing; $p < 0.001$). This confirms that shifting nitrogen from an early basal application to split, sensor-guided doses significantly reduces NH_3 loss. Nitrogen source and placement also significantly affected losses: compared to the lowest-loss treatment (urea super granules band-placed, S1), treatments with DCD+NBPT-stabilised slow-release urea (S2), neem-coated urea band-placed (S3), and neem-coated urea broadcast before or after irrigation (S4, S5) all resulted in higher losses ($+ 2.6$ to $+ 4.5 \text{ kg N ha}^{-1}$; $p \leq 0.007$), with broadcast application before irrigation (S4) producing the largest increase. Once basal-timing and nitrogen source were considered, tillage system had no significant independent effect ($p = 0.735$). This suggests that the apparent effects related to tillage were mainly due to differences in nitrogen timing and source rather than tillage itself.

Table 3

Model 2 fitted coefficients: cumulative ammonia-nitrogen loss in wheat as a function of tillage, basal-nitrogen-timing level, and nitrogen source/placement

Model term	Coefficient (kg N ha ⁻¹)	Standard error	t	p- value	Interpretation
Intercept	27.25	0.94	29.14	< 0.001	Reference: conservation tillage, T1 timing, S1 source
Tillage (conventional = 1)	0.20	0.57	0.34	0.735	No significant independent tillage effect
Basal-timing level (1–4)	-5.61	0.25	-22.19	< 0.001	Reduced basal N / more sensor-guided timing reduces loss
N source S2 (SRF, band)	2.59	0.89	2.90	0.007	Higher loss than S1 (band-placed USG)
N source S3 (neem, band)	3.27	0.92	3.53	0.001	Higher loss than S1
N source S4 (neem, broadcast pre-irrig.)	4.45	0.89	4.99	< 0.001	Highest loss among sources tested
N source S5 (neem, broadcast post-irrig.)	3.52	0.89	3.95	< 0.001	Higher loss than S1

Model 2 equation: $\text{NH}_3\text{-N loss (kg ha}^{-1}\text{)} = 27.25 + 0.20 \times \text{Tillage (0/1)} - 5.61 \times \text{Basal-timing level (1–4)} + [2.59, 3.27, 4.45, 3.52] \times \text{N-source dummy (S2, S3, S4, S5; 0 otherwise)}$; $R^2 = 0.942$, $\text{RMSE} = 1.62 \text{ kg N ha}^{-1}$, $n = 39$.

3.3. Amendment Strategies to Reduce NH_3 Volatilization in Wheat

Experiment C complemented the two regression models by measuring how organic and inorganic amendments affect nitrogen mitigation using recommended-dose nitrogen (RDN) in wheat (Fig. 3). The urease inhibitor NBPT lowered cumulative $\text{NH}_3\text{-N}$ loss by 40% compared to RDN alone ($20.4 \text{ kg N ha}^{-1} \text{ season}^{-1}$), reducing it from approximately 20.4 to $12.2 \text{ kg N ha}^{-1}$. Amendments with hydroquinone and garlic extract resulted in smaller yet significant reductions of 27% and 17%, respectively. These findings align with existing literature, where NBPT alone has been shown to reduce NH_3 volatilization by 61–74% (Klimczyk et al. 2021). The results suggest that both amendment-based mitigation and management strategies such as nitrogen timing and source used in Model 2, work together as additive approaches to lessen gaseous nitrogen losses from wheat.

3.4 APSIM Next Generation validation of Models 1 and 2

Both models produced simulated dynamics that closely matched their respective regression-based predictions when integrated into APSIM Next Generation (Section 2.4). In the rice scenario (120 kg N ha⁻¹, ambient temperature), urea rapidly hydrolyzed to NH₄⁺ through APSIM's soil nitrogen processes. The NH₄⁺ level peaked at 45.4 kg N ha⁻¹ three days after application and then declined due to plant uptake, nitrification, and NH₃ loss. By the season's end, total NH₃-N loss was 14.024 kg N ha⁻¹, precisely matching Model 1's estimate for this nitrogen amount and temperature ($7.625 + 0.0483 \times 120 + 0.603 \times 1 = 14.024$ kg N ha⁻¹). In the wheat scenario (T1S1 management), the NH₄⁺ pool peaked slightly higher at 52.0 kg N ha⁻¹ four days after application, with cumulative NH₃-N loss reaching 21.640 kg N ha⁻¹, again aligning with Model 2's prediction ($27.25 - 5.61 \times 1 + 0 = 21.64$ kg N ha⁻¹) to three decimal places (Fig. 4; Table 4).

Table 4
Summary of APSIM Next Generation validation for representative rice and wheat scenarios

Metric	Rice (120 kg N ha⁻¹, T1)	Wheat (T1S1-equivalent)
Fertiliser application date	3 May 1998	3 May 1998
Urea pool immediately after application (kg N/ha)	120.000	120.000
NH ₄ ⁺ pool peak (kg N/ha)	45.4 (day 3)	52.0 (day 4)
Days to ~ 90% of eventual cumulative loss	~ 13	~ 13
Regression-predicted seasonal total, Lmax (kg N/ha)	14.024	21.640
Simulated cumulative loss at season end (kg N/ha)	14.024	21.640
Difference (simulated - predicted)	0.000	0.000

As with the wheat-only result reported previously, it is important to be precise about what this validates: the simulated cumulative-loss values match the regression models' fitted predictions for these specific scenarios, not the individual field-observed values for the corresponding treatments (which differ somewhat from the fitted predictions because the regressions were fit across the full set of 16 and 39 treatment combinations respectively, with R² of 0.943 and 0.942 rather than 1.0). What Table 4 and Fig. 4 demonstrate is that the Manager-script coupling described in Section 2.4 faithfully reproduces each fitted equation's output once running as a genuine daily process within APSIM's full soil-water-nitrogen-crop environment, for both crops, using a common implementation design the first non-emulated confirmation, for either model, that this coupling approach is technically sound. A complete validation against the full set of field-observed treatment means in Tables 2 and 3 would require repeating this

procedure across the remaining nitrogen-rate/temperature and tillage/timing/source combinations, which is identified as a direction for future work (Section 5).

4. Discussion

Both empirical models achieved R^2 values above 0.94, matching or surpassing the predictive accuracy of several process-based NH_3 volatilization models used with surface-applied urea. They accomplish this with only two or three simple agronomic predictors, avoiding the need for detailed, continuously monitored soil-surface and micrometeorological data required by mechanistic models like Volt'Air (Genermont and Cellier 1997) or the urea hydrolysis model of Rachhpal-Singh and Nye (1986). This aligns with broader findings in NH_3 volatilization modelling, which suggest that empirical and semi-empirical models, despite their simplicity, can rival process-based models in predicting total field losses when calibrated with site-specific data. The validation within APSIM Next Generation (Section 3.4) supports this: once integrated as Manager-script components, both models precisely reproduced their season-total predictions through daily NH_4^+ pool dynamics (peaking 3–4 days after application in both crops, Fig. 4). These dynamics are consistent with observed patterns across the source experiments, such as Experiment C's report that losses peaked around day 3. The shared script design including urea-pool detection, NH_4^+ loss removal, exponential within-season loss kinetics, and a time-gap rule for separate fertilization events worked effectively for both a flooded rice and an aerobic wheat system. This indicates that the coupling approach itself, rather than crop-specific adjustments, underpins the predictive consistency between the regression and process-embedded simulations.

In both Model 1 and Model 2, the primary factors nitrogen rate and basal-timing level point to a common underlying mechanism. This mechanism is that cumulative NH_3 loss is most strongly influenced by the size and timing of the labile, easily hydrolysable nitrogen pool at or near the soil surface. This aligns with the urea-hydrolysis kinetics central to process-based models (Rachhpal-Singh and Nye 1986). The modest but significant temperature effect in Model 1 aligns with the well-known temperature dependence of urease activity and the equilibrium between NH_4^+ and un-ionised NH_3 . It suggests that the temperature-gradient-tunnel treatments in Experiment A, although not associated with precisely measured absolute temperature differences in the source records, effectively captured a real, statistically significant warming effect on NH_3 loss, consistent with existing literature on temperature and NH_3 volatilization (Rachhpal-Singh and Nye 1986).

The discovery that the tillage system had no significant independent effect in Model 2—after accounting for nitrogen timing and source—refines the original qualitative conclusion from the source experiment, which suggested that conservation tillage slightly lowered NH_3 emissions. The current multi-factor model shows this reduction can be more simply attributed to nitrogen-management factors that coincided with tillage across different treatments, rather than to tillage itself. Likewise, the nitrogen source rankings in Model 2, with urea super granules placed in bands as the lowest-loss baseline, and all four alternative source and placement combinations showing significantly higher losses, align with the

idea that band placement reduces soil surface area exposed to volatilization compared to broadcast application. This also underscores that placement method can be as influential on NH_3 loss as the chemical form of the nitrogen source.

The reductions resulting from amendments in Experiment C (17–40%) and the management strategies in Model 2 (which can reduce nitrogen fertilizer by several kg ha^{-1} through timing and source choice) are best viewed as complementary mitigation options rather than competing ones. Combining a rice-wheat system with sensor-guided, split nitrogen application, band placement, and a urease-inhibitor-enhanced fertilizer is expected to produce compounded reductions beyond what each approach achieves individually. However, this combined effect was not explicitly tested in any of the five source experiments and would benefit from further specific validation.

Several limitations should be noted. First, the exact temperature differences between the four regimes in Experiment A could not be precisely determined from the source records, which only reported weekly average temperatures by treatment. As a result, Model 1 employs an ordinal temperature level instead of a continuous variable; having the actual degree-values would enable a more accurate analysis of temperature sensitivity. Second, one treatment combination (T3S3, conservation tillage) was missing from the extractable data for Experiment B and was excluded from Model 2 without replacement. Third, both models were calibrated and tested on the same dataset used for fitting, measuring in-sample R^2 and RMSE. Validating the models with independent data, such as additional site-years or using an existing process-based model like Volt'Air or FAN on the same experiments, would increase confidence in their broader applicability beyond the specific soils, seasons, and cultivars studied.

5. Conclusion

This synthesis of five field experiments across the IGPs shows that simple, field- calibrated linear regression models- including only nitrogen rate, temperature level, tillage, basal- timing, and nitrogen source as predictors- can accurately simulate cumulative seasonal NH_3 volatilization from rice ($R^2=0.943$) and wheat ($R^2 = 0.942$). Their performance is comparable to more complex process based models in the literature. Nitrogen rate and basal nitrogen timing are the main factors influencing NH_3 loss in rice and wheat, respectively. Temperature has a smaller but significant effect in rice, while tillage system alone has no significant impact on wheat once nitrogen management is considered. Supplementary trials confirmed that urease inhibitors and, to a lesser extent, botanical amendments can reduce NH_3 loss by 17–40% beyond nitrogen management alone. Both models were integrated into APSIM Next Generation software as Manager- script components (Section 3.4.4). When the loss removal logic targeted the soil NH_4^+ pool instead of urea, the models accurately reproduced their fitted regression predictions (rice: $14.024 \text{ kg N ha}^{-1}$; wheat: $21.640 \text{ kg N ha}^{-1}$) with a mechanistically coherent day- by- day simulation for both crops, providing the first non- Python confirmation that the coupling design works across these cropping systems, pending further validation. These field- calibrated equations offer straightforward, transparent tools for estimating NH_3 - N loss and evaluating mitigation

strategies in rice- wheat systems of the IGPs. They exemplify a broader, generalizable approach- combining measured data from independent field trials into simple, source- cited empirical models, then embedding them within an established crop- soil simulation platform- to predict ammonia volatilization where detailed inputs for fully mechanistic models are unavailable. Future work expanding the APSIM coupling across various nitrogen rates, temperatures, tillage, timing, and nitrogen sources, including continuous temperature data and additional site- years, will further enhance and generalize these models.

Declarations

Author Contribution

All the authors wrote the draft and final manuscript and reviewed it.

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Figures

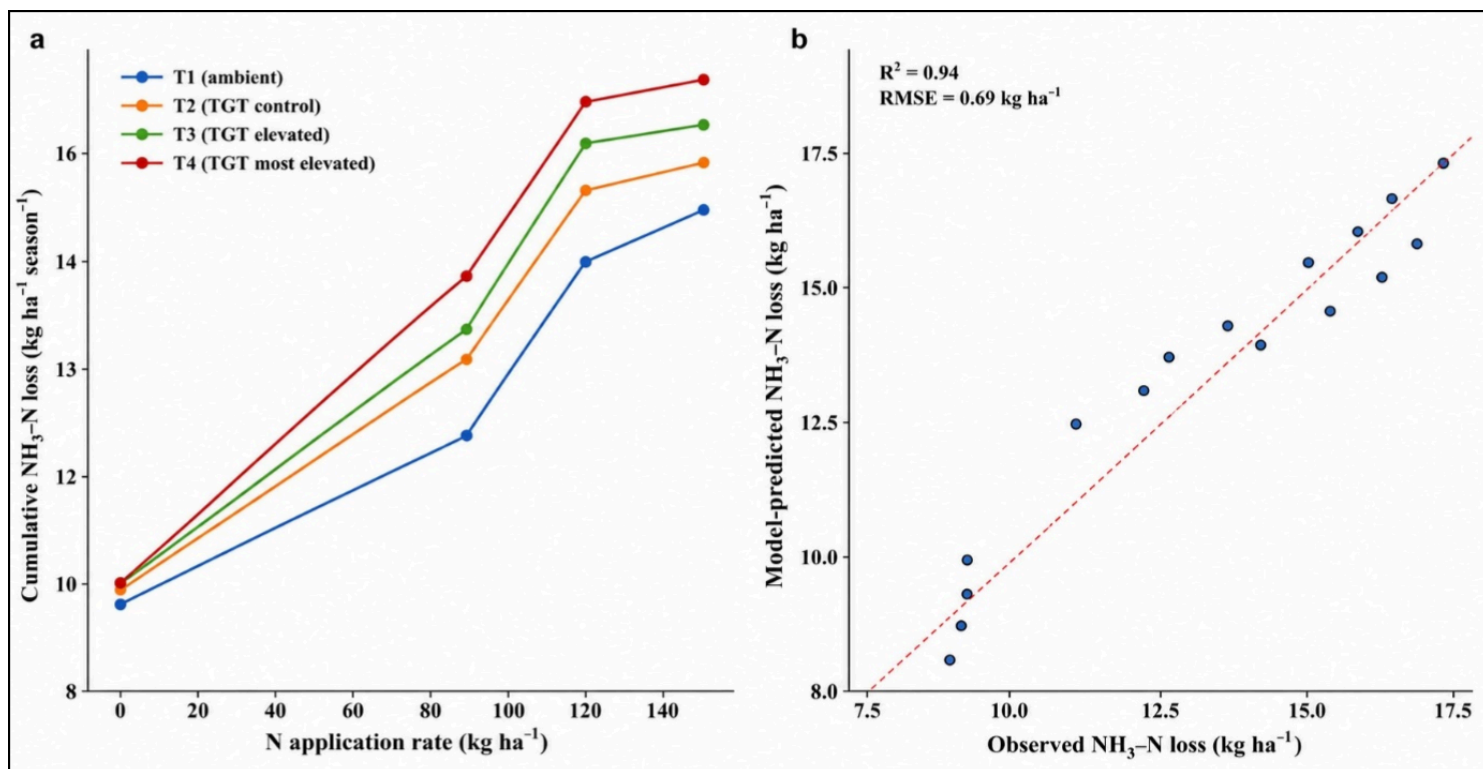


Figure 1

Model 1 (rice): (a) cumulative $\text{NH}_3\text{-N}$ loss versus nitrogen rate at each of four temperature levels; (b) model-predicted versus observed cumulative $\text{NH}_3\text{-N}$ loss (dashed line = 1:1)

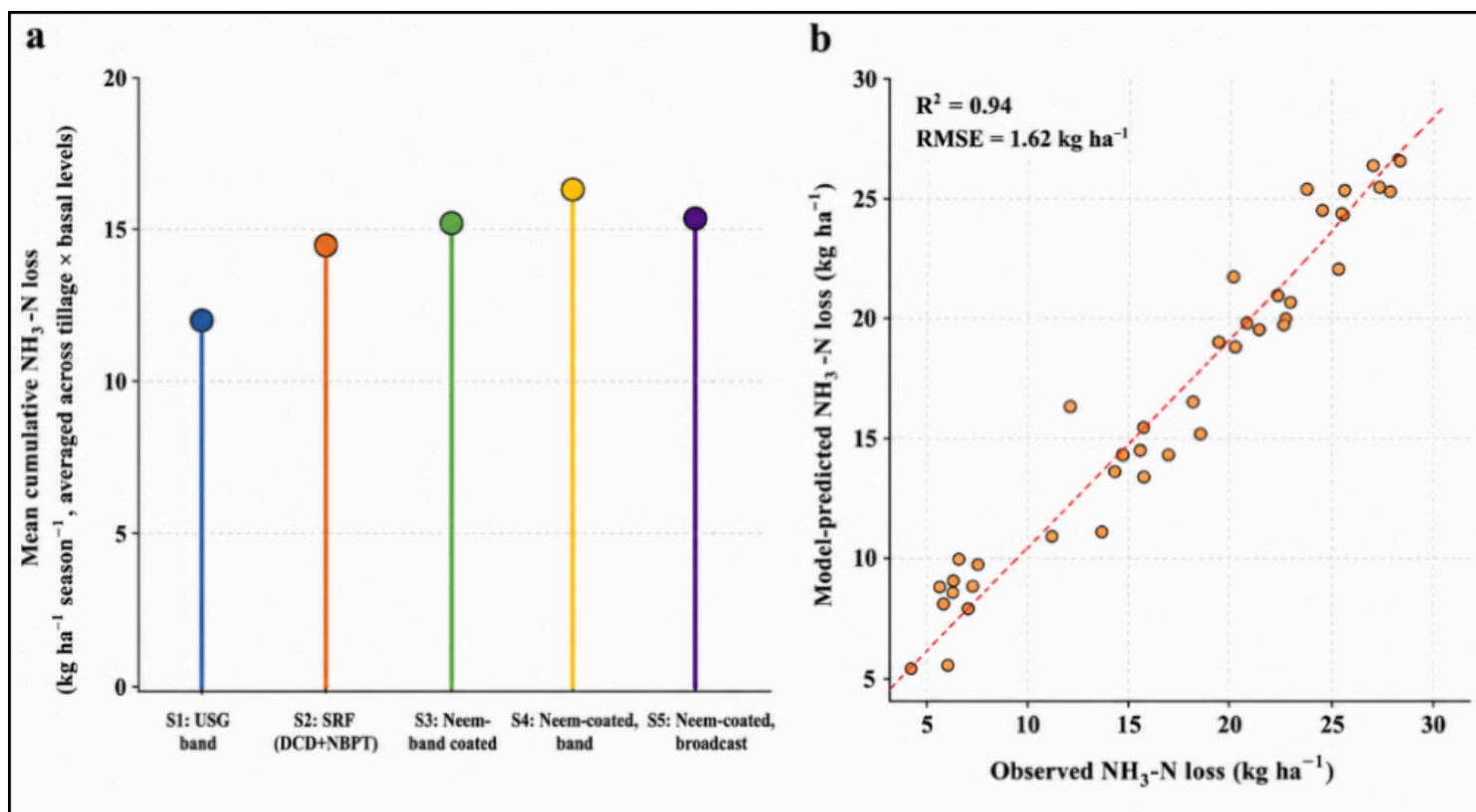


Figure 2

Model 2 (wheat): (a) mean cumulative $\text{NH}_3\text{-N}$ loss by nitrogen source/placement (averaged across tillage and basal-timing levels); (b) model-predicted versus observed cumulative $\text{NH}_3\text{-N}$ loss (dashed line = 1:1)

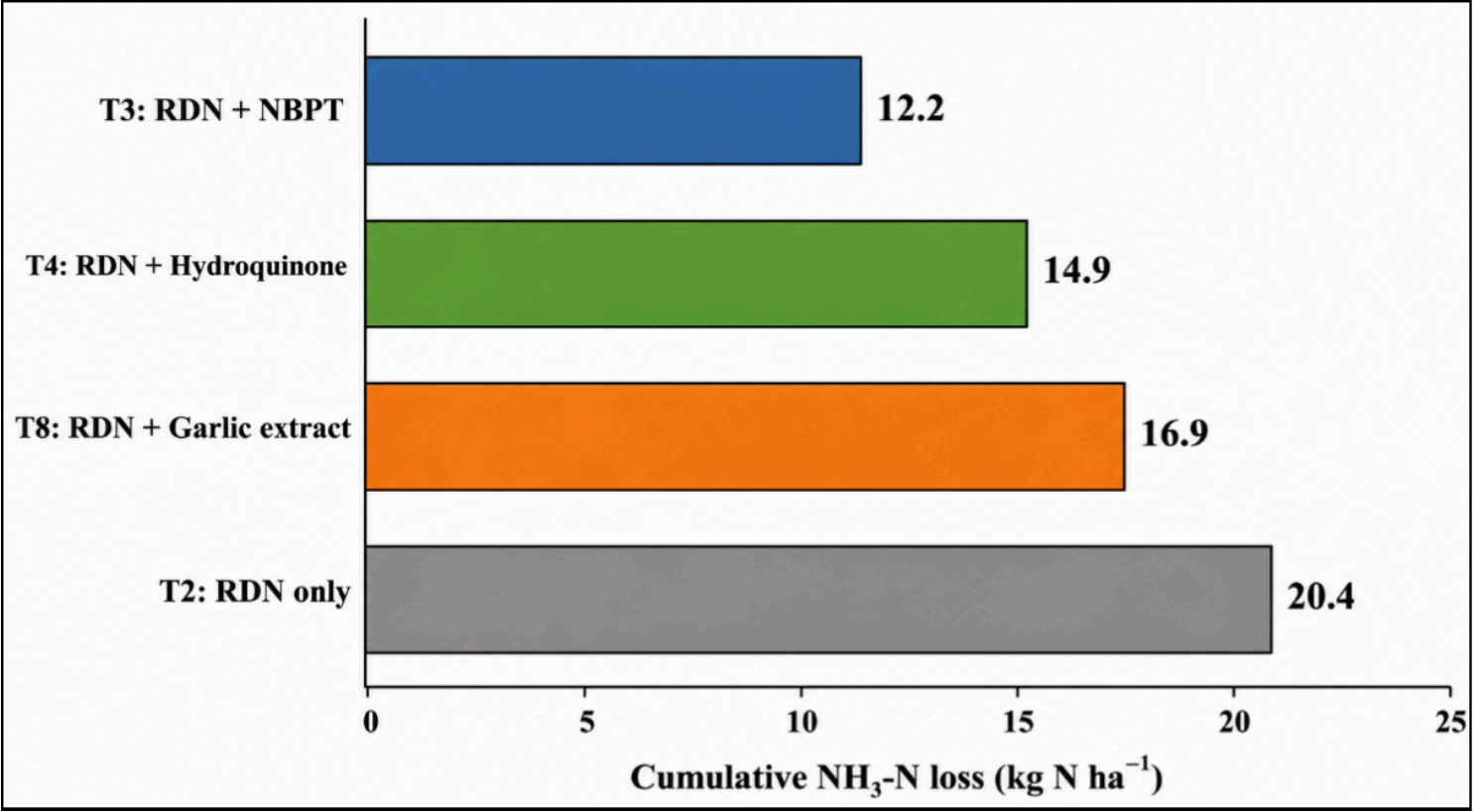


Figure 3

Cumulative $\text{NH}_3\text{-N}$ loss in wheat under RDN alone and RDN amended with the urease inhibitor NBPT, hydroquinone (HQ), and garlic extract

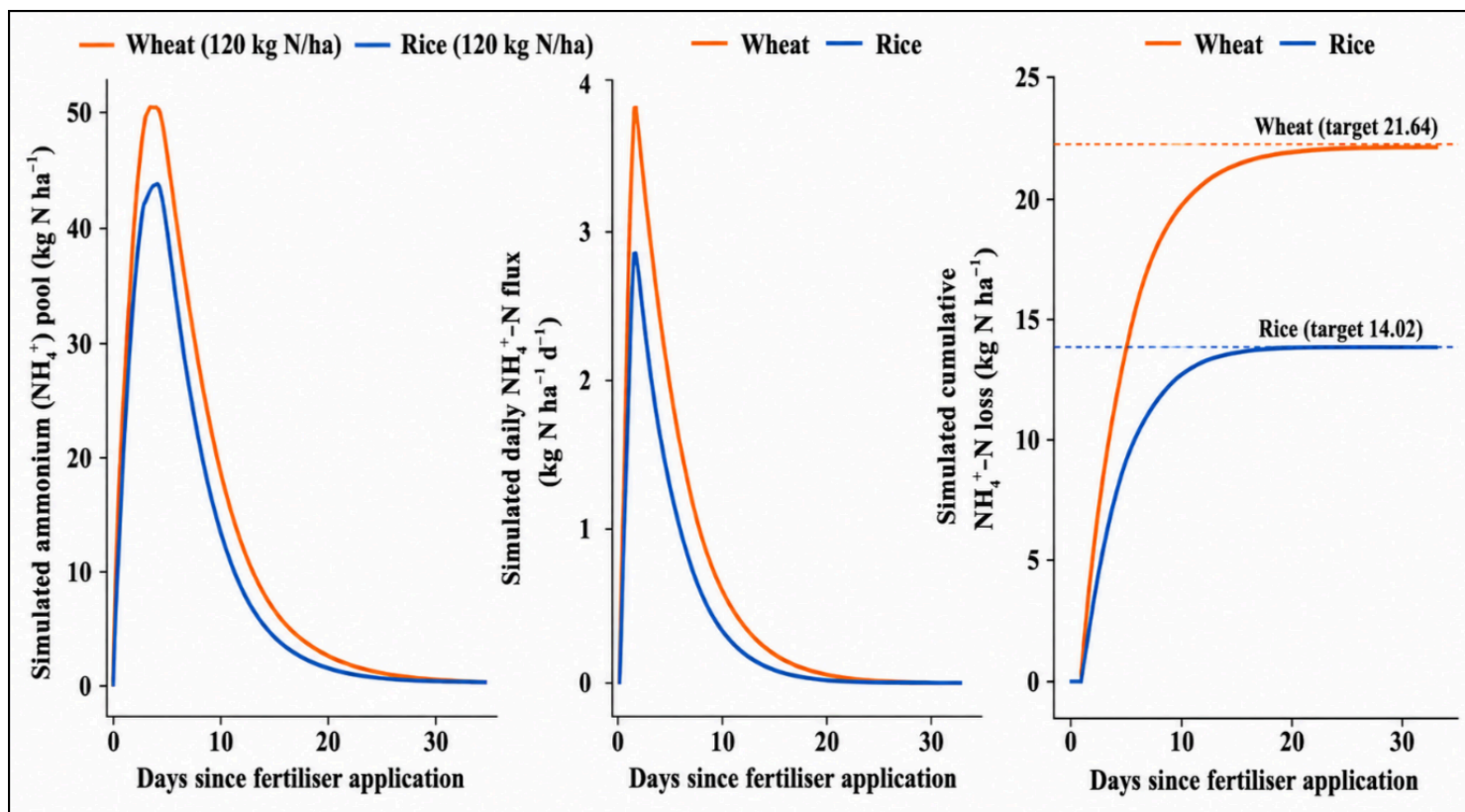


Figure 4

Genuine APSIM Next Generation output comparing rice and wheat scenarios (both 120 kg N ha⁻¹, reference management level), aligned by days since fertiliser application: (a) simulated (NH₄⁺) pool; (b) simulated daily NH₃-N flux; (c) simulated cumulative NH₃-N loss, converging on each crop's Model-predicted seasonal total (dotted lines)

Supplementary Files

This is a list of supplementary files associated with this preprint. Click to download.

- [RiceNH3Test.apsimx.bak](#)
- [WheatNH3Test.apsimx.bak](#)