

Supporting Information

A Mechanistic Model for Determining Factors that Influence Inorganic Nitrogen Fate in Corn Cultivation

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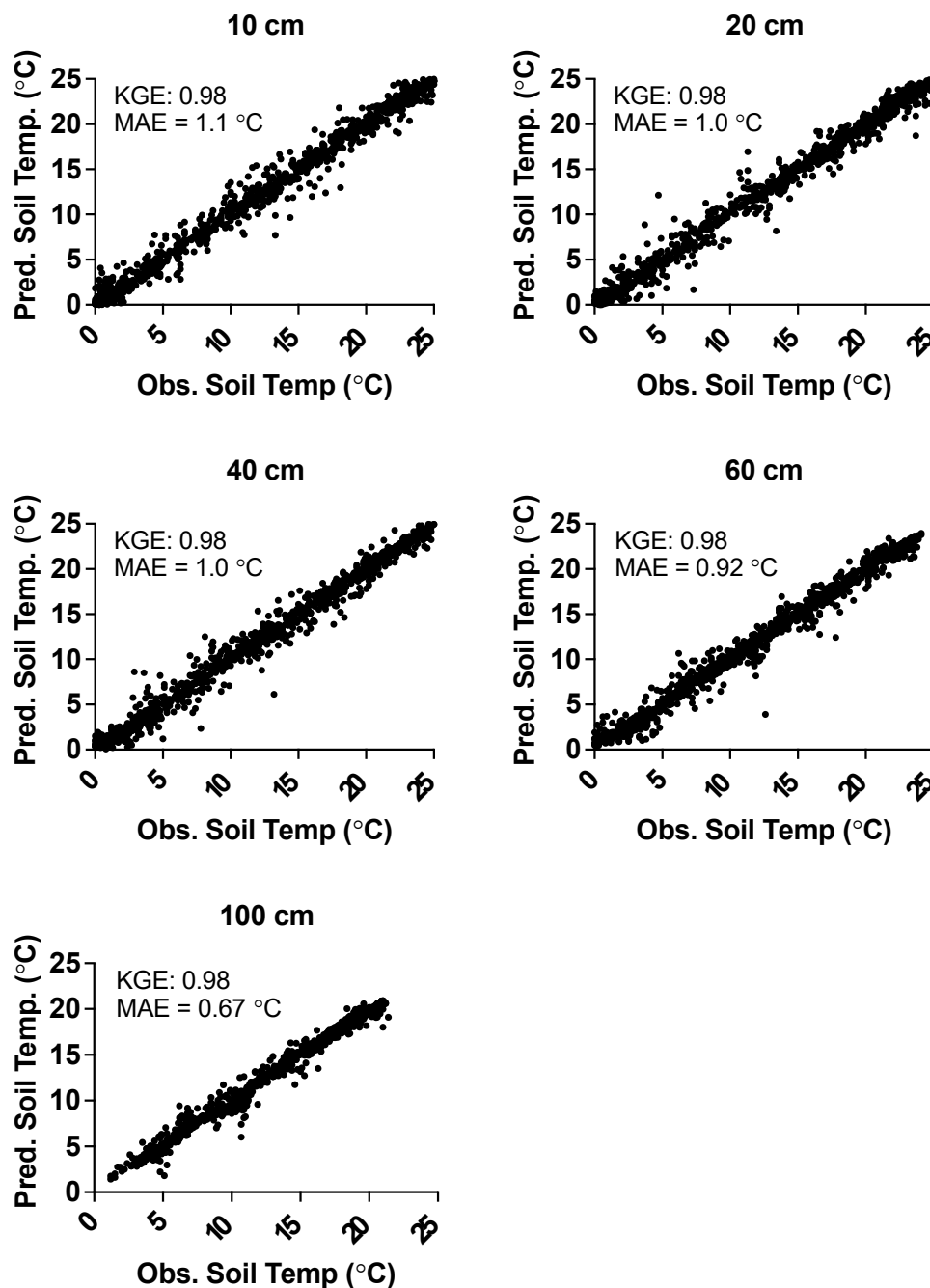


Figure S1. A random forest regression models were created to predict the soil temperature at depths of 10, 20, 40, 60, and 100 cm for dates where temperature data was not available. Features used to train the model included daily precipitation, high and low daily air temperature, daily solar radiation, and the day of year. Each regressor was trained using a 70 – 30 training and validation split and contained 100 trees. Each regressor was evaluated for accuracy by KGE and MAE. Plots display the predicted (red) vs observed (black) data for each of the soil temperature regressors.¹

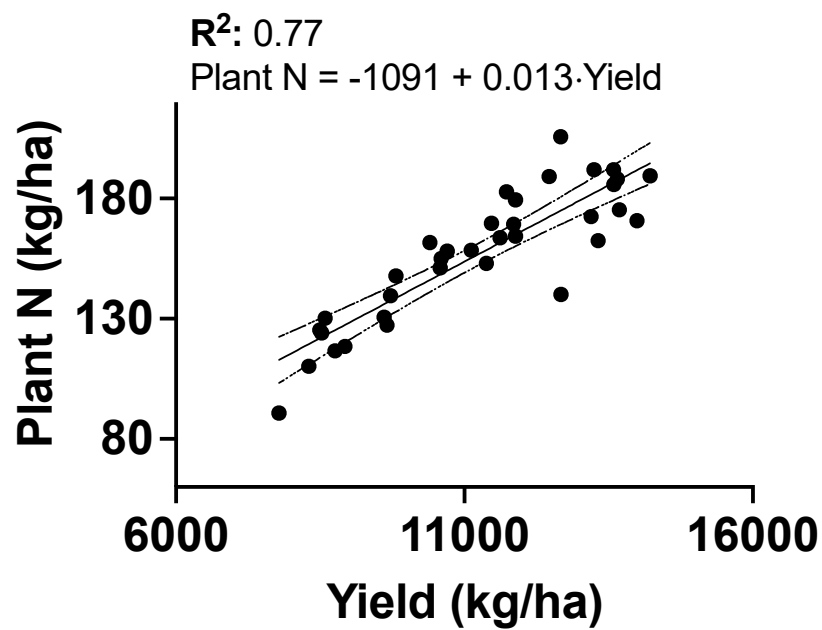


Figure S2: A linear regression was created from historical data at the ISU research farm to predict plant nitrogen content (kg/ha) from yield totals.¹ The plot displays this regression and the 95% confidence interval bands.

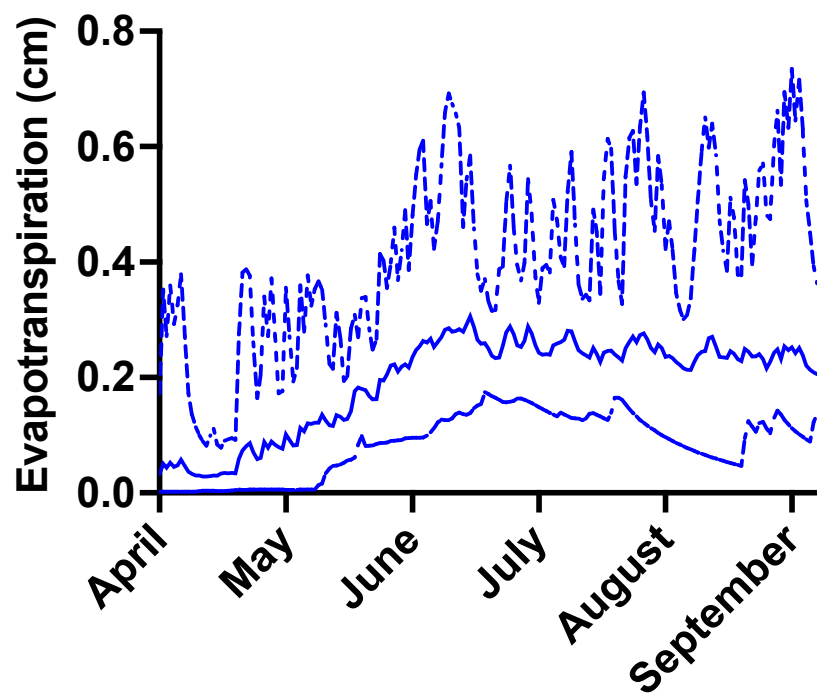


Figure S3. The modeled daily evapotranspiration across the study years. The line displays the mean and the shaded region displays the range.

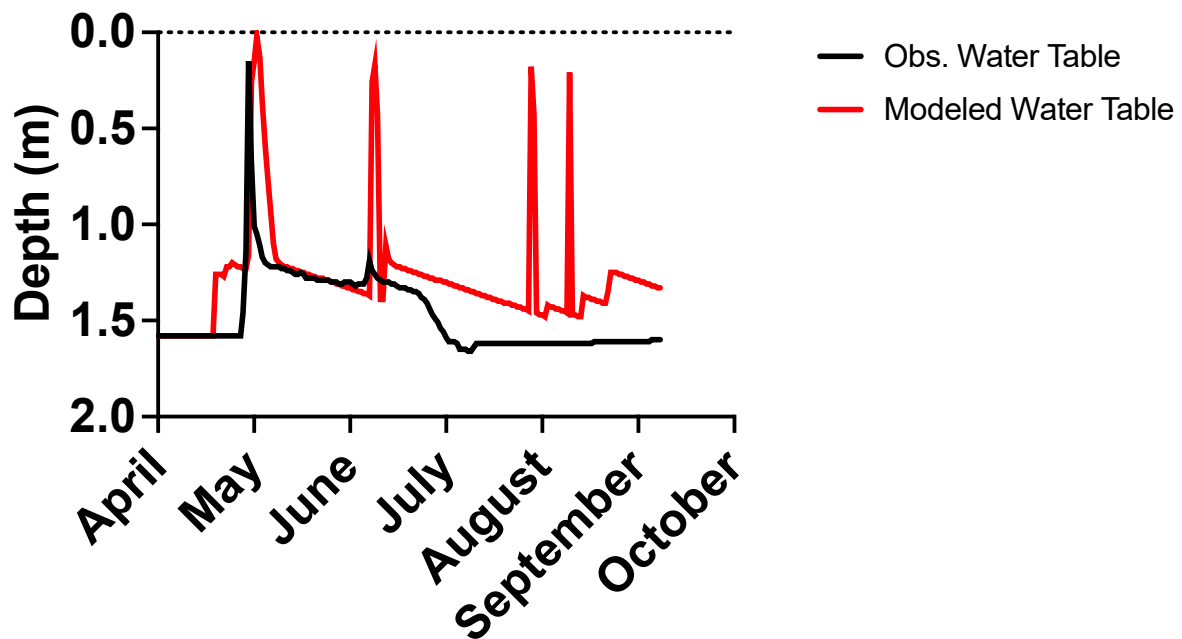


Figure S4: Example modeled water table depth vs. observed data from 2012 at the study site.¹

RootBox Description:

RootBox is an L-system; a model that is used to compactly describe a branched geometry, where a number of production rules are iterated to create a graphically interpretable model.² The production rules include elongation and lateral branching, which are governed by the following critical descriptors: maximum root length (cm), initial growth rate (cm/d), spacing between branches (cm), the number of branches, length of basal and apical zones (cm), root radius (cm), and branching angles (degrees) (Table S1). Randomness is introduced into RootBox through random selection of descriptors over a predesignated range within a simulation. Modification of the descriptor ranges can allow for the generation of realistic geometries of specific plants, such as corn. Iterating the L-system over time allows for a three-dimensional representation of a growing root system. The differential development of root systems due to environmental conditions, such as soil properties, nutrient availability, and water availability is complex and still under investigation.^{3,4} Thus, one root architecture simulation was generated for all NO_3^- simulations and it was assumed that root architecture was constant regardless of soil parameters and availability of nutrient and water.

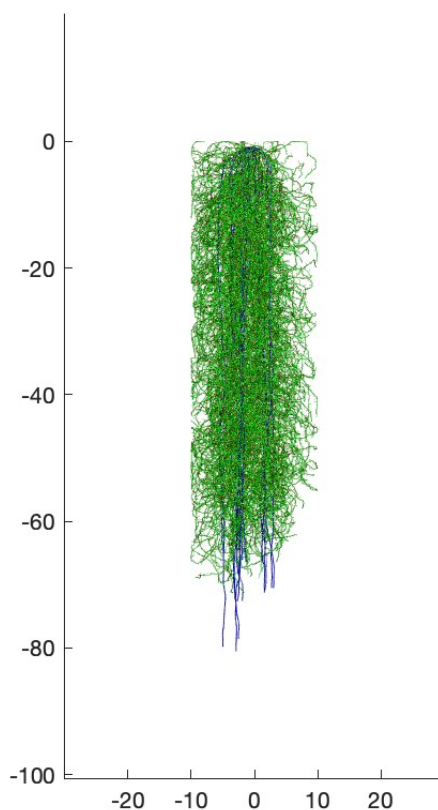


Figure S5: Corn root architecture at day 120 developed using RootBox 6 with primary roots (blue) and secondary lateral roots (green). Values from Table S1 were used to develop this architecture.

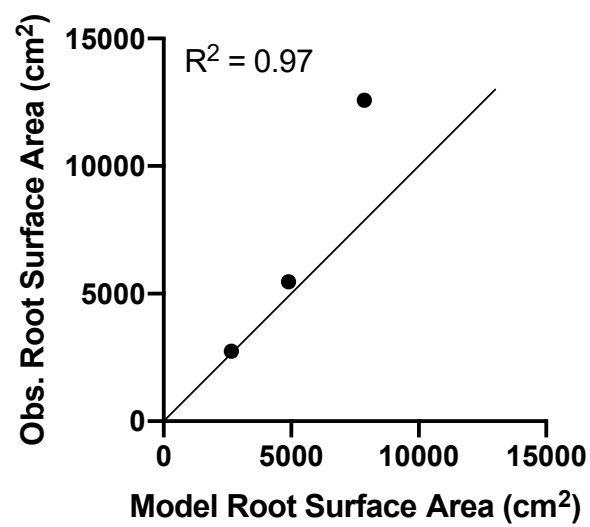


Figure S6: Root surface area validation. RootBox simulated values of total root surface area plotted against empirical measurements.⁵

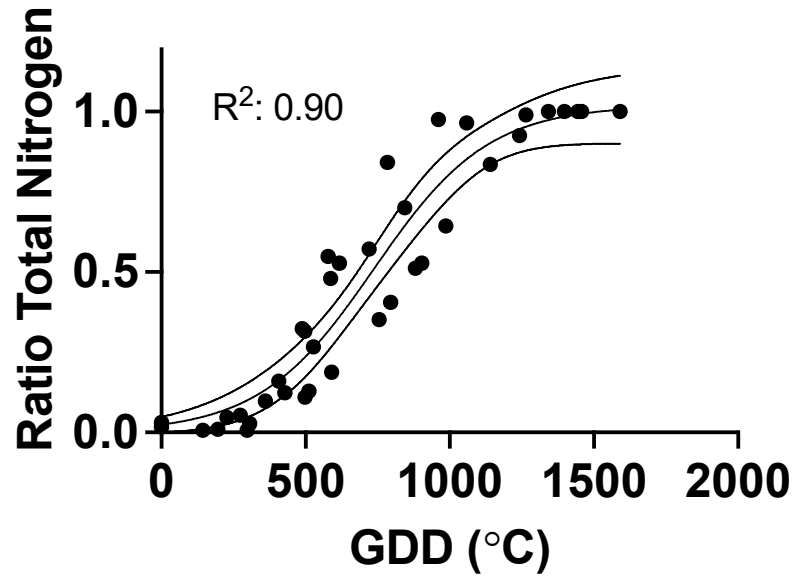


Figure S7. A logistic growth curve was made to model uptake of nitrogen by the plant by accumulated GDD (°C) using empirical data points found in the literature.⁵⁻⁷ Data used to create this model are the portion of total plant nitrogen accumulated by accumulated GDD (°C). This curve was used to describe the nitrogen uptake rate of the plant in the mechanistic model. Plot displays the individual data points, fitted curve, and the 95% confidence intervals of the curve.

Table S1. Table displaying the calibrated rate coefficients for mineralization/immobilization, denitrification, evaporation, and plant water uptake for each of the ten study years. Calibrated coefficients minimized error between the simulated plant nitrogen and drainage nitrogen totals and the empirically measured plant nitrogen and drainage nitrogen totals. They also led to evapotranspiration values that matched previous reports for corn in the literature.

Year	Mineralization (unitless)	Denitrification (unitless)	Transpiration (unitless)	Evaporation (unitless)	Plant N Error	Drain N Error
2008	2.10E-03	2.30E-02	1.50E-03	5.00E-03	0.55%	-0.30%
2009	6.25E-04	4.20E-03	1.50E-03	5.00E-03	16.83%	3.29%
2010	1.00E-03	1.76E-02	1.50E-03	3.25E-02	3.05%	2.34%
2011	1.40E-03	4.20E-03	1.00E-03	5.00E-04	2.85%	-0.95%
2012	8.33E-04	6.46E-02	1.00E-03	5.00E-04	12.15%	-1.27%
2013	1.00E-03	4.20E-03	1.50E-03	5.00E-03	7.00%	-2.70%
2014	1.90E-03	4.20E-03	1.00E-03	5.00E-04	-3.49%	6.96%
2015	2.10E-03	3.44E-02	1.50E-03	1.00E-03	13.40%	-0.86%
2016	4.49E-05	4.20E-03	1.00E-03	1.00E-03	19.86%	6.02%
2017	5.00E-04	3.44E-02	1.00E-03	5.00E-04	48.60%	2.27%

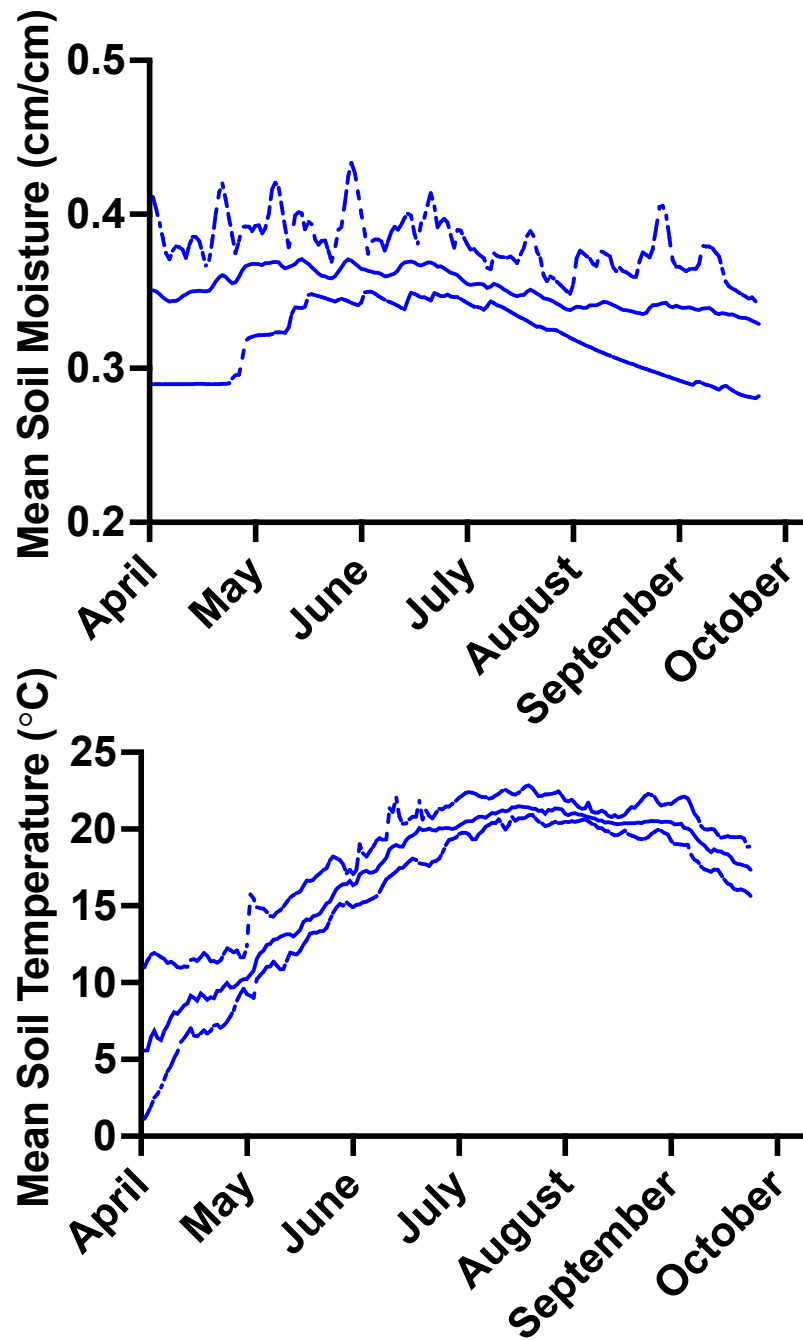


Figure S8. The mean (solid line) and range (shaded region) across the soil profile and study years for soil moisture (top) and soil temperature (bottom).¹

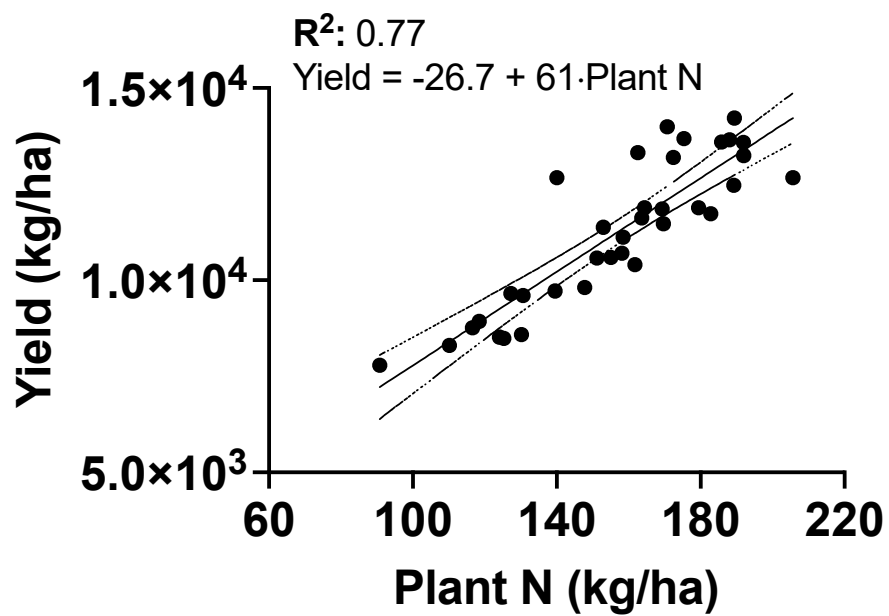


Figure S9. A linear regression was created from historical data at the ISU research farm to predict yield totals (kg/ha) from plant nitrogen totals.¹ The plot displays this regression and the 95% confidence interval bands.

Economic Model:

An economic model was developed to estimate the net income from predicted corn grain yields. Corn grain yields were predicted from total plant nitrogen under the fertilizer application timing and rate scenario using the regression developed in Figure S8. Predicted yields with a zero-nitrogen application rate were then subtracted from predicted yields for each scenario to estimate the yield increases from using a specific application rate of nitrogen. Return to nitrogen fertilizer (\$/ha) was then calculated using the following equation⁸:

$$\text{Return to Nitrogen} = (\text{yield increase} * \text{grain price}) - (N \text{ application rate} * \text{fert. cost})$$

Grain prices and fertilizer costs were \$4.40 per bushel and \$0.60 per kg, respectively and were estimated as current prices for corn grain and anhydrous ammonia at the time of the analysis.^{9,10} Absolute values for return on nitrogen could differ based on the fluctuation of these prices.

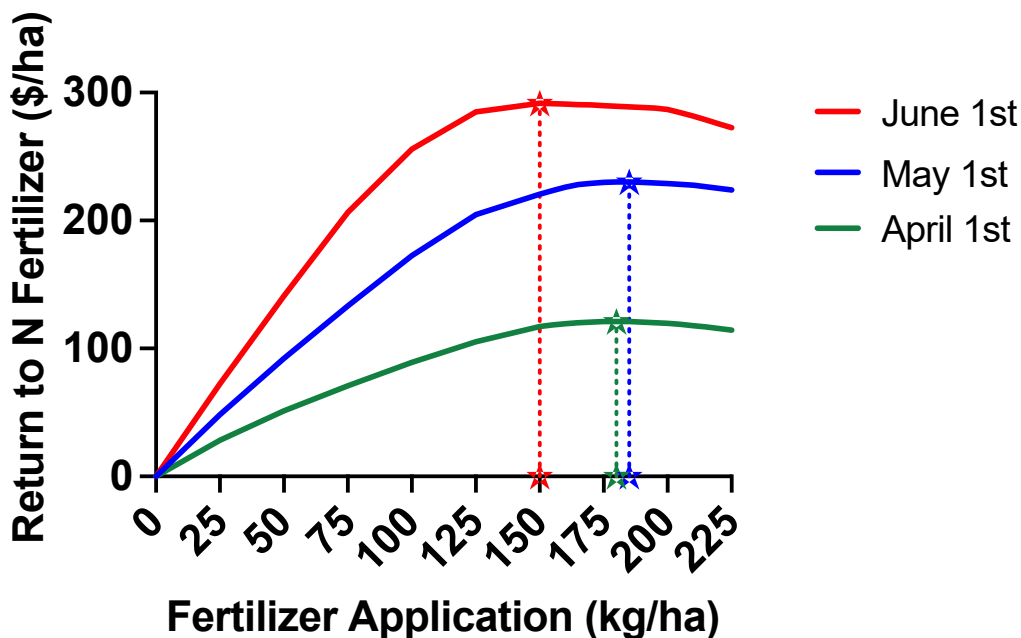


Figure S10. The mean net income return to nitrogen (\$/ha) across study years for simulated crop yields across fertilizer application rates when fertilizer is applied on April 1st, May 1st, and June 1st. Stars indicate the maximum return to nitrogen (MRTN), which is the maximum economic output under the application timing scenarios and the fertilizer application rate where the MRTN is achieved.

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