A validation of APSIM nitrogen balance and leaching predictions

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Abstract

Systems models are vital tools for addressing the growing need to understand the implications of management decisions on nitrogen (N) cycling and leaching in New Zealand. The Agricultural Production Systems sIMulator (APSIM) is a suite of modules that enables the simulation of systems covering a range of plant, animal, soil, climate and management interactions. While there has been extensive testing and calibration of the APSIM plant and soil modules in Australian conditions, they have not been comprehensively tested in New Zealand. Previous tests of APSIM have shown that modifications to some of APSIM's parameters describing the movement of mineral N through the soil profile may be required to improve leaching predictions under New Zealand conditions. APSIM simulations, both with and without the modifications, are compared with data collected from a different field experiment at Lincoln, Canterbury. Results indicate that the modifications improve model performance for this dataset. They also show that APSIM may underestimate the rate of N mineralisation in the soil and that further modifications to APSIM are required to better suit the soil and climate conditions present within New Zealand.

Additional keywords: modelling, potatoes, ryegrass, soil water

Introduction

The two primary approaches taken to understand and quantify the implications that management decisions have on N cycling and leaching are measurements and modelling. Although measuring nutrient losses can be used to quantify the impacts of agriculture at the catchment scale, it can be prohibitively time consuming, too costly and too variable to be practical at the farm or paddock scale (Addiscott, 1995). A recent review of a number of modelling approaches to estimating N and phosphorous (P) losses in New Zealand highlighted the variety of models currently in use (Cichota and Snow, 2009). Models range from the paddock scale (e.g. SPASMO, Green *et al*. (2003)), though to farm scale (e.g. OVERSEER, Wheeler *et al*. (2003)), to the catchment and region scale (e.g. AquiferSim, Lilburne *et al*. (2006)).

Systems models are one approach used to address the growing need to understand the implications of management decisions on N cycling and leaching in New Zealand. The Agricultural Production Systems sIMulator (APSIM) is a suite of modules that enable the simulation of systems covering a range of plant, animal, soil, climate and management interactions. While there has been extensive testing and calibration of the APSIM plant and soil modules in Australian conditions, they have not been extensively tested in New Zealand.

Previous tests of APSIM have shown that modifications to APSIM's parameters that control the extent of mixing of percolating water may be required to improve estimates of the leaching of mineral N under New Zealand conditions (Sharp *et al*., 2011). Furthermore, APSIM may underestimate the rate of N mineralisation in the soil under cool conditions (Lilley *et al.,* 2003; Verburg *et al.,* 2007). This paper undertakes a validation of the modifications proposed in Sharp *et al*. (2011) by comparing APSIM simulations with data collected from a different 3-year field experiment at Lincoln, Canterbury, conducted during the same time frame but on a different site. The experiment in question was a potato crop followed by another crop and was originally designed to explore the movement of applied N fertilisers through the surface soil and subsoil.

Materials and Methods

The experimental site was located at Lincoln, Canterbury (43°37'19"S; 172°28'10"E). The soil at the site is classified as a Pahau silt loam (New Zealand classification – Mottled Argillic Pallic, (Hewitt, 1998) or Aqui Haplustalfs (Soil Survey Staff, 2006)).

On 14 October 2004, a 20 m x 20 m plot was marked out and 400 kg N ha^{-1} as calcium ammonium nitrate (CAN) was hand broadcast and then washed in with 2.4 mm of water applied using a watering can. Potatoes (*Solanum tuberosum* L. cv. 'Desiree') were planted across the plot in rows on 15 October 2004 at a rate of approximately 46,000 tubers ha^{-1}. The potatoes were harvested in April 2005 and Italian Ryegrass (*Lolium multiflorum* L. cv. Andy) was planted after cultivation. The ryegrass was mowed at regular intervals. On 11 November 2006, a second application of 400 kg N ha^{-1} was applied to the site as CAN. The relatively high application of N to the ryegrass was applied to generate a leaching pulse, an objective of the original experiment. The potatoes were drip irrigated fortnightly after crop emergence at a rate in excess of crop demand (1.75 x evapotranspiration, ET) to ensure drainage occurred. Irrigation was applied to potatoes with one drip line either side of each row of potatoes and emitters spaced at 30 cm applying (11 mm hr^{-1}). Ryegrass was irrigated between November and May in the first year after establishment using overlapping sprinklers applying water at a rate of 8.5 mm hr^{-1} across the plot. After the second application of fertiliser, approximately 34 mm per week was applied until February 2007. From October 2007 until the end of the trial, 17 mm per week was applied.

Measurements of soil mineral N, crop DM, soil water content and leachate nitrate concentration were made at regular intervals throughout the trial. Soil samples were taken at 0.2 m intervals from the soil surface to 1.2 m and analysed for mineral N. Crop dry matter yields were calculated at harvest for the potato crop and when mowing the ryegrass. Soil water below 0.2 m was measured in 0.2 m increments using a neutron probe, with tubes installed to a depth of 3 m; the 0 to 0.2 m depth was measured using time domain reflectometry (TDR) installed vertically. Leachate was collected from ceramic cup solution samplers installed at depths of 1 m, 3 m, 5 m and 7 m, with three installed at each depth (Dann *et al*., 2010). Nitrogen leaching was calculated using the soil solution nitrate concentration measured from samples collected in the ceramic cups and the drainage calculated by APSIMs water balance. This procedure aimed to reduce uncertainty around drainage estimates.

The observed data were compared with simulations developed in APSIM 7.3. APSIM allowed the integration of several crop models with an underlying soil module which simulates soil water movement and nutrient supply. The crop modules used were 'potato' and 'AgPasture ryegrass'. The soil water module SoilWat was used (http://www.apsim.info/Wiki/SoilWat.ashx). The soil description (e.g. soil texture) and initial values were provided from data collected at the start of the experiment. Drained upper limit (DUL) was estimated using the highest stable water content observed in the time course of soil water measurements. These values of DUL were used to estimate Lower limit (LL) and saturation (SAT) from empirical relationships that were fitted to a range of measurements of DUL, LL and SAT taken in Canterbury silt loam soils.

Within APSIM's SoilWat module the saturated and unsaturated flows of soil water are used to calculate the redistribution of solutes throughout the soil using a 'mixing' algorithm (http://www.apsim.info/Wiki/SoilWat.ashx). Essentially solute movement is calculated as the product of the water flow and the solute concentration in that water. The solute concentration of the water leaving a layer is calculated from the solute concentration of water and coming into that layer and the extent of mixing between water draining through the layer and the water already in the layer. In APSIM 7.3 it is assumed both saturated and unsaturated flow have mixing efficiency factors of 1.0 which assumes drainage water is fully mixed with the water present in the layer. However, Sharp *et al.* (2011) have shown predictions of N leaching to be improved by reducing the mixing coefficient for saturated flow from 1.0 to 0.7. The aim of this paper is to test whether that change gives improved model performance on another independent data set. APSIM was therefore run with both the original value of 1.0 and with the reduced mixing value for saturated water movement (*flux_eff*) of 0.7, as used in Sharp *et al.* (2011).

Model outputs were evaluated and compared using the methods described in Smith *et al.* (1997). These included the root mean square error (RMSE); modelling efficiency (EF) i.e. whether the simulated data described the trend in the measured data better than the mean of the measured data; coefficient of determination (CD) i.e. a measure of the proportion of total variance in the observed data that is explained by the predicted data; relative error (E) i.e. any bias in the total difference between simulation outputs and measured values; and sample correlation coefficient (r) i.e. whether simulated values follow the same pattern as observed values. The statistical significance of RMSE and E was evaluated assuming a deviation corresponding to the 95% confidence interval of the observed values ($\mathrm{RMSE}_{95\%}$ and $E_{95\%}$).

Results

APSIM estimated that the system would produce a potato crop of 13,990 kg DM ha^{-1}, while a mean observed value of 12,390 kg DM ha^{-1} (standard deviation = 2,408 kg ha^{-1}) was obtained, indicating a good agreement between measured and predicted values. APSIM estimated that over the course of the ryegrass ley (April 2005 to December 2007) 14,571 kg DM ha^{-1} would be harvested under the original setup and 15,385 kg DM ha^{-1} would be harvested with the modified parameterisation. A mean observed value of 30,213 kg DM ha^{-1} was obtained, indicating a poor agreement between measured and predicted values.

There is a good agreement between estimated and measured soil water content values (Figure 1). The RMSE was 6.3, which is less than the $RMSE_{95\%}$ of 12.0, indicating that the simulated values fall within the 95% confidence interval of the measurements. In addition, the APSIM outputs gave a positive EF value (0.31), demonstrating that the simulated values describe the pattern in the observed data better than the mean of the observations. The calculated value of E (-1.8) also falls within the range of $E_{95\%}$ (± 11.7) indicating there is no bias in the predicted values. When looking more closely at the individual soil layers, as shown in Figure 2, there is good agreement between predicted and simulated values throughout the soil profile. The only exception is in the top layer when under the potato crop, where APSIM overestimates the soil water content in the top 20 cm of soil (Figure 2). One possible explanation for these differences may be changes in the soil surface area to volume ratio and soil bulk density in the top layer of the soil created by the creation of ridges and furrows, which cannot be simulated in APSIM. However, this hypothesis requires further investigation.

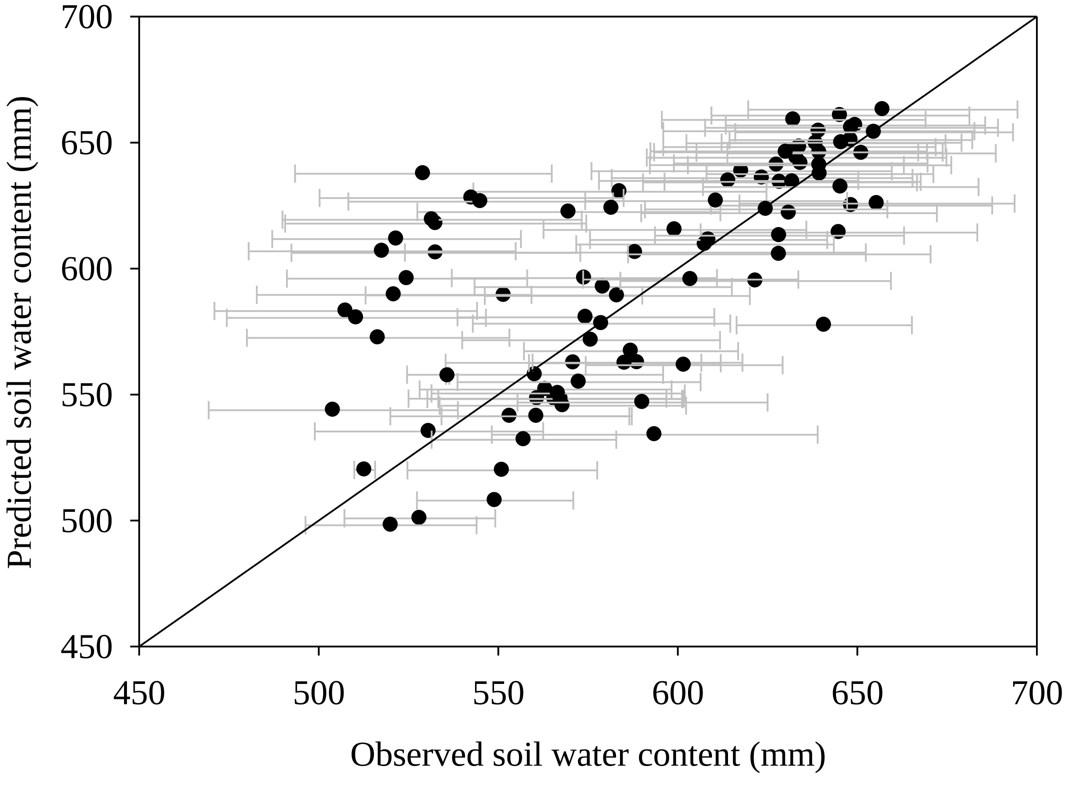

Figure 1: Observed against predicted total soil water content to 3 m, with associated standard deviation and 1:1 reference line**.**

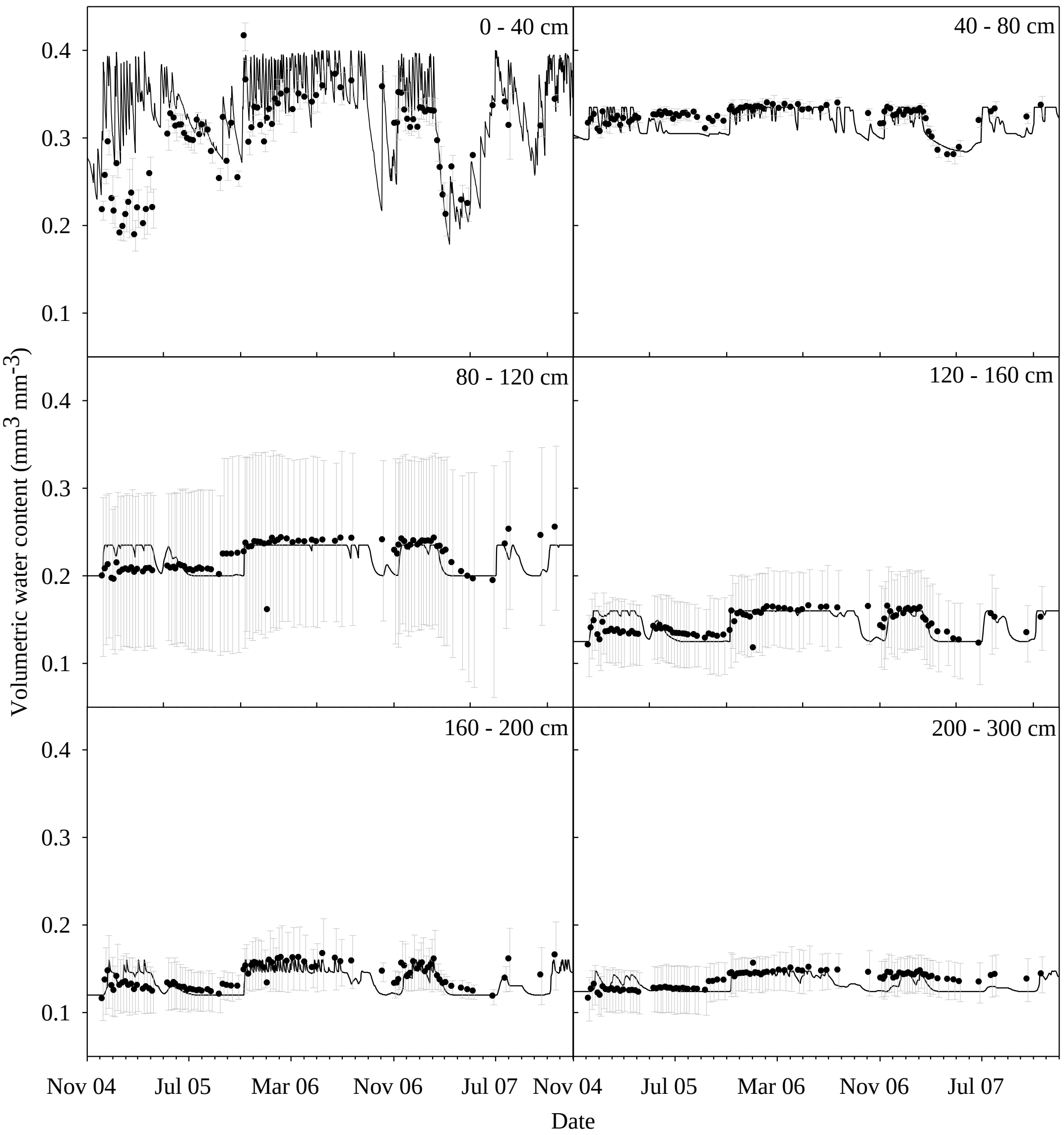

Figure 2: Observed (●), with associated standard deviation and predicted (-) volumetric soil water content through time in soil layers of increasing depth.

At all depths, the modification of *flux_eff* to a value of 0.7 improves the fit (RMSE) of APSIM outputs to the measured data, although none achieve values less than $\mathrm{RMSE}_{95\%}$, indicating that the simulated values were not within the 95% confidence interval of the measurements (Table 1). Similarly, the EF statistic for the simulated values were all negative, demonstrating that the simulated values did not describe the pattern in the observed data better than the mean of the observations, but all increased with the change to the mixing coefficient (Table 1). At depths of 1 m, 3 m and 5 m, the value of CD was increased above 1 by decreasing *flux_eff*, indicating that the deviation of the predictions from the mean of the observed values was less than that observed in the measurements. This suggested that the improved model describes the experimental data better than the mean of the measurements. Table 1 also shows that at all depths, except 7 m, the outputs from the original model (*flux_eff* = 1.0) show bias (E and $E_{95\%}$). However, when the changes were applied to the model, the values of E fell within the range of $E_{95\%}$, suggesting the bias is no longer present.

Table 1: Evaluation of model outputs for leaching at 1 m, 3 m, 5 m and 7 m and the differing mixing values for saturated water movement (*flux_eff*), using the methods described in Smith *et al.* (1997).

Depth	*flux_eff*	RMSE	$RMSE_{95\%}$	EF	CD	E	$E_{95\%}$
1 m	1.0	119.83	±13.77	-4.90	0.71	-52.25	±9.67
	0.7	62.97	±13.77	-0.64	2.06	14.94	±9.67
3 m	1.0	123.73	±6.55	-8.84	0.36	-61.26	±35.96
	0.7	86.99	±6.55	-3.87	1.12	-11.58[1]	±35.96
5 m	1.0	121.43	±6.83	-6.27	0.49	-41.16[1]	±51.89
	0.7	89.20	±6.83	-2.92	1.09	0.121	±51.89
7 m	1.0	157.37	±5.04	-11.86	0.19	-95.49	±43.67
	0.7	118.16	±5.05	-6.25	0.45	-37.29[1]	±43.67

[1] Denotes those values for RMSE and E that fall within $RMSE_{95\%}$ and $E_{95\%}$.

Table 1 shows results over the whole simulation. However, if model outputs for the leaching data from a depth of 1 m, for example, are broken down into separate years it is possible to identify where the APSIM simulations show the most difference from the observed values. Table 2 shows that in year 1 of the simulation, the outputs were greatly improved by reducing the mixing coefficient, with both the RMSE and E falling within $RMSE_{95\%}$ and $E_{95\%}$ respectively and EF becoming positive. This suggests that in the first year APSIM output values fell within the 95% confidence interval of the observed, there was no bias in the simulations and the simulated values describe the pattern in the observed data better than the mean of the observations. However, the model did not perform well in the second and third years (Table 2).

The modified APSIM setup showed an improved adherence to the data for soil mineral N over the entire simulation (RMSE = 75.97) compared with the original setup (RMSE = 80.25). However, neither fell within the 95% confidence interval of the data ($RMSE_{95\%}$ = 62.49). In addition, the bias was removed in the sample by reducing *flux_eff* (E = 46.86, $E_{95\%}$ = ± 51.38) compared with the original setup (E = 57.94, $E_{95\%}$ = ± 51.38). Figure 3 shows that from March 2004 the simulation outputs, both original and modified, underestimate soil mineral N. This may be due to APSIM under-predicting the rate of mineralisation. This is most evident in autumn-winter 2004 and to a lesser extent 2006 when no fertiliser was applied and measured soil mineral N increased substantially more than that predicted (Figure 3).

Table 2: Evaluation of model outputs for leaching at 1 m in years 1, 2 and 3 and the differing mixing values for saturated water movement (*flux_eff*), using the methods described in Smith *et al.* (1997). Note a year is taken to run from 1 September to 31 August.

Year	*flux_eff*	RMSE	$RMSE_{95\%}$	EF	CD	*E*	$E_{95\%}$
1	1.0	85.88	±39.58	-1.33	0.20	-47.89	±28.42
	0.7	33.62[1]	±39.58	0.64	0.78	27.01[1]	±28.42
2	1.0	763.85	±29.28	-58.85	0.02	-1529.93	±39.77
	0.7	711.41	±29.31	-50.94	0.02	-1589.43	±39.77
3	1.0	92.93	±28.02	-1.42	0.51	84.45	±22.46
	0.7	112.65	±28.02	-2.51	0.38	94.61	±22.46

[1] Denotes those values for RMSE and *E* that fall within $RMSE_{95\%}$ and $E_{95\%}$.

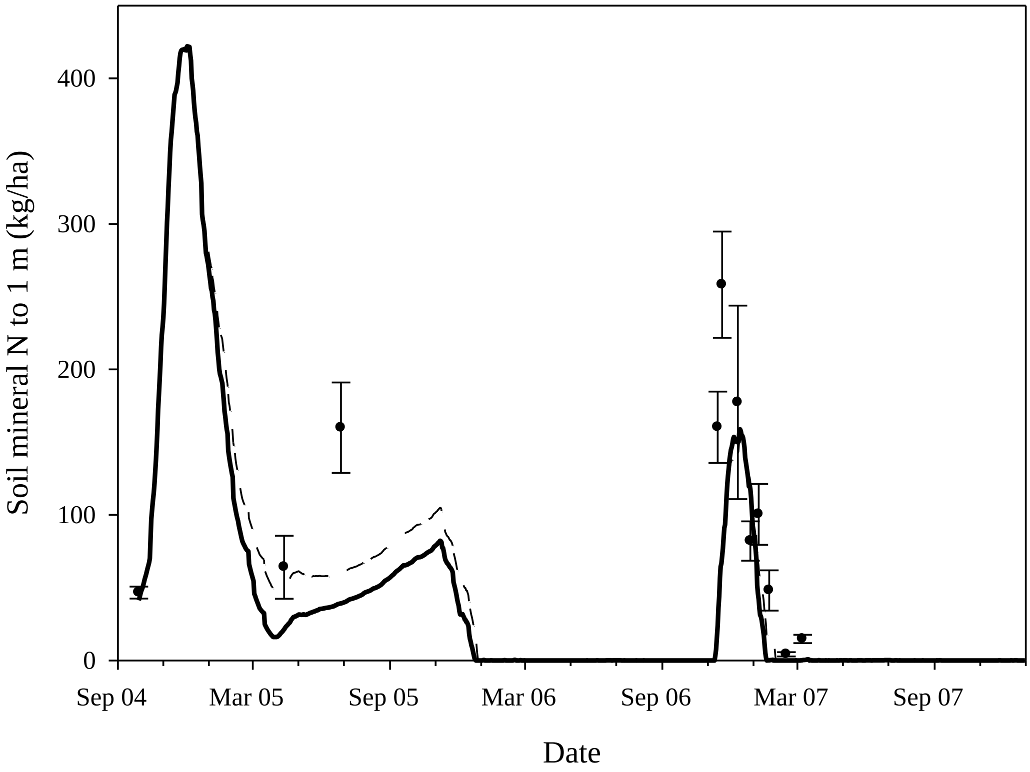

Figure 3: Observed (●), with associated standard deviation, predicted original (-) and predicted modified (--) soil mineral nitrogen to 1 m through time.

The underestimation in the rate of mineralisation by APSIM may have resulted in the poor estimation of ryegrass harvested. This can be seen in Figure 4 which shows the growth limiting factor due to N stress for ryegrass. It shows that through the majority of the ryegrass ley the plants are experiencing N stress. To assess how APSIM would have performed if it had have predicted higher rates of mineralisation APSIM was re-run including a rule that added 2 kg ha^{-1} nitrate to the top layer of soil when the total amount of nitrate in the top 1 m of soil fell below 5 kg ha^{-1}. This ad hoc rule bears no relationship to mineralisation processes but has the same overall effect of mineralisation, putting more mineral N into soil solution. Putting this additional N into the system decreased the N stress the ryegrass experienced (Figure 4) and increased APSIM's estimated total harvest to 29,748 kg ha^{-1}, giving much better agreement to observed values (30,213 kg ha^{-1}). The change had no significant effect on the soil water content, both throughout the whole profile and in the top layer. As an example, figure 5 demonstrates this in the top layer (0-400 mm) over several months in the spring-summer 2005-06. In addition there was no significant change to estimations of soil nitrate nitrogen or leaching.

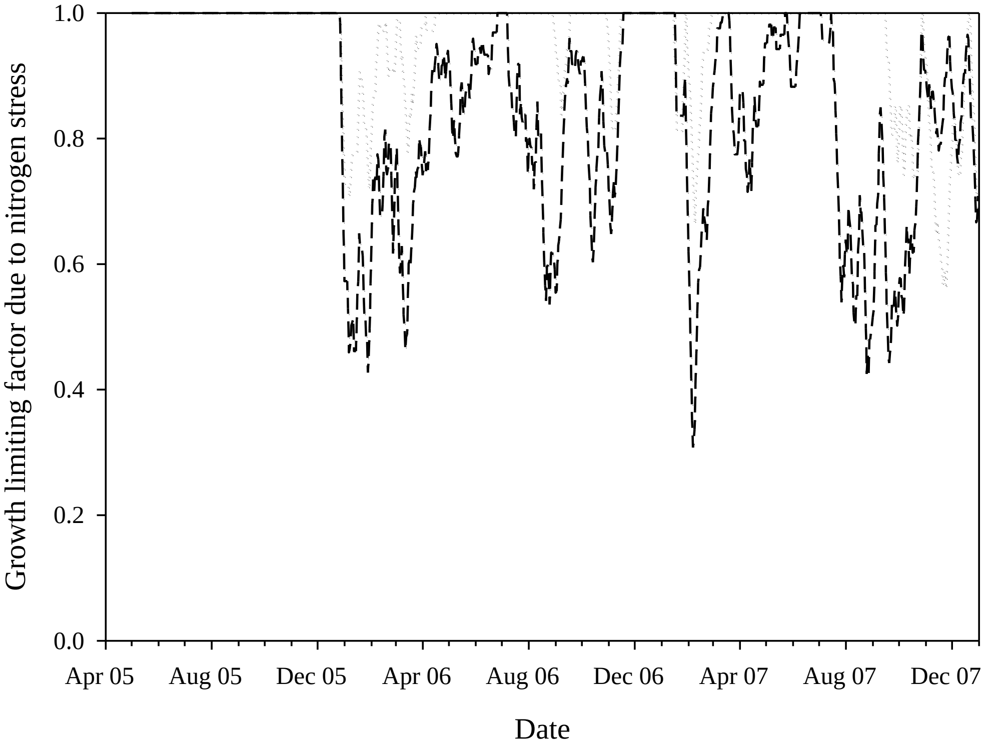

Figure 4: Ryegrass growth limiting factor, due to nitrogen stress, through time. Predicted modified (--) and predicted modified with the additional nitrate fertiliser (···). Note values less than one indicate nitrogen stress

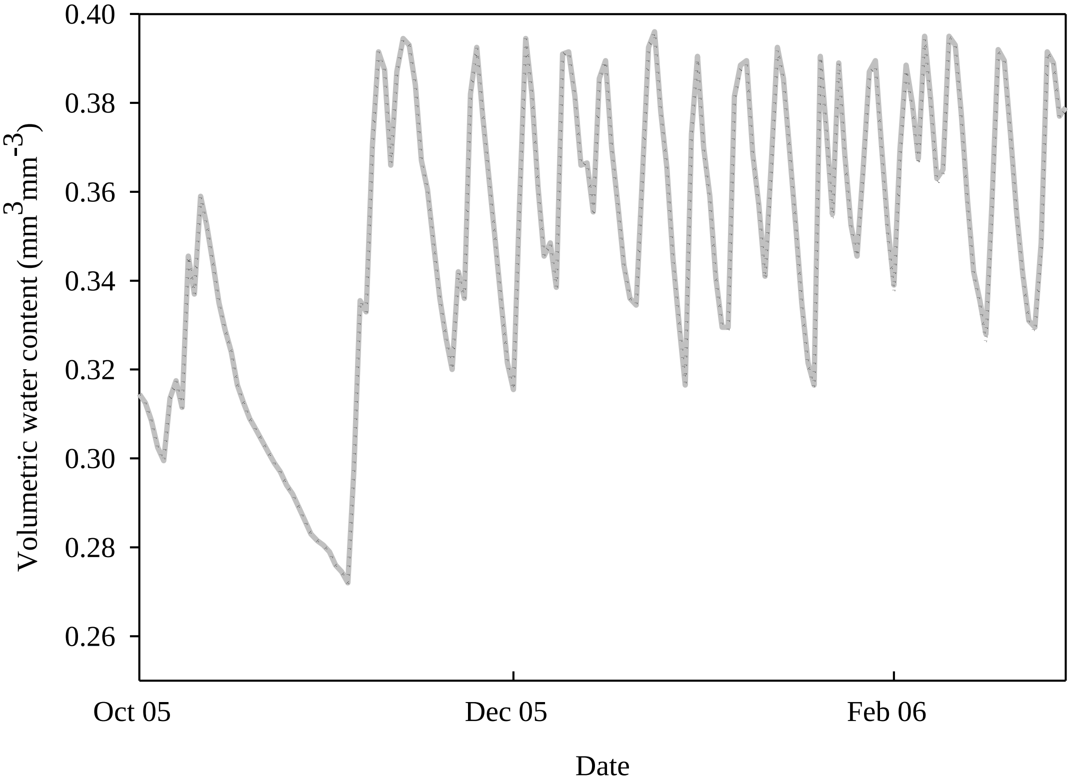

Figure 5: Volumetric soil water content through time in the 0-400 mm soil layer for predicted modified (grey –) and predicted modified with the additional nitrate fertiliser (⋯).

Discussion

Results show that APSIM accurately simulated potato yield, while it gives a poor approximation of ryegrass yield. The simulations conducted in this paper and later modifications to the model suggests this was due to the underestimation of soil mineral N in the final 2 years of the simulation. This caused the ryegrass model to predict N stress and substantially reduced its yield predictions.

Confidence can be placed in APSIM's estimates of drainage. APSIM gave a good prediction of soil water content in all layers except in the top layer when under the potato crop (Figure 2). Through all of the soil layers, APSIM simulations track the observed data through time and respond accordingly to the increases and decreases in soil water content with the wetting and drying of soil (Figure 2). The estimations of soil water content changed very little when ryegrass biomass production was increased to values similar to those observed in the field experiment by the addition of N. Given that there is confidence in the irrigation and rainfall data inputs and the soil water content is well approximated by APSIM simulations, it can be inferred that drainage from the system is simulated appropriately.

The primary source of N loss from the system was nitrate leaching. With the original setup, predictions of annual leaching in the first year exceed the observed. However, when the solute mixing efficiency factor (*flux_eff*) is reduced to a value of 0.7, as in Sharp *et al.* (2011), a slightly improved fit to the experimental leaching data is achieved (Table 2). When examined on a year-on-year basis an improved fit to leaching data is only seen in the first year and there is a very poor fit in the second and final years of the trial (Table 2). This is similar to the findings in Sharp *et al.* (2011) who found the reduction in *flux_eff* fixed an over prediction of leaching in the first year of simulations but left an under prediction of leaching in subsequent years. The agreement in these two sets of findings provides some verification that the *flux_eff* parameter should be set to 0.7 to give accurate leaching predictions in free draining alluvial soils in Canterbury, however further testing is required.

APSIM underestimates mineral N after the first year of simulations (Figure 3). This is particularly evident during the autumn and winter months, where measured mineral N is increasing. This suggests that mineralisation of organic N is occurring. However, in both the original and modified simulations, APSIM underestimates both the amount and rate of mineralisation. This is consistent with the findings of other authors who have suggested that APSIM may underestimate N mineralisation at lower temperatures (Lilley *et al.*, 2003; Verburg *et al.*, 2007; Sharp *et al.*, 2011). APSIM's SoilN module, which controls carbon and N dynamics within APSIM, was initially parameterised and tested in tropical-subtropical Australia (Probert *et al.*, 1995; Probert *et al.*, 1998) and consequently may not perform as well in cooler temperate climates. It is therefore recommended that SoilN and the subsequent rates of N mineralisation in APSIM are validated in both temperate and non-temperate climates to ensure better approximation of soil N dynamics.

In conclusion, APSIM was successful at simulating the N balance of this crop rotation in the first year only. Analysis showed that APSIM over-estimates the leaching of mineral N through the soil profile and when adjustments are made, estimates of leaching are much improved in the first year. Further analysis suggested the poor performance of the N balance in the final 2 years was due to underestimates in N mineralisation within APSIM and further work is required to adapt APSIM to New Zealand conditions.

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