

Comparison of models for predicting nitrification, denitrification and nitrous oxide emissions in pastoral systems

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Abstract: Intensification of agricultural systems has resulted in remarkable increases in productivity. However in grazed systems only about 10-20% of the N ingested by grazing animals is retained in animal products. The remainder is returned in excreta to the paddock in a spatially non-uniform fashion as dung and urine and then either accumulates in the soil or is lost via leaching or gaseous emissions. The amount of N lost from these patches via leaching and gaseous emissions is highly dependent on site-specific factors. Routine direct measurements are impractical given the scale and variability so simulation models are an essential alternative to estimate likely N losses. Various simulation approaches are in use or are being developed to predict N leaching and N₂O emissions. The models vary in the level of detail or number of nitrogen pools and transformation processes considered, as well as on how the processes are described. Other processes within the models, such as water and heat transport within the soil also affect the modelled N transformations and losses. While most models have been tested and validated for some processes or outputs in a particular range of systems, soils and climates, there is a lack of information on how models compare in other aspects. We discuss key differences and similarities between the N transformation components of the APSIM and DNDC models with respect to their simulation of nitrification, denitrification and N₂O emissions under pastoral systems.

Agreement between daily N₂O emissions from urine patches simulated by APSIM and DNDC was variable, Figure 1. For the Horotiu soil the index of agreement (IA) between measurements and APSIM or DNDC were 0.4 and 0.13, and for the Templeton soil 0.77 and 0.47. Agreement between total emissions over the experimental period was better for the APSIM model than the DNDC, based on default model parameters. For the Horotiu soil, N₂O emissions over 3 months were 4.9 kg/ha, and simulations with APSIM and DNDC gave values of 7.4 and 13.7 kg/ha. For the Templeton soil over 1 year measurements were 2.8 kg/ha and simulations with APSIM 1.9 kg/ha and with DNDC 16.3 kg/ha. Adjusting default values to NZ conditions can, however, improve the prediction capacities of the models.

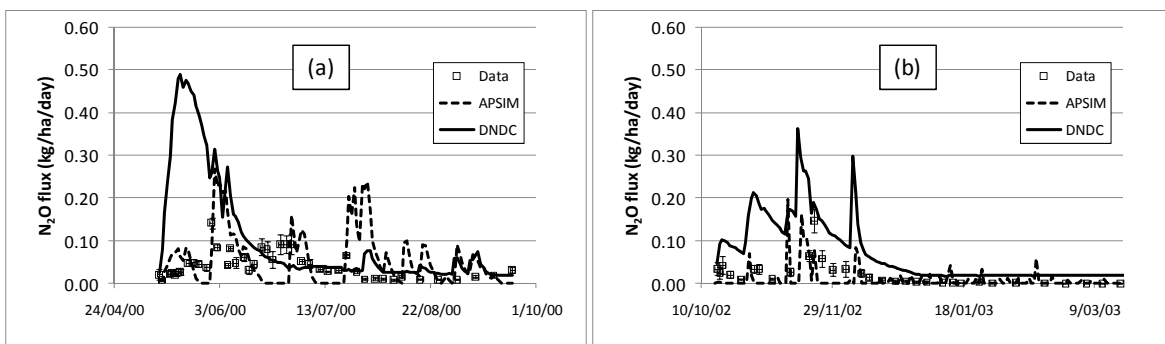


Figure 1. Measured and simulated N₂O emission from a urine patch by APSIM and DNDC a) Horotiu silt loam over 4 months and b) Templeton silt loam over 1 year from New Zealand (data taken from de Klein et al., 2003)

Keywords: APSIM, DNDC, nitrous oxide, nitrification, denitrification

1. INTRODUCTION

Nitrogen cycling in terrestrial ecosystems is complex and includes microbial processes such as mineralisation, nitrification and denitrification, plant physiological processes (nitrogen uptake and assimilation) and physicochemical processes (leaching, volatilisation). These various processes are affected by environmental conditions such as soil oxygen and moisture contents, temperature, mineral N content, available carbon and pH. The complexity of these various interconnected processes combined with a large spatial and temporal variation in transformation rates involved in nitrogen cycling processes bedevils quantification of N losses via leaching, volatilisation and nitrous oxide (N₂O) emissions from all agricultural systems but is particularly challenging in pastoral systems because the grazing ruminants effectively redistribute the nitrogen from the plants into high-concentration excreta patches. The resulting heterogeneity in the soil-plant system means that whole paddocks cannot appropriately be modelled at a process level using paddock averages.

Various models have been developed that integrate process-based knowledge of nitrogen and carbon cycling in the soil-plant atmosphere continuum. Such models offer the potential to decipher the contribution of individual components to the total system and can help to better understand how environmental conditions combined with management strategies interact to control nitrogen cycling and N losses. Inter-model comparison offers another possibility for better understanding the complex and interacting processes.

The Agricultural Production Systems Simulator, (APSIM; Keating *et al.*, 2003), and DeNitrification DeComposition, (DNDC; Li *et al.*, 1992) are models that provide process-level descriptions of nitrogen cycling and provide, besides many other outputs, daily values for N transformation rates and losses. These two models have different strengths in scale and loss pathways. APSIM has been developed to simulate the biological and physical processes in farming systems, initially with an emphasis on cropping systems, but lately also for pasture systems with the possibility of simulating at the urine patch as well as multi-paddock scale (Li *et al.*, 2010; Vogeler *et al.*, 2010). DNDC model has been initially developed for simulating N₂O, CO₂ and N₂ emissions and denitrification from cultivated and grassland sites, but later improved for simulation water flow and nitrate leaching (Li *et al.*, 2006) and other systems such as perennial pastures and N₂O emissions from dairy-grazed pasture in New Zealand (Saggar *et al.*, 2004). In both models, processes such as nitrification and denitrification are represented as functions of nitrogen and available carbon, and modified by dimensionless factors for soil water content and temperature. The description of N transformations in these two models is, however, conceptually different. While in APSIM the processes of nitrification and denitrification are described via empirical reaction equations, expressed via a Michaelis-Menten type equation, DNDC is a microbial growth model.

The objective of this model comparison is to identify primary differences in simulated nitrogen transformation rates in soils under varying environmental conditions including temperature, soil water content, soil organic carbon, pH, and initial NH₄ and NO₃ concentration. To begin, a short description of the two models is given. To eliminate the effect of water flow on these transformation processes simulations were first done under static conditions. In the second comparison rainfall and drainage were included. Finally model predictions were compared to published laboratory and field measurements.

2. MODEL DESCRIPTION AND SIMULATION SETUP

2.1. APSIM

APSIM is a framework of biophysical modules that simulate biological and physical processes in farming systems (Keating *et al.*, 2003). The SoilN module simulates the dynamics of N and C on a daily time-step in soil layers, with C and N mineralisation, C and N immobilisation, N nitrification, N denitrification and nitrate and ammonium adsorption and movement explicitly described in each layer. These N processes are controlled by soil water content, temperature and pH and water flow which are simulated within either the SoilWat (Probert *et al.*, 1998) or SWIM (Verburg *et al.*, 1996) modules. For all simulations APSIM Version 7.4 was used.

2.2. DNDC

DNDC consists of several sub-models for simulating thermal-hydraulic flows, plant growth, aerobic decomposition, fermentation and denitrification. The model usually operates on a daily time-step, except following a rainfall event where denitrification is calculated on an hourly time-step. To allow nitrification and denitrification to occur simultaneously in aerobic or anaerobic microsites, a dynamic 'anaerobic balloon' balloon' is used (Li *et al.*, 2000). Substrates such as carbon, NH₄ and NO₃ are split into aerobic and

anaerobic soil micro-sites. The NZ-DNDC (Saggar *et al.*, 2007), a modification of DNDC (Version 8.6K) was used within this model comparison.

2.3. N transformations simulations in uniform soil

To compare N transformations from the two different simulation approaches, APSIM and DNDC, simulations were set up with uniform soil under a range of static environmental conditions. The soil was a bare sandy loam with a depth of 200 mm. The bulk density of the soil was 1 Mg m^{-3} , total porosity was 59%, θ at field capacity and permanent wilting point was 0.43 and $0.23 \text{ m}^3 \text{ m}^{-3}$ and the C:N ratio of the humus fraction was 12. Factors that were changed included water flow regime (either static or dynamic), the initial concentration of NH_4 (100 or 500 kg/ha) with 10 kg NO_3 /ha, or 1 kg NH_4 /ha with 100 kg NO_3 (uniform within the soil), θ of 0.3, 0.45, and $0.55 \text{ m}^3 \text{ m}^{-3}$, soil temperature of 10, 15 and 30°C , soil organic carbon content of 3 and 6%, pH of 6 and 8, with or without rainfall of either 20 mm on day 1, or at 5 mm/day. The simulations were run for 10 days and simulation output included cumulative and daily values of nitrification, denitrification, and N_2O and N_2 emissions.

2.4. Nitrification simulation - comparison against measurements

Nitrification simulated with APSIM and DNDC were compared to two incubation studies done under controlled conditions in a silt loam (Di and Cameron, 2004) and a loam and clay loam (Rovita and Killorn, 2007). The nitrification was inferred from the temporal decrease of NH_4 in the soil.

2.5. Simulation of N_2O emissions from urine patches-comparison with measured N_2O data

APSIM and DNDC were used to simulate N_2O emissions following urine application to two different soil types in two different seasons. The simulations were compared to selected experimental results, described in detail by de Klein *et al.* (2003). In short, the selected experiments were done in the Waikato region of New Zealand on a free draining Horotiu silt loam and in the Canterbury region on a moderately drained Templeton silt loam. Urine, at a concentration of about 600 kg/ha, was applied in autumn 2000 to the Horotiu soil and in spring 2002 to the Templeton soil.

2.6. Statistical analysis

To evaluate the agreement between simulation results of APSIM and DNDC, as well as between the models and measurements the correlation coefficient and the Index of Agreement (IA) proposed by (Willmott *et al.*, 1985) as an alternative to correlation coefficients. IA is a relative and varies between 0 for no agreement at all and 1 for a perfect match.

3. RESULTS

3.1. N transformations simulations in uniform soil

Nitrification

Nitrification of the initial NH_4 (NH_4ini) in the soil as simulated by APSIM and DNDC were quite different with a high initial nitrification rate and a steep decline in NH_4 simulated by DNDC and a relatively constant nitrification rate over the 10 day simulation run for APSIM. This is shown in Figure 2a for a simulation run under static conditions, a temperature of 10°C and NH_4ini of 500 kg/ha. In general, the agreement improved with decreasing NH_4ini and increasing temperature (Figure 2b). This is mainly due to a much greater response of APSIM to temperature, as can be seen from the simulated nitrification of NH_4 of 30 kg/ha over a period of 10 days (Figure 3a) with the 12 combinations of factors (pH, OC, θ). In contrast DNDC reacted more strongly to θ , showing decreasing nitrification with increasing θ over the range of water contents studied (Figure 3b). DNDC also showed a reduction in nitrification rate as pH increased from 6 to 8 (data not shown), whereas that pH range is considered to be uniformly optimal with APSIM's default settings.

Denitrification

Denitrification from the simulations done under dynamic conditions and with an initial NO_3 concentration of 100 kg/ha shows increasing rates with time for DNDC, while decreasing rates for APSIM (Figure 4). For denitrification DNDC shows a stronger influence of temperature and organic carbon than does APSIM (Figure 5). While in APSIM denitrification only occurs at $\theta \geq$ field capacity, and thus equals zero in the simulations done at θ of 0.3, in DNDC denitrification is triggered by rainfall \geq 5 mm.

N₂O emissions

Simulated N₂O emissions from DNDC and APSIM show a similar trend as did denitrification, with an increasing rate for DNDC and a slightly decreasing rate for APSIM over the 10 days (Figure 4b). Similar to denitrification DNDC shows a larger response to temperature and organic carbon content (data not shown).

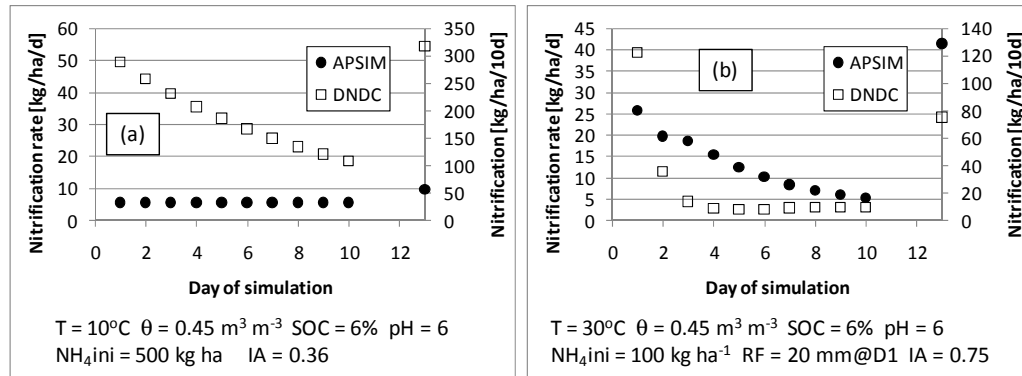


Figure 2. Nitrification rate simulated by APSIM and DNDC over 10 days in a silt loam under a) static conditions and b) a rainfall event of 20 mm on day 1. Also shown, on the right axis, is the total nitrification over 10 days.

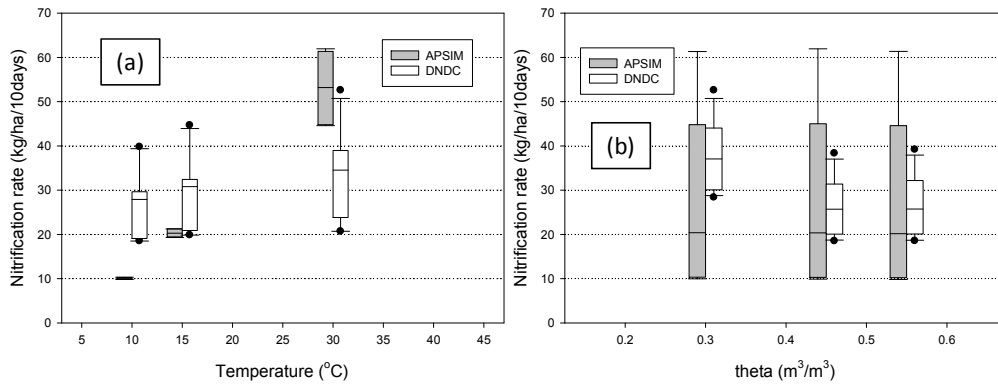


Figure 3. Nitrification over 10 days as simulated by APSIM and DNDC for a sandy loam with an initial NH₄ of 30 kg/ha under dynamic conditions as influenced by a) temperature and b) soil water content. The boxes show the 25th, 50th, and 75th percentiles, and the whiskers the 5th and 95th percentiles model outputs from 12 different combinations of a) pH, OC and θ and b) pH, OC, and T.

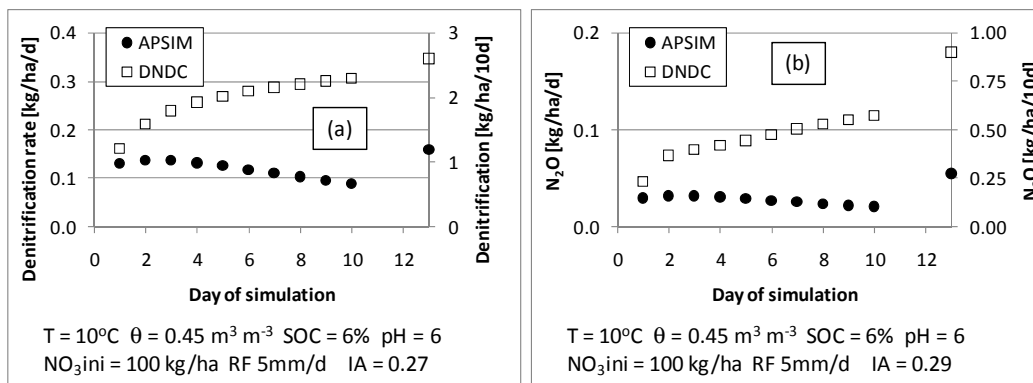


Figure 4. a) Denitrification rate and b) N₂O emission simulated by APSIM and DNDC over 10 days in a silt loam with a rainfall of 5 mm/day.

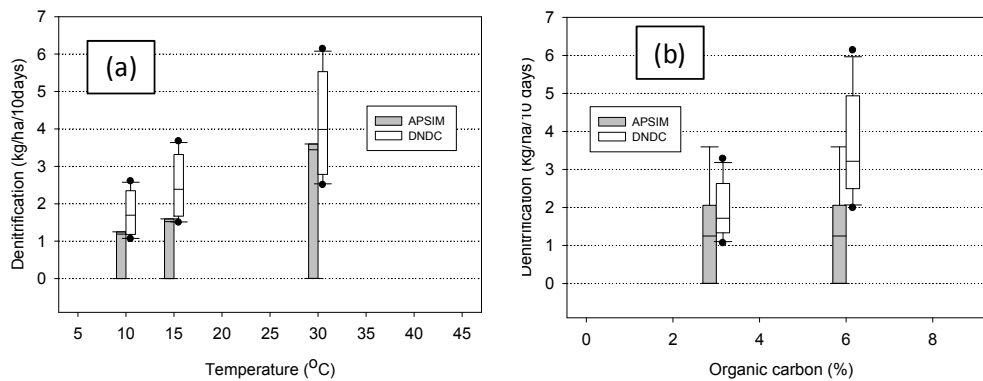


Figure 5. Denitrification over 10 days as simulated by APSIM and DNDC for a sandy loam under dynamic conditions as influenced by a) temperature and b) soil organic carbon content as influenced by a) temperature and b) soil organic carbon content (SOC). Each temperature and organic carbon content comprises model outputs from 12 different combinations of a) pH, OC and θ and b) pH, θ , and T.

3.2. Nitrification simulation - comparison with measured data

Neither of the models showed a close agreement with the nitrification data. The closest agreement between models and data was for APSIM compared to the Di and Cameron (2004) data at 20 °C and the Rovita and Killorn (2007) loam data (Figure 6). APSIM badly under predicted nitrification at 8 C (Figure 6a) and had the wrong direction of response to the clay compared to the loam soil (Figure 6b). DNDC consistently over-predicted nitrification rates and showed little effect of NH_4 concentration, soil or temperature on the nitrification rate. (Figure 6).

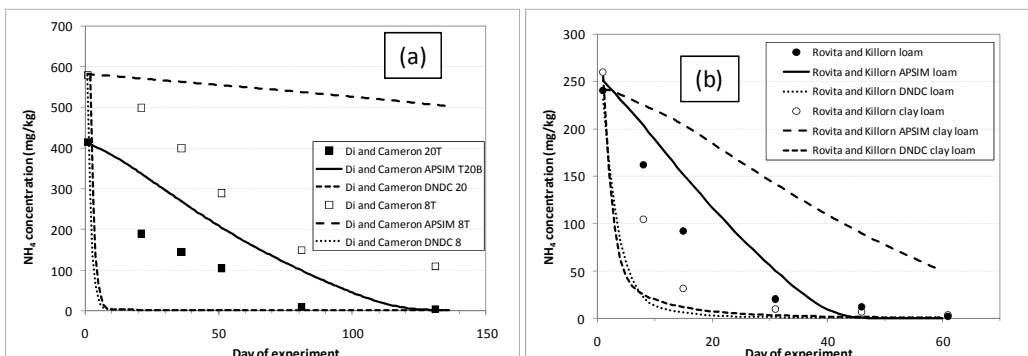


Figure 6. Comparison of measured and simulated nitrification by APSIM and DNDC for a) a silt loam from New Zealand (Di and Cameron, 2004) and b) a loam and clay loam from Iowa, USA (Rovita and Killorn, 2007).

3.3. Simulation of N_2O emissions from urine patches - comparison with measured N_2O data

Agreement between N_2O emissions simulated by APSIM and measured from urine patches on the Horotiu soil was reasonably good considering the large variability in measured values (Figure 1 and Table 1). While the simulation of the variation in N_2O emissions with time is not as good, with low IA's (Table 1) the agreement of the total N_2O emission over the period of about 4 months is reasonably good. Measured emissions ranged from 3.9 – 6.4 kg/ha and were slightly higher at 7.4 kg/ha for APSIM. For the simulations it was assumed that the N_2O produced within the top 200 mm is released into the atmosphere, as suggested by Li *et al.* (2007) for denitrification. The agreement between N_2O emissions measured and predicted by DNDC is very poor for the Horotiu soil, with total emissions of 13.7 kg/ha, more than double the measured amount and a large surge shortly after urine application. For the Templeton soil the agreement between APSIM and measurement was better for both the IA and the total N_2O emission, with measurements ranging from 1.7 to 4.6 kg/ha and APSIM simulation of 1.9 kg/ha. DNDC, using default parameters, again over-predicted emissions, but the daily trend in N_2O emission was similar to the measured data, indicated by the higher IA for the Templeton soil than the Horotiu soil.

The question arises why APSIM and DNDC show a similar trend in N₂O emissions from urine patches for the Templeton soil, but a large initial discrepancy for the Horotiu soil, especially shortly following urine application. Initial nitrification under the urine patches is, as suggested from the results presented above, higher in DNDC than APSIM, due to both the high initial NH₄ concentration and the average temperatures of 13 (Horotiu) and 11.8°C (Templeton) within the first 14 days. Denitrification is also likely to be higher in DNDC compared with APSIM (Figure 5), but more similar for the Templeton soil with an organic carbon content of 3%, compared with the Horotiu soil with an OC of 5.8%. However more analysis is required to fully understand the interactions between nitrification and denitrification, and the many other interconnected processes that affect the fate of N in pastoral systems, including volatilisation, movement of NO₃ and NH₄ in the soil, and their uptake by plants, as well as the partitioning of the denitrified N into N₂ and N₂O, and how this finally influences N₂O production and emissions as simulated by APSIM and DNDC.

Table 1. Comparison of measured (average and range), and simulated gaseous N emissions from a urine patch by APSIM and DNDC for a Horotiu silt loam over 4 months and a Templeton silt loam over 1 year from New Zealand (de Klein *et al.*, 2003) with units of kg/ha.

	N ₂ O					N ₂ /N ₂ O	NH ₃	
	measured	APSIM (20cm)	DNDC (50 cm)	IA APSIM	IA DNDC	DNDC	APSIM	DNDC
Horotiu	4.9 (3.9-5.1)	7.4	13.7	0.4 (0.37-0.48)	0.13 (0.09-0.19)	19.0	4.6	28.8
Templeton	2.8 (1.7-4.6)	1.9	16.3	0.77 (0.64-0.83)	0.47 (0.31-0.67)	20.2	7.7	18.8

4. CONCLUSIONS

This paper presents a comparison of the two different models, APSIM and DNDC to simulate nitrogen transformation rates, including nitrification, denitrification and N₂O emissions in soils. The comparison included simulation done in uniform soils under static and dynamic conditions, as well as comparison to measured data from published laboratory and field data.

The APSIM- and DNDC-simulated nitrification and denitrification rates over 10 days were quite different. While in APSIM temperature had a larger effect on nitrification, in DNDC the NH₄ concentration and the soil water content had more effect. Denitrification DNDC shows a stronger influence of temperature and organic carbon than does APSIM, and in DNDC is triggered by rainfall whereas in APSIM by soil water content. The agreement between simulated nitrification rates and measured data shows variable results. In general DNDC largely over-predicts the measured nitrification rate. APSIM simulations agree under some environmental conditions with measurements but not in others. The comparisons suggest further work is required to better understand the influence of soil organic matter and allophone content on nitrification rates.

Agreements between measured and simulated N₂O emissions from urine patches were reasonably good, especially considering that the models were run with default parameter values. Agreement between total emissions over the experimental period was better for the APSIM model than the DNDC. For the Horotiu soil, N₂O emissions over 3 month were 4.9 kg/ha, and simulations with APSIM and DNDC gave values of 7.4 and 13.7 kg/ha. For the Templeton soil over 1 year measurements were 2.8 kg/ha and simulations with APSIM 1.9 kg/ha and with DNDC 16.3 kg/ha.

In conclusion it should be stressed that for both models only default values for the many model parameters were used. Fine tuning of model parameter values based on measurements and improved understanding is likely to increase the prediction capability of the models, and maybe also the agreement between the two models. For example the model performance could be improved for APSIM by increasing the nitrification rate based on the soil organic carbon content (Snow *et al.*, 2011), and for DNDC by altering the partitioning of the soil organic carbon and increasing the volatilisation rate (Giltrap *et al.*, 2010).

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REFERENCES

- De Klein, C., Barton, L., Sherlock, R.R., Li, Z., and Littlejohn, R.P., 2003, Estimating a nitrous oxide emission factor for animal urine from some New Zealand pastoral soils.: *Australian Journal of Soil Research*, v. 41, p. 381-399.
- Di, H.J., and Cameron, K.C., 2004, Effects of temperature and application rate of a nitrification inhibitor, dicyandiamide (DCD), on nitrification rate and microbial biomass in a grazed pasture soil.: *Australian Journal of Soil Research*, v. 42, p. 927-932.
- Giltrap, D.L., Singh, J., Saggar, S., and Zaman, M., 2010, A preliminary study to model the effects of a nitrification inhibitor on nitrous oxide emissions from urine-amended pasture: *Agriculture, Ecosystems and Environment*, v. 136, p. 310-317.
- Keating, B., Carberry, P., Hammer, G., Probert, M., Robertson, M., Holzworth, D., Huth, N., Hargreaves, J., Meinke, H., Hochman, Z., McLean, G., Verburg, K., Snow, V., Dimes, J., Silburn, M., Wang, E., Brown, S., Bristow, K., Asseng, S., Chapman, S., McCown, R., Freebairn, D., and Smith, C., 2003, An overview of APSIM, a model designed for farming systems simulation: *European Journal of Agronomy*, v. 18, p. 267-288.
- Li, C., Aber, J., Stange, F., Butterbach-Bahl, K., and Papen, H., 2000, A process-oriented model of N₂O and NO emissions from forest soils: 1. Model development: *Journal of Geophysical Research D: Atmospheres*, v. 105, p. 4369-4384.
- Li, C., Farahbakhshazad, N., Jaynes, D.B., Dinnes, D.L., Salas, W., and McLaughlin, D., 2006, Modeling nitrate leaching with a biochemical model modified based on observations in a row-crop field in Iowa.: *Ecological Modelling*, v. 196, p. 116-130.
- Li, C., Frolking, S., and Frolking, T.A., 1992, A model of nitrous oxide evolution from soil driven by nitrous oxide evolution from soil driven by rainfall events. Model structure and sensitivity.: *Journal of Geophysical Research*, v. D9, p. 9776-9799.
- Li, F.Y., Snow, V.O., Holzworth, D.P., and Johnson, I.R., 2010, Integration of a pasture model into APSIM, Proceedings of the 13th Australian Agronomy Conference, Lincoln, New Zealand (www.regional.org.au/au/asa/2010/farming-systems/simulation-decision-support/6993_lifyrevis.htm). Joint New Zealand - Australian Agronomy Society Conference, November 2010: Lincoln, New Zealand.
- Li, Y., White, R., Chen, D., Zhang, J., Li, B., Zhang, Y., Huang, Y., and Edis, R., 2007, A spatially reference water and nitrogen management model (WNMM) for (irrigated) intensive cropping systems in the North China Plain: *Ecological modelling* v. 203, p. 395-423.
- Probert, M.E., Dimes, J.P., Keating, B.A., Dalal, R.C., and Strong, W.M., 1998, APSIM's water and nitrogen modules and simulation of the dynamics of water and nitrogen in fallow systems: *Agricultural Systems*, v. 56, p. 1-28.
- Rovita, D., and Killorn, R., 2007, Kinetics of nitrification in selected Iowa soils treated with Stay-N 2000: *Communications in Soil Science and Plant Analysis*, v. 38, p. 1949-1963.
- Saggar, S., Andrew, R.M., Tate, K.R., Hedley, C.B., Rodda, N.J., and Townsend, J.A., 2004, Modelling nitrous oxide emissions from dairy-grazed pastures: *Nutrient Cycling in Agroecosystems*, v. 68, p. 243-255.
- Saggar, S., Giltrap, D.L., Li, C., and Tate, K.R., 2007, Modelling nitrous oxide emissions from grazed grasslands in New Zealand.: *Agriculture Ecosystems and Environment*, v. 119, p. 205-216.
- Snow, V.O., Shepherd, M.A., Cichota, R., and Vogeler, I., 2011, Urine timing: Are the 2009 Waikato results relevant to other years, soils and regions?, *in* Currie, L.D., and Christensen, C.L., eds., *Adding to the Knowledge Base for the Nutrient Manager*. <http://flrc.massey.ac.nz/publications.html>. Occasional Report No. 24. Fertilizer and Lime Research Centre, Massey University, Palmerston North, New Zealand, p. 14.
- Verburg, K., Ross, P.J., and Bristow, K.L., 1996, SWIMv2.1 User Manual. Divisional Report No 130: Canberra, Australia, CSIRO Division of Soils, 107 p.
- Vogeler, I., Cichota, R., Snow, V.O., Muirhead, R., and De Klein, C., 2010, A modelling analysis to determine N-risk indicators, *in* Edwards, G.R., and Bryant, R.H., eds., *Australasian Dairy Science Symposium: Christchurch, NZ*, p. 221-224.
- Willmott, C.J., Ackleson, S.G., Davis, R.E., Feddema, J.J., Klink, K.M., Legates, D., R., O'Donnell, J., and Rowe, C.M., 1985, Statistics for the Evaluation and Comparison of Models: *Journal Geophysical Research*, v. 90, p. 8995-9005.