# SOILPH - A NEW APSIM MODULE FOR MANAGEMENT OF SOIL ACIDIFICATION

Z.Hochman<sup>1</sup>, S. Braithwaite<sup>1</sup>, M.E. Probert<sup>1</sup>, K. Verburg<sup>2</sup> and K.R. Helyar<sup>3</sup>

<sup>1</sup>CSIRO Tropical Agriculture/APSRU, <sup>2</sup>CSIRO Land and Water, <sup>3</sup>NSW Agriculture.

## Abstract

APSIM (Agricultural Production Systems Simulator) is a software system that can be flexibly configured to simulate diverse production systems. The new SOILpH module adds to the capabilities of APSIM by: 1) Employing a proton budgeting framework which tracks the production and consumption of protons, weak acids and alkalis in the N and C cycles; 2) Calculating the flow of protons into, and out of, soil layers by incorporating elements of the SPAM (Soil Profile Acidification Module) model; 3) Using empirical functions to calculate pH buffer capacity and pH-AI relationships and; 4) Using standard solubility constants to allow for reactions of  $CO_2$ ,  $CaCO_3$ , AI silicates and others. With the SOILpH module, APSIM has the capability to calculate the rate and distribution of acidification in cropping systems. This development allows APSIM to be used as a modelling framework for research and management of soil acidification.

### Key words: Soil acidification, modelling, soil pH, pH buffering, aluminium, cropping systems.

Soil acidification is a major threat to sustainability of Australian agriculture where 35 million ha are highly acidic with pH 4.8, and a further 55 million ha have the a potential to degrade to that level (1). In many agricultural systems the most important components contributing to acidification are loss of nitrate via leaching, changes in soil organic matter content and product removal (6).

This paper provides a description of a cropping system model with a capability for simulating soil acidification. This capability was achieved by integrating an agricultural systems simulation model with other calculation methods and stand-alone models currently employed in acidification studies.

Helyar and Porter (6) developed a proton budget framework for tracking the production and consumption of protons. This conceptual model is useful for determining the relative importance of the various acidifying processes in different agricultural systems and environments (3, 4, 11). Its usefulness has to this date been restricted due to three limitations:

• Long-term data on the change in soil pH and the pH buffer capacity are required to calculate the total acidification of an agricultural system.

• Nitrate leaching cannot be reliably measured, especially in long-term experiments. It is therefore calculated by difference, which assumes that all acidification that cannot be accounted for by other processes is due to the nitrification of ammonium followed by nitrate leaching with a strong alkali cation.

• Changes in pH buffer capacity over time are ignored as acid added over a period of time can be estimated by the term (delta pH \* final pHBC) where measured data are available for these terms. However, to simulate acidification through time, when the levels of organic matter or soluble aluminium change over the period of study, it is necessary to be able to simulate change in pHBC in response to such changes.

APSIM (Agricultural Production Systems Simulator) is a software system that allows models of crops, pastures, trees, soil water, nutrients (N), and erosion to be flexibly configured to simulate diverse production systems (10). APSIM already had the capability to simulate the major processes that contribute to soil acidification: the soil nitrogen (SoilN) module describes urea hydrolysis, mineralisation, immobilisation, nitrification and denitrification (12); nitrogen (N) uptake is simulated by the crop modules; N transport and leaching is simulated by the water balance modules Soilwat (12) or SWIM [Soil Water Infiltration Movement (15)] and the decomposition of residues is calculated by the residue module,. Combining the Helyar and Porter framework with the APSIM model allows all proton balances (including

nitrate leaching) to be calculated by tracking proton inputs and outputs from soil layers for any cropping system that can be simulated by APSIM.

The need to simulate changes in pHBC, through time is resolved using empirical relationships that describe pH buffering as a function of hydrogen ion concentration, effective cation exchange capacity, exchangeable aluminium and percent organic carbon (7). An alternative approach to pH buffering, based on a geochemical description of the buffer capacity, is described elsewhere in these proceedings (14). This approach will allow a more dynamic simulation of chemical processes such as weathering, cation exchange, and aluminium complexion and dissolution and is required at pH values below 4.0 where the empirical functions used in this model extrapolate poorly.

Modelling acidification in discrete soil layers (defined by depth relative to the soil surface) accounts for the fact that acids and alkali are added to the soil in particular locations. For example nitrification occurs dominantly in the surface organic rich layer. Additionally, transport of ions in the mass flow of water is responsible for transfer of acid and alkali within the soil profile. The balance of uptake of cations and anions at different depths also causes a redistribution of acidity within the plant soil continuum as roots excrete organic acids to maintain a constant internal pH. These processes are accounted for in SPAM (Soil Profile Acidification Module) a mechanistic model for calculating the rate of movement of acid down the soil profile (5, 9, 13). The new SOILpH module adapts the functions developed in SPAM to calculate daily net flow and root excretion for each soil layer.

### The SOILpH module

In SOILpH a proton budget is calculated daily for each soil depth layer and the crop is treated as a separate component of the overall system. Hydrogen ion accumulation (kmol H<sup>+</sup>/ha) in a soil layer is calculated with the overall equation:

where:

**lime\_dissl** is calculated from the size of the lime pool in a soil layer and a function describing the solubility of lime as a function of soil pH (2) and the flow of water through the soil layer.

**ash\_alk\_wt** is calculated from a user supplied value for ash alkalinity of mature crop residue. This value is multiplied by the APSIM predicted weight of residue returned to the soil.

**netflow** is the net mass flow in water of  $H_2$ +,  $HCO_3$ -,  $CO_{32}$ -, and Al3+ out of a soil layer. The functions used are as detailed in (13) though the daily rather than annual mass flow is calculated. Mn reactions have not been included in the model at this stage but are known to be significant in weakly weathered soils containing sources of easily reducible  $MnO_2$ .

Note that in Helyar and Porter's framework N\_uptake terms are not included, as they do not represent a change in the reference for the soil/crop system. In SOILpH the N uptake terms are included because the system consists of soil layers and uptake of nh4 or no3 is an export out of a soil layer. The advantage of having formula (ii) in an APSIM module is that all the terms on the right hand side of equation (ii) can be calculated from values that are output by APSIM's SoilN or crop modules.

**root\_ex\_acid** is the proton equivalence of organic acid excreted by roots to allow crops to keep a constant internal pH while taking up more cations than anions. For each soil layer cations and anions other than N are defined as either available or unavailable for uptake (*eg.*, P is available only in layers close to the soil surface). The daily uptake of non-N nutrients is simplified as the product of their final concentration in the mature crop and the daily accumulation of crop drymatter. In SOILpH, N uptake is part of the equation for calculating acid excretion from roots. The N uptake terms in the N cycle must therefore reappear with an opposite sign in the root excretion formula, which is part of the carbon cycle. Thus for the whole soil/crop system the N\_uptake values are balanced out as is assumed in the Helyar and Porter framework.

**org\_acid\_acc** is the acid added when soil organic matter is increased. This function is the same as that used in (6) except that the increase in organic matter is calculated by APSIM's SoilN module.

To convert the proton balance in a soil layer into a change in soil pH, the SOILpH module uses empirical equations that were developed and tested on a wide range of agricultural soils in NSW and New Zealand (7, 8). The equations are used to calculate a lime requirement index (LRI, pH ha/t lime) as a function of pH, exchangeable aluminium, effective cation exchange capacity and the organic carbon fraction (7). LRI is then converted to pH buffering capacity (pHBC, kmol H+/ha/pH unit) using the equation:

pHBC = 20/(LRI \* 1.2)

*where:* the constant, 20, converts t CaCO3 /ha into kmol H+/ha and the constant, 1.2, allows for the incomplete lime reaction 12 months after liming in the field sites used to derive the LRI equations (M. Conyers, *pers. comm.*) The SOILpH module keeps track of all the parameters used to calculate pHBC so that it can update its value over time to keep up with changes in factors that modify buffering.

For linking acidification to crop production losses it is also necessary to predict soil aluminium. Empirical formulae [8; K. Helyar unpublished Lime-it (rotations) equations] are employed in SOILpH for calculating Alexch and AICa.

At the time of writing the SOILpH module was complete and configured in APSIM though the only crop module set up to run with SOILpH is the wheat crop module NWheat. Functions for the response of crop roots to acidification will need to be developed for each crop module. This is currently being done with the NWheat module (Senthold Asseng, pers. comm.) an effort that should serve as a template for other crops.

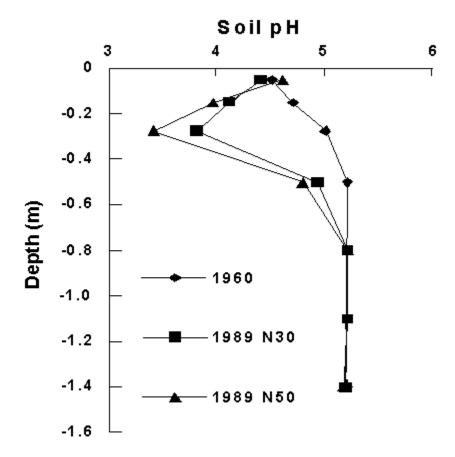
Depth	CLL <sup>4</sup>	USL <sup>®</sup>	BD⁴	pH	ECEC	Organic C
(mm)	(mm/mm)	(mm/mm)	(g/cc)		(cmol/kg)	(%)
0-100	0.186	0.32	1.56	4.5	3.76	0.82
100-200	0.196	0.30	1.56	4.7	3.28	0.50
200-350	0.215	0.34	1.52	5.0	4.2	0.29
350-650	0.231	0.34	1.46	5.2	4.6	0.17
650-950	0.237	0.35	1.42	5.6	4.6	0.13
950-1250	0.282	0.35	1.46	5.6	4.6	0.13
1250-1550	0.301	0.33	1.50	5.6	4.6	0.19

Table 1. Key soil properties at start of simulations

"Crop Lower Limit, the lower limit of crop water availability.

<sup>b</sup> Upper Storage Limit, where pore water pressure is at or above -0.1 bar.

<sup>e</sup>Soil Bulk Density, measured at USL.



# Figure 1

## Simulation results

As a first test of the SOILpH module it was subjected to a range of "experiments" to determine whether it "behaves" logically and realistically. A sample of the results of this type of test is provided in Fig. 1. Here a typical moderately acid soil was described (Table 1) and a cropping system of continuos wheat was simulated over a 30-year period using weather data from a 619 mm average annual rainfall site in Goondiwindi, Qld. The simulation started in 1960 and two management options were contrasted: annual

application of 30 kg/ha N was compared with 50 kg/ha N. In both cases the N source was urea. As anticipated the higher rate of N fertiliser was more acidifying. The higher pH of the top soil layer in the high N treatment was consistent with higher levels of wheat residues being returned to the soil surface and a build up in the surface organic matter fraction (data not presented).

#### Conclusion

The SOILpH module has reached a stage of develop-ment where it is ready for evaluation against existing field data sets. With the SOILpH module, APSIM has the potential to be used for investigating the effects of management options such as cropping rotations and fertiliser use on long term acidification rates and pro-ductivity. Other applications include the evaluation of the susceptibility of different environments (soil climate combinations) to acidification by alternative cropping systems.

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