

# Modelling nitrogen leaching: Are we getting the right answer for the right reason?

M. van der Laan<sup>a\*</sup>, J.G. Annandale<sup>a</sup>, K.L. Bristow<sup>a,b</sup>, R.J. Stirzaker<sup>a,b</sup>, C.C. du Preez<sup>c</sup>,  
P.J. Thorburn<sup>b</sup>

<sup>a</sup> Department of Plant Production and Soil Science, University of Pretoria, Private Bag X20, Hatfield 0028, South Africa

<sup>b</sup> CSIRO Sustainable Agricultural National Research Flagship and CSIRO Land and Water, Australia

<sup>c</sup> Department of Soil, Crop and Climate Sciences, University of the Free State, Bloemfontein 9300, South Africa

\*Corresponding author. Permanent address: University of Pretoria, Private Bag X20, Hatfield, 0028, South Africa. Tel.: +27 12 420 3665. E-mail address: [michael.vanderlaan@up.ac.za](mailto:michael.vanderlaan@up.ac.za)

## ABSTRACT

The complexities and challenges in quantifying N leaching have led to development of a range of measurement and modelling techniques, but none are widely applied. Observations that N moves more slowly than water through the soil profile has resulted in different approaches being used to simulate impeded N movement in crop models: (i) by accounting for nitrate ( $\text{NO}_3^-$ ) adsorption to the soil, (ii) by considering incomplete mixing between resident and draining soil water fractions or (iii) a combination of both. We compare and discuss strengths and weaknesses of these approaches. Our inability to directly measure model parameters (especially with regards to simulating N dynamics), and the risk of compensating errors during model testing and calibration, often results in low confidence in simulated N leaching. We caution that our current ability to simulate N leaching is in most cases not yet well enough developed for reliable and accurate predictions. We recommend a more strategic approach involving better linking measurement and modelling to improve understanding of the critical soil processes that control N leaching as one way of further improving our understanding and quantification of N leaching.

Keywords: APSIM, DSSAT, nitrate, SWB-Sci

## 1. Introduction

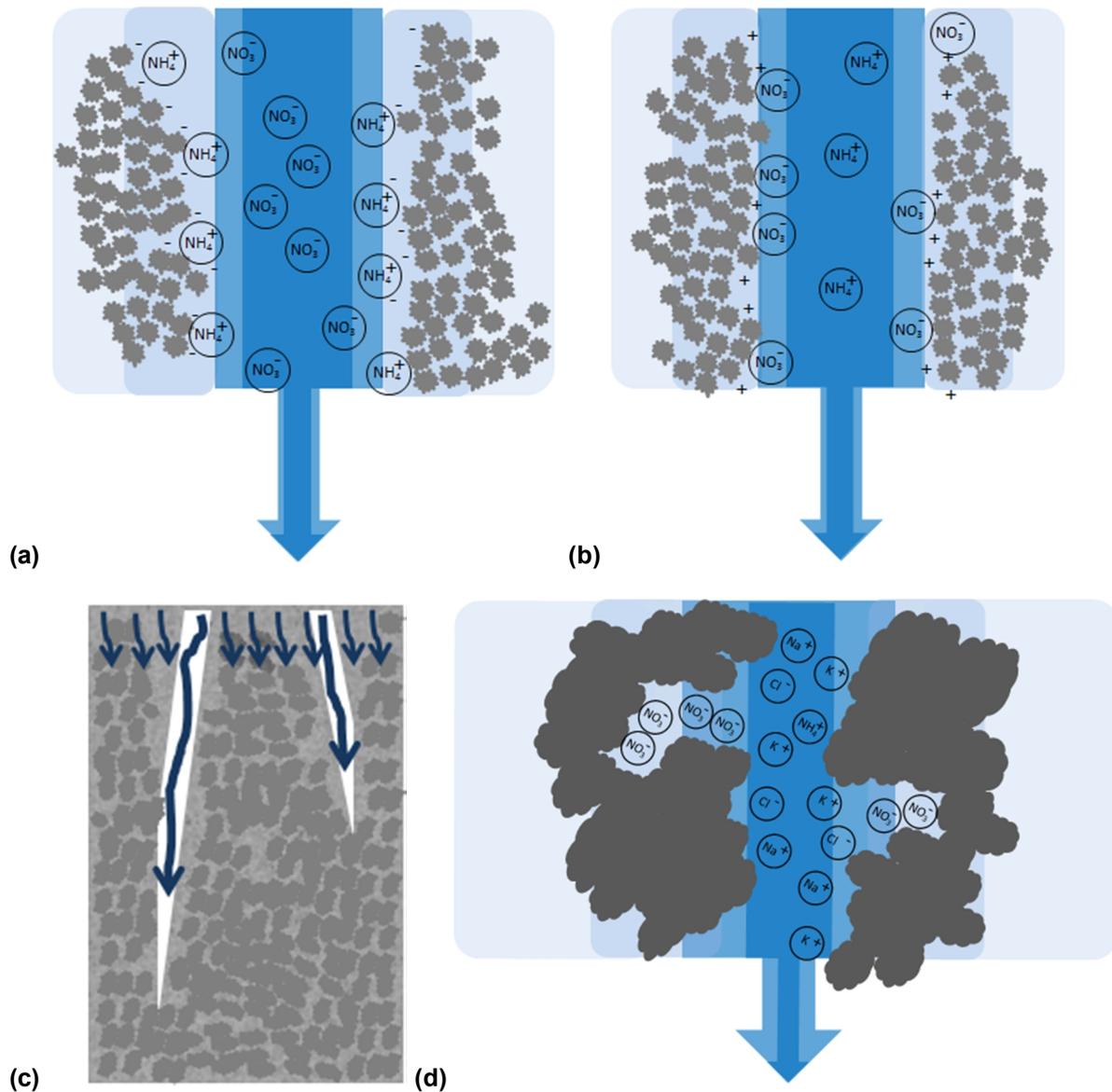
A major negative impact of agriculture on the environment results from the leaching of nitrogen (N) from the rootzone to groundwater. Quantifying leaching losses is highly challenging as a result of the uncertainties associated with estimating deep drainage, estimating N concentrations in the different pore water fractions that are draining, and accounting for any incomplete mixing between the resident and draining soil water as well as any preferential flow interactions (Figure 1). A range of methods to measure and model N leaching from agricultural soils have been developed, but currently no standard approach is widely applied.

Mechanistic crop models represent our current best understanding of physical, chemical and biological processes and interactions, and are a synthesis of knowledge gained from years of research and experience (Ma et al., 2000). For most crop models, the majority of testing and validation effort has been done for aboveground variables, most likely due to a primary interest in crop productivity and because aboveground variables are easier to measure. A large number of crop models have been applied to investigate N leaching losses at the local to field scale, including RZWQM (Ma et al., 1998), GLEAMS (Webb et al., 2001), APSIM (Keating et al., 2003), CropSyst (Stöckle et al., 2003), CERES, CROPGRO and CANEGRO within the DSSAT framework (Daroub et al., 2003; Van der Laan et al., 2011), and SWB-Sci (Van der Laan et al., 2010). HYDRUS (Šimůnek et al., 2008), although not a crop model, has also been used extensively to simulate N leaching (Phogat et al., 2013).

Simulation of the soil water balance in these various models follows either a detailed mechanistic approach [e.g. Richards' equation (Richards, 1931)] or a simpler cascading or 'tipping bucket' soil water balance approach (Reddy, 1983). Despite various shortcomings, the simpler models are more commonly used because (1) they are easier to parameterise, (2) long standing and geographically widespread use has resulted in large databases of soil input data, (3) options for deriving soil input data from simple soil measurements are often available, and (4) they have a shorter run time (Huth et al., 2012). There is, however, still uncertainty in whether the simpler empirical representation of soil water movement is effective in accurately simulating N leaching.

Notwithstanding the extensive research on N leaching, our inability to accurately measure N leaching under field conditions has limited our ability to fully understand and simulate the complex processes involved. In soil, inorganic N often moves more slowly than the infiltrating water, and the need to consider mobile and less mobile (or immobile) water phases arising from the range in pore-water velocities associated with the infiltrating water is widely accepted as important in modelling solute fluxes (Turner, 1958; Clothier et al., 1995; Coats and Smith, 1964; Ventrella et al., 2000; Ilseman et al., 2002). Adsorption of  $\text{NO}_3^-$  or ammonium ( $\text{NH}_4^+$ ) to soil particle surfaces can also result in impeded movement of N, most notably for soils with a high anion/cation exchange capacity. In addition, the modelling of N leaching is complicated by the dynamic nature of N in the soil-plant-atmosphere continuum (see section 3.1). Uncertainties related to parameterisation, initialisation and representation of the key processes controlling N dynamics in different cropping

systems has resulted in limited applicability and low confidence in simulations of N leaching.



**Fig. 1.** Schematics showing processes that can impede nitrate ( $\text{NO}_3^-$ ) and ammonium ( $\text{NH}_4^+$ ) leaching in soil: a)  $\text{NH}_4^+$  adsorption on soil cation exchange sites; b)  $\text{NO}_3^-$  adsorption on soil anion exchange sites; c) bypass flow under saturated conditions, through, for example, soil cracks and old root channels; and d) incomplete mixing between the infiltrating water and soil water located in smaller soil pores. Darker shades of blue represent faster soil pore water velocities.

In this paper we review approaches embedded in several commonly used crop models to simulate N leaching. While models that use Richards' equation for soil water flow are briefly discussed, the focus is on cascading soil water balance models which are commonly used to model various components of cropping systems. We discuss strengths and weaknesses of the various approaches, and highlight challenges in model parameterization and initialization that lead to uncertainty in the simulated data, and the possibility of getting the right answer for the wrong reason. We also address the question whether a monitoring and model assisted learning approach to adaptive N management would be more useful at this stage given the current uncertainties in our ability to simulate N leaching.

## **2. Common approaches used to model N leaching**

### *2.1 Model descriptions*

**HYDRUS** has been extensively used to investigate N leaching from cropping systems. The HYDRUS model uses numerical methods to solve the Richards' equation for variably saturated water flow, the convection-dispersion equation for solute transport in the liquid phase and diffusion equations for solute transport in the vapor phase (Šimůnek et al. 2008). A two-region, dual porosity formulation which partitions the liquid phase into separate mobile and immobile regions can also be used to account for physical non-equilibrium solute transport as can occur in well-structured soils. Provision for attachment/detachment of solutes to the solid phase is

also made. Flow can occur in a vertical, horizontal or inclined direction. This model needs to be linked with a crop model to enable root growth, crop water and N uptake, and soil N transformations (Hu et al., 2008). While greater accuracy may be expected as a result of the highly mechanistic nature of this model, higher user skill level requirements, the difficulty in obtaining accurate site specific soil properties at the appropriate scale and the need to couple the model with a crop model limits its widespread application. Hydrus has been especially useful for exploring different mechanisms of N movement under different scenarios in two-dimensional furrow and micro-irrigated systems (Cote et al. 2003; Gärdenäs et al. 2005; Crevoisier et al., 2008).

The United States Department of Agriculture's **RZWQM** (Root Zone Water Quality Model) is a one-dimensional model containing special features to simulate solute movement. This includes rapid transport of surface applied chemicals to deeper depths through macropores and the preferential transport of chemicals within the soil matrix via mobile-immobile zones (Ma et al., 2000). Equilibrium soil chemistry is also accounted for. Soil water redistribution is simulated using a mass-conservative numerical solution of the Richards' equation. A partial-piston displacement, partial-mixing approach is used to calculate solute transport at 1 cm deep increments during infiltration and at coarser increments during redistribution (Ma et al., 2000). A hybrid DSSAT-RZWQM model (DSSAT is discussed below) has also been developed to improve the crop growth algorithms and the number of crops that can be modelled in RZWQM (Li et al. 2008). Various tests have shown the model provides adequate estimates of soil NO<sub>3</sub>-N, but over- or under-predictions did occur in some cases (Cameira et al., 1998; Kumar et al., 1998; Ma et al., 1998; Farahani et al., 1999;

Jaynes and Miller, 1999;). Ma et al. (1998) observed that soil water  $\text{NO}_3^-$  at a 200 cm depth was over-predicted and attributed this to 'over-simplification of model assumptions such as no retardation of  $\text{NO}_3^-$ , immobility of ammonium, and use of first-order degradation rates'. Ghidry et al. (1999) observed that using soil macropore information and accounting for soil cracking greatly improved estimates of solute leaching.

For simpler cascading soil water balance crop models, the lower limit (also referred to as permanent wilting point), drained upper limit (also referred to as field capacity) and saturation volumetric water content (VWC) values are specified for each soil layer. These parameters are used to determine the amount of infiltrating water in a soil layer above the drained upper limit that will 'cascade' to the layer below. A user-defined factor determines what fraction of the water volume above the drained upper limit can drain to the layer below during each daily time-step. During the simulation of infiltration, the amount of water 'in' a layer can exceed the saturated VWC within a time step using this approach. This is because the total volume of water being added to and draining through a layer in a daily time-step is temporarily placed in that layer (and mixed) before the fraction above saturation is passed to the layer below. In situations where large quantities of water are cascading through the soil profile, considerable solute 'dilution' can occur when the infiltrating water has a low solute concentration resulting in 'low efficiency' solute movement (Verburg, 1996). This approach, therefore, unintentionally accounts for some degree of 'incomplete mixing' between the draining and resident soil water fractions within each layer of soil.

In **APSIM** (**A**gricultural **P**roduction **S**ystems **s**IMulator) it is possible to use two different models for the soil water and solute balance – SoilWat and SWIM3 (Huth et al., 2012). SoilWat is a cascading model while SWIM3 is based on numerical solutions to the Richards' and Convection-Dispersion equations. The description below was obtained from Probert and Verburg (1996). During saturated water flow, solute movement is simulated using a 'mixing' algorithm in SoilWat in which all water and solute entering a layer is fully mixed with what is already there, following which an 'efficiency factor' is used to calculate the amount of solute leaving the layer. SoilWat also considers unsaturated upward and downward flows driven by water content gradients, and a second user-specified efficiency factor is used to influence the amount of solute which moves with the water from one layer to another as a result of unsaturated flow. Originally, only  $\text{NO}_3^-$  and urea movement was considered, but this has been changed so that SoilWat can now accommodate any solute. A convection-dispersion equation is used to simulate solute movement in SWIM3, especially  $\text{NO}_3^-$ ,  $\text{NH}_4^+$ , urea and  $\text{Cl}^-$  movement (Huth et al., 2012). APSIM's ability to estimate N leaching has been assessed using measured field data, with varying levels of accuracy being achieved (Stewart et al. 2006; Thorburn et al. 2011). Using APSIM-SWIM, Stewart et al. (2006) noted that for one of the sites studied, the discrepancy between measured and simulated matric potential at 50 cm was a result of the inability of the model to account for soil cracking and the resultant preferential flow pathways. The authors further observed that while there was reasonable agreement between the magnitude of observed and simulated cumulative  $\text{NO}_3\text{-N}$  fluxes, temporal fluxes were not accurately reproduced. This was attributed to the presence of the preferential flow pathways. Comparative work done of APSIM-SoilWat and APSIM-SWIMv2 has shown that while comparisons are difficult as a

result of different boundary conditions or driving forces being represented, both soil water balance approaches could predict soil profile water content and conservative tracer movement satisfactorily (Bond et al., 1996; Bristow et al., 1996). Mention is not made of the efficiency factor value used in this study or how it was estimated. Each had strengths and weaknesses for simulating different circumstances, and user experience was noted to play an important role for both approaches.

**CropSyst** (Cropping Systems Simulation Model; Stöckle et al., 2003) and **SWB-Sci** (research version of the Soil Water Balance model; van der Laan et al., 2010) use a simple cascading soil water balance approach and account for incomplete N mixing based on the approach developed by Corwin et al. (1991). This approach utilizes a mobility coefficient ( $\gamma$ ) which represents the fraction of the liquid phase that is subject to piston-flow displacement, with the fraction  $1-\gamma$  representing the liquid phase that is bypassed. Both  $\text{NO}_3^-$  and  $\text{NH}_4^+$  leaching are taken into account. Van der Laan et al. (2010) observed that when using this approach in SWB-Sci, simulated draining  $\text{NO}_3^-$  concentrations aligned closely with draining concentrations measured in passive samplers intercepting draining water, while simulated resident soil water concentrations aligned closely with concentrations measured in active samplers ('resident' soil water is collected using a suction force).

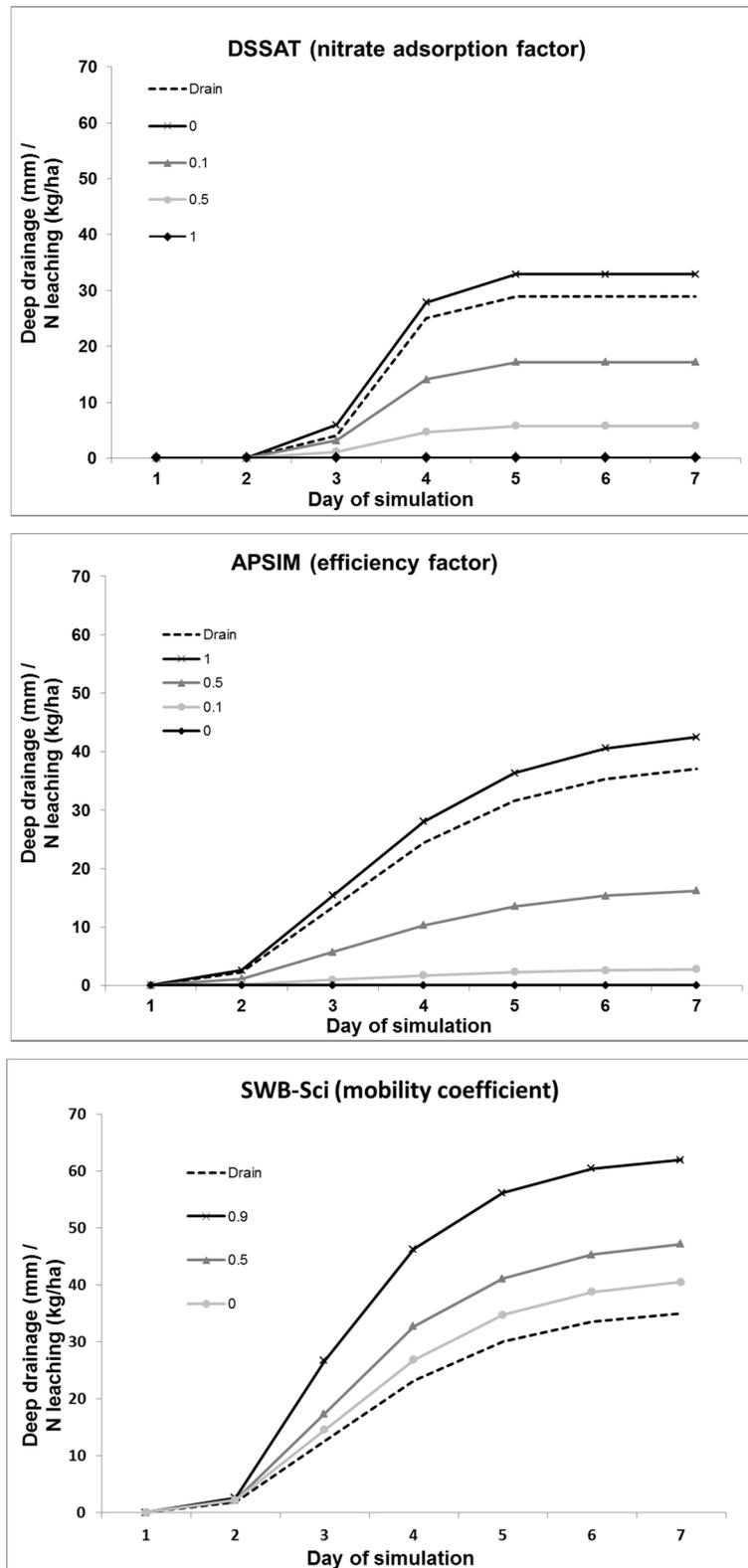
For the **DSSAT** (Decision Support System for Agrotechnology Transfer; Daroub et al., 2003) crop model framework, only  $\text{NO}_3^-$  (not  $\text{NH}_4^+$  or urea) movement is considered. No incomplete mixing processes for  $\text{NO}_3^-$  are included, but adsorption of  $\text{NO}_3^-$  to soil surfaces is accounted for using a  $\text{NO}_3^-$  Adsorption Factor ( $\text{cm}^3 \text{g}^{-1}$ ) (Bowen et al., 1993), which is based on the  $\text{NO}_3^-$  movement retardation factor work

of Wild (1981). This factor is used to determine the concentration of  $\text{NO}_3^-$  in the water of a soil layer that is subjected to leaching. DSSAT has two soil organic matter (SOM) modules, the original SOM module based on the PAPRAN model, and a SOM module based on the CENTURY model which divides SOM into more fractions, each with a variable C:N ratio and can mineralise and immobilize N (Jones et al., 2003). It is expected that the latter module will give better estimates of soil  $\text{NO}_3^-$  levels, and therefore N leaching. Similarly to DSSAT, in the **STICS** model (Simulateur multi-disciplinaire pour les Cultures Standard; Sierra et al., 2003), a critical value [ $C_{\text{critNO}_3}$  ( $\text{kg NO}_3\text{-N ha}^{-1} \text{ mm}^{-1} \text{ water cm}^{-1} \text{ soil depth}$ )] is used to account for  $\text{NO}_3^-$  adsorption on soil and the prevention of this fraction of  $\text{NO}_3^-$  from being transported to lower soil layers.  $\text{NO}_3^-$  above the  $C_{\text{critNO}_3}$  is assumed to mix completely between resident and draining soil water for that layer. Asadi and Clemente (2003) observed that DSSAT underestimated N leaching in an acid sulphate soil but that estimates were still acceptable; no indication on how the  $\text{NO}_3^-$  Adsorption Factor was used is given. For STICS, Sierra et al. (2003) demonstrated that  $\text{NO}_3^-$  transport was overestimated when  $C_{\text{critNO}_3}$  was not accounted for.

The leaching of nitrite ( $\text{NO}_2^-$ ) is not addressed in any of the models discussed above, probably because modellers assume that only minute concentrations of  $\text{NO}_2^-$  occur due to the rapid conversion of  $\text{NH}_4^+$  to  $\text{NO}_3^-$ , and because the leaching mechanism for the two anions ( $\text{NO}_3^-$  and  $\text{NO}_2^-$ ) is similar. The impact of liming on  $\text{NO}_3^-$  adsorption is also not considered in any of the models we reviewed. A lack of consideration of soil chemistry, in general, on soil hydraulic properties is seen as a weakness of these models (Huth et al., 2012).

## 2.2 Comparison of approaches

The effectiveness of the different approaches to simulate N leaching is difficult to assess given the challenges in accurately measuring N leaching under field conditions. It has been recognised that while more complex, mechanistic models have their strengths they do not always result in more accurate simulations (De Willigen, 1991). As a result of the different approaches used, the ability of the user-defined factors to account for incomplete mixing between the draining and resident soil water and/or soil  $\text{NO}_3^-/\text{NH}_4^+$  adsorption is expected to be uncertain. We tested this through a simple comparative simulation study using three cascading soil water balance crop models (DSSAT, APSIM, SWB-Sci) representing the main N leaching approaches used. A soil profile with the same characteristics was initialized for each of the models. The soil had 11 layers with a drained upper limit/field capacity =  $0.21 \text{ m}^3 \text{ m}^{-3}$ , lower limit/permanent wilting point =  $0.12 \text{ m}^3 \text{ m}^{-3}$ , initial VWC =  $0.19 \text{ m}^3 \text{ m}^{-3}$ , bulk density =  $1.1 \text{ Mg m}^{-3}$ , initial  $\text{NO}_3^- = 20 \text{ mg kg}^{-1}$  and initial  $\text{NH}_4^+ = 0 \text{ mg kg}^{-1}$ .  $\text{NO}_3^-$  was treated as a conservative tracer for these simulations by 'switching off' all other N transformation pathways (eg. mineralisation, immobilisation, denitrification etc.). Drainage factors and saturation VWC (=  $0.56 \text{ m}^3 \text{ m}^{-3}$  for the APSIM and DSSAT models and  $0.59 \text{ m}^3 \text{ m}^{-3}$  for the SWB-Sci model) were calibrated to give approximately 35 mm of deep drainage during the seven day simulation period. The simulation was run using a daily time-step with an irrigation event of 60 mm applied on day two (Figure 2).



**Fig. 2.** Influence of adjusting the impeded nitrate ( $\text{NO}_3^-$ ) leaching factor on cumulative N leaching during a simulated drainage event using the DSSAT (nitrate adsorption factor), APSIM (efficiency factor) and SWB-Sci (mobility coefficient) models (— $\times$ — represents complete mixing). Cumulative drainage is also shown.

Adjusting the relevant N leaching factor gave similar results for  $\text{NO}_3^-$  leaching using the DSSAT and APSIM models. A nitrate adsorption factor of  $1 \text{ cm}^3 \text{ g}^{-1}$  resulted in zero leaching for the DSSAT simulation and a saturated flow efficiency factor of 0 resulted in zero leaching for the APSIM simulation, while in SWB-Sci it was not possible to simulate zero N leaching. Increasing the mobility coefficient in SWB-Sci increased  $\text{NO}_3^-$  leaching loads, and much higher leaching loads could be simulated using this model compared to DSSAT, and to a lesser extent APSIM. A mobility coefficient of 0 resulted in cumulative leaching similar to that of the DSSAT and APSIM models under conditions of complete mixing. The reason for this is that following the initial rapid movement of water through the soil profile during which incomplete mixing is represented by the Corwin et al. (1991) approach, complete mixing is simulated between the draining and resident soil water fractions in the time-steps thereafter, resulting in relatively higher  $\text{NO}_3^-$  concentrations in the draining water. SWB-Sci therefore does not have the same capability to impede  $\text{NO}_3^-$  movement during slower drainage as can be done by changing the N-leaching factors in DSSAT and APSIM. For all three approaches complete mixing led to the highest N leaching as expected; estimates were similar for the DSSAT and APSIM models but much higher for SWB-Sci. The drainage curves were similar for APSIM and SWB-Sci, but different for DSSAT, for which drainage had ceased by day five, indicating a noticeable difference in the cascading water balance approach used between DSSAT and the other models.

These results suggest that the DSSAT and APSIM models can be more easily fitted to simulate reduced leaching due to incomplete mixing or soil inorganic N adsorption when irrigation or rain water with low  $\text{NO}_3^-$  concentrations is draining through a soil

profile with higher ambient levels of  $\text{NO}_3^-$ . The approach used in SWB-Sci, on the other hand, may be more effective in simulating higher leaching for the same scenario for a soil where piston-flow is dominant. Preferential flow will also be better represented using the Corwin (1991) approach, but this approach will not account for impeded  $\text{NO}_3^-$  leaching in soils with a high anion exchange capacity.

This simple comparison highlights how important it is for users to understand the detail of a particular approach being used to model N leaching in the crop model they are using, and whether the approach adopted captures the key processes that control N movement in their system of interest.

### **3. Model parameterisation and initialisation**

Confidence in model parameterisation and initialisation depends on the accuracy of measured input data, soil heterogeneity and the impact of any assumptions made. Mechanistic models, for example those that solve Richards' Equation for water flow, generally utilise parameters that are more easily measurable, for example, saturated hydraulic conductivity. The measurement of these parameters in the laboratory or field is often a laborious and costly exercise, and pedotransfer functions which estimate hydraulic properties from basic soil properties such as texture and bulk density are commonly used as a result (Van Alphen et al. 2001). While there is uncertainty relating to pedotransfer estimates, an advantage is that sampling density can be increased when using basic soil properties to estimate hydraulic properties (Van Alphen et al. 2001). Alternatively, soil parameters can be estimated from regular observations of soil water content, including periods of wetting, redistribution

and drainage and drying down by plants (Huth et al. 2012). For cascading water balance models calibration procedures are more heavily reliant on user expertise and experience, which can have a major impact on the accuracy and reliability of simulated outputs. In modelling pesticide and bromide leaching using the GLEAMS model, Rekolainen et al. (2000) observed that the simulated results of different users for the same scenario can differ markedly from each other, even for calibrated simulations. Botterweg (1995) also demonstrated that different users applying the same measured data could influence the calibration process significantly, while still obtaining a reasonable fit using a different understanding of the system being simulated.

### *3.1 Challenges in establishing an impeded N transport factor through calibration*

Due to the strong linkage between N and water, and the complexities involved in calibrating a crop model, including the possibility of compensating errors, multiple forms of measurement to generate data for calibration purposes are the best approach to minimise this type of error. For example an over-estimation of N mineralisation from SOM can be compensated for by an over-estimation of N leaching losses when only crop N uptake and intermittent soil inorganic N measurements are made to calibrate and test models (Figure 3). The same applies for the other N out-/inflows. Carry-over effects from previous seasons can also have an important impact and should be fully considered when determining the length of the trial in which measurements will take place and by prioritising the measurement of initialisation data. Using the RZWQM, Farahani et al. (1999) over-estimated  $\text{NO}_3^-$  leaching by 79% and concluded that when model parameterisation relied on a single

season's data for calibration, the narrowness of prevailing conditions during that season could bias input values. The authors recommended the use of experimental observations from multiple seasons to overcome this.

### *3.2 Using sensitivity analysis to assess the importance of model inputs*

Sensitivity analyses aim to identify model inputs that most significantly influence model results (Vanclooster et al. 1995). By way of example, to better understand the relative importance of the mobility coefficient used in SWB-Sci, selected model parameters and initialisation values for the Van der Laan et al. (2010) study were increased or decreased by 15% and the influence on drainage volume (mm) and N leaching ( $\text{kg ha}^{-1}$ ) was assessed (Table 1). This exercise demonstrated that the drainage factor was the most sensitive parameter for this simulation scenario, with a reduction of 15% leading to under- estimates of 64 and 62% for cumulative drainage and N leaching, respectively. A similar conclusion regarding the importance of correctly estimating the soil drainage parameter was drawn by Vanclooster et al. (1995) for the WAVE-model.

Simulated results were also sensitive to bulk density as it is used to calculate saturation VWC in the model and led to large differences in estimated drainage. Interestingly, reducing bulk density by 15% led to a 26% increase in drainage, but only a 4% increase in N leached. The reason for this is that a smaller mass of profile inorganic N was initialised by the model to be in the soil profile as bulk density is used to convert the user-specified inorganic N concentration to inorganic N mass. In comparison, altering the mobility coefficient or the radiation use efficiency of the crop

by 15% had very little influence on model estimates of cumulative deep drainage and N leaching at the end of the season. Output was also very sensitive to initial VWC and soil profile inorganic N levels, with VWC having an even larger influence than the drainage factor. Clearly a particular model's ability to simulate the water balance correctly is of paramount importance in estimating N leaching losses. Reduced initial inorganic N levels resulted in increased drainage as a result of poorer crop growth/reduced ET as a result of N deficiencies.

Sensitivity analyses can be very useful in informing researchers and modellers on what the most important model inputs are and on the most important measurements that need to be made as part of a monitoring programme. They also highlight the importance of soil variability in estimating leaching loads, and will assist in determining when a lumped parameterization approach versus separate simulations for different soil types are more appropriate for a particular field (Huth et al., 2012).

**Table 1**

Sensitivity analysis for four model parameters and two initialisation values for the SWB-Sci model used in the leaching study by Van der Laan et al. (2010).

Parameters	Original value	-15%	15%	-15%→ % change		+15%→ % change	
				Drainage	N leach	Drainage	N leach
Mobility coeff (0-1)	0.3	0.26	0.35	1	-1	-1	0
Drain factor (0-1)	0.95	0.81	1.0*	-64	-62	32	20
Bulk density (kg m <sup>-3</sup> )	1100	940	1270	26	4	-32	-20
Rad use eff (kg MJ <sup>-1</sup> )	0.0017	0.002	0.0014	1	7	-1	-2
<b>Initialisation values</b>							
Initial VWC (m <sup>3</sup> m <sup>-3</sup> )	0.187 <sup>#</sup>	0.159 <sup>#</sup>	0.215 <sup>#</sup>	-73	-68	94	72
Initial inorg N (mg kg <sup>-1</sup> )	16.4 <sup>#</sup>	14.0 <sup>#</sup>	18.9 <sup>#</sup>	24	3	-35	-23

#### 4. Discussion and recommendations

For models utilising a cascading soil water balance approach, N leaching approaches differ significantly, and in each case have needed to be greatly simplified while still aiming to account for the complex processes that control the flux of inorganic N. None of the crop models described incorporate all the major leaching processes. For example, DSSAT addresses chemical adsorption, SWB-Sci addresses incomplete mixing, while APSIM-SoilWat lumps both processes together using an efficiency factor. The inclusion of all the important processes into each model could in theory lead to greater accuracy, for example including an incomplete mixing algorithm into DSSAT and an  $\text{NO}_3^-$  adsorption algorithm into SWB-Sci, but this still leaves the dilemma of how to parameterise these processes. All the models are therefore predisposed during the calibration phase to get the right answer for the wrong reason due to feedbacks and compensating errors. Modellers are faced with a conundrum: the more accurately the processes are described, the greater the error we can introduce through incorrect parameterization. As noted by Stirzaker et al. (2010), 'it is often therefore better to have a simpler model which we understand, and understand the limitations of, than a complex one we do not understand'.

Ultimately the accuracy of our estimates of N leaching, and improved understanding of the driving processes, will be achieved through linking measurement and modelling exercises more closely together to overcome the challenges highlighted in this paper. The approach of running detailed, multi-season experiments to parameterise models is not a solution for most model users. However, simple cost-effective  $\text{NO}_3^-$  monitoring, such as that used by Van der Laan et al. (2010) and

Fessehazion et al. (2011), could provide inputs and updates into the model and prevent the potential gross errors highlighted in Table 1. As many of the input parameters required to simulate N leaching in crop models cannot be measured directly, calibration with measured data is key, particularly for models where important processes are represented empirically. A model parameter and initialisation value sensitivity analysis can also assist in identifying key parameters or variables that should be measured to generate useful calibration data.

The appeal for more measurement is not primarily for the purpose of more accurate model parameterisation. Moreover, our measurement tools are largely inadequate for the task. Essentially it is the interplay between pragmatic measurement and strategic modelling that offers a way forward. For example field monitoring of nitrate could help us understand which processes are dominating in our system and modelling can provide insight into how different processes interact and what types of measurements are likely to provide the most useful data (Van der Laan et al., 2010). That would allow knowledge obtained through monitoring to be fed back into improving the functional utility of the model and confidence in the output. The linkage works because monitoring can give reliable data at a point in time, but is subject to potentially huge spatial variability. Modelling can accumulate errors over time, but when reinitialised from time to time can provide more reliable output since it is constrained by the principles of conservation of mass and energy.

It is essential that authors clearly describe all the parameters and initialization values used in setting up their simulations, and whether these were best guess estimates, were derived from measured data or were obtained through calibration. Too often,

the critical factors controlling N leaching are omitted or poorly described in published papers. This is most likely as a result of oversight by authors or a lack of understanding of how greatly these factors influence the model predictions

## **5. Conclusions**

A proper understanding of the N leaching approaches used in crop models, and the processes they aim to represent, is essential for improving the accuracy and application of crop models. Major uncertainties still lie with the parameterization of our N leaching models and whether various processes are accurately simulated. This results in low confidence in N leaching estimates and the possibility of compensating errors.

Many of the published papers on N leaching do not include adequate information about the processes being simulated and the parameterization and initialisation of the models, making the simulated results difficult to interpret. The onus is on all of us who use and/or report on models to simulate N leaching to include sufficient details about how N leaching was modelled to assure the reader we are getting the right answer for the right reason.

We also recommend a more strategic approach involving better linking measurement and modelling to enhance understanding and quantification of the critical soil N processes as one way of further improving our confidence in predicting N leaching.

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