CHAPTER 5

MODELLING THE EFFECTS OF NITROGEN AND PHOSPHORUS STRESS ON CROP GROWTH USING SWB-Sci: AN EXAMPLE USING MAIZE

ABSTRACT

Increasing fertilizer prices and environmental pressures associated with declining water quality and eutrophication necessitate the careful management of nitrogen (N) and phosphorus (P) in cropping systems. For this reason, N and P subroutines have been included into the SWB-Sci model. Modified approaches for modelling crop P uptake, stress effects and banded P fertilizer applications were required. The testing of these new subroutines using data from a maize trial in Kenya is presented. In most cases, but not all, the model performed well in simulating total dry matter production, leaf area index, and N and P uptake. The comparison of measured and simulated N:P ratios was also used successfully to assess model performance, and is recommended as an approach when modelling crop N and P uptake mechanistically. It is clear that data quality should always be scrutinized so that poor quality measurements do not incorrectly undermine reported model performance. Further work on plant available P in different soils and the longevity of banded fertilizer P is needed. In its current form, SWB-Sci can now be used to gain further insights into the dynamics of carbon, N and P in agro-ecosystems, and play a role in developing economical and environmentally responsible fertilization strategies.

5.1 INTRODUCTION

In sub-Saharan Africa, low soil fertility, especially with regard to nitrogen (N) and phosphorus (P) is a major constraint on crop production (Sanchez et al., 1997). Improving management of N and P in cropping systems is therefore important to mitigate against escalating fertilizer costs and loss of nutrients from agricultural systems to waterways, which can lead to eutrophication and a deterioration of fresh water quality. Managing this type of pollution involves N and P, as one of these nutrients is most often the limiting factor for algal growth.

The contribution of agriculture to Non-Point Source (NPS) nutrient pollution is technically difficult and challenging to monitor, and modelling has been identified as a useful tool in increasing our understanding and management of NPS pollution. For these reasons, new N and P subroutines have been included into SWB-Sci, a mechanistic, local-scale, generic crop model, originally developed as an irrigation scheduling tool. Accurate simulation of nutrient uptake is dependent on accurate crop growth modelling (Daroub et al., 2003). SWB-Sci has undergone extensive water balance validation and has been found to accurately simulate crop growth, water use and soil volumetric water content (VWC) for a range of crops, including vegetable crops such as pumpkin, squash and tomato; field crops such as sunflower, maize, soybean, potatoes and canola; the pasture crops lucerne and fescue; and tree crops (Jovanovic et al., 1999; Jovanovic and Annandale, 2000; Steyn, 1997; Jovanovic et al., 2002; Annandale et al., 2003; Tesfamariam 2004). A salt subroutine was also included into SWB-Sci to study the long-term sustainability of using gypsiferous mine water to irrigate crops (Annandale et al., 2001; Beletse, 2008).

In the past, general acceptance of N as the limiting factor for crop growth has resulted in a greater focus in simulating N in crop models; but in low input systems, P can often be limiting (Probert and Keating, 2000). Phosphorus sorption to the soil matrix and the complex adaptations that plants have undergone to acquire P in soil (Raghothama, 1999), makes the mechanistic modelling of P uptake highly challenging. Furthermore, little attention has been given to the dependence of crop growth on P uptake (Greenwood et al., 2001). Comprehensive crop models that have been used to model P include the DSSAT models CERES and CROPGRO (Daroub et al., 2003) and APSIM (Probert, 2004).

Approaches used to model N and P in SWB-Sci are based on those from well-tested models, as discussed below. Several modifications to simulate P demand and uptake, stress effects and banded P fertilizer applications were, however, required. The testing of these subroutines using a historical dataset from Kenya, for a dryland maize trial receiving different rates of N and P, is presented in this paper. The conventional approach of using statistical analysis as well as a new approach using shoot N:P ratios are used to assess model performance. Finally, the model is also used to assess the importance of adequate N and P fertilization to reduce unwanted deep drainage.

5.1.1 Review of model development

N and P simulation approaches and algorithms were obtained primarily from CropSyst (Cropping Systems Simulation Model; Stöckle et al., 2003) for N, and GLEAMS (Groundwater Loading Effects of Agricultural Management Systems; Leonard et al., 1987) for P. SWAT (Soil Water Assessment Tool; Neitsch et al., 2002) and APSIM (Agricultural Production Systems Simulator; Keating et al., 2003) were also used to a limited extent. All major processes are simulated, including organic matter mineralization, immobilization, nitrification, denitrification, volatilization, N fixation, P and NH_4^+ sorption, soluble N and P runoff and leaching, and inorganic and organic fertilization. The effects of various physical and chemical factors such as soil water content, temperature and pH are also included. The water balance is simulated using the 'cascading' approach and crop growth is simulated as a daily dry matter increment that is either radiation or transpiration limited (Jovanovic and Annandale, 2000). When available soil water does not meet potential transpiration demand, water stress occurs and is calculated as the ratio between actual and potential transpiration. A water stress index is also used to slow down the accumulation of growing day degrees.

Crop N uptake is calculated as the lesser of crop N demand and potential N uptake. Maximum, minimum and critical crop N concentrations (kg kg^{-1}) are calculated daily. When crop concentrations are below the critical N concentration, growth is reduced.

If concentrations fall below the minimum N concentration growth ceases (Stöckle et al., 2003). In SWB-Sci, in contrast to CropSyst which calculates yield using a harvest index approach, a harvestable dry mass increment is calculated on a daily basis once the crop has reached the reproductive stage to determine yield. Modifications to the code were therefore required to estimate translocation of N from vegetative crop organs to the grain on a daily basis and also to estimate N deficiency effects on grain development.

5.1.2 Modelling crop P uptake, stress effects and banded P fertilizer applications

As a more mechanistic, generic crop approach was required to estimate potential P uptake, crop P demand and P deficiency stress effects, new algorithms based on the CropSyst approach for calculating N uptake and demand were developed. Users are required to define plant P concentration at emergence, as well as optimal crop P concentrations for the vegetative and reproductive growth phases. Crop P demand is calculated by multiplying the daily dry matter increment by optimal P concentration. A possible P deficit in the crop is also accounted for when calculating daily crop P demand. After water or radiation limited growth has been calculated, growth can be further reduced by either N or P deficiency stress, depending on which is greater. Simulation of the effect of deficient soil P on crop growth follows the approach of Daroub et al. (2003), using equation 1:

$$\text{P Stress Factor} = 1 - [1 - (\text{Potential P Uptake/P Demand})]^4 \qquad (1)$$

The *P Stress Factor* ranges from 0 for total stress to 1 for no stress, and is not directly proportional to the ratio of potential uptake to demand (Daroub et al., 2003). Grain P mass is simulated as the total P taken up after the commencement of flowering.

Initial model testing indicated that the availability of banded fertilizer P could not adequately be modelled by adding this fertilizer input to the plant-available *Labile P* pool using the GLEAMS approach. When banded fertilizer P was added to the *Labile P* pool in the model, it quickly became unavailable to the plant by moving to the plant-unavailable *Active P* pool. For this reason, modifications were made to include a *Banded P* pool. In APSIM, banded P is also accounted for separately from labile P and assigned a higher value in terms of crop availability (Probert, 2004). Plant availability from the banded P pool in APSIM is influenced by soil water and temperature. While little is known about the dissolution of fertilizer P applied in the soil as a band, deep bands (> 15 cm) have been observed to maintain their integrity well beyond the growing season of application (Stecker and Brown, 2001). Band half lives have been calculated by Zerkoune (1996) to range from 1.4 to 3.8 years and band longevity estimated to range from 2.6 to 6.5 years by Eghball (1989). In the absence of good supportive data it was decided to incorporate a simple routine to simulate banded P dissolution by moving a set fraction (currently 0.005) of *Banded P* to *Labile P* daily while the modelled soil layer water content in which the band was placed was wetter than the permanent wilting point. No dissolution is allowed to take place when the soil water content is below the permanent wilting point.

Crop P uptake has also been modified to reflect the higher availability of *Banded P* by setting the soil P buffering effect (through adsorption) as zero for this *Banded P* pool. Additionally, a *Layer Uptake Factor* was included, as calculated by Equation 2:

$$\text{Layer Uptake Factor} = (\text{Labile P}+\text{Banded P})\times\text{Active Upake Factor}\times\text{Water Content Function} \quad (2)$$

Where the *Water Content Function* represents the influence of the amount of water in the soil, (*Labile P* + *Banded P*) is the amount of plant available P in kg ha^{-1}, and the *Active Uptake Factor* is a species specific factor reflecting a crop’s ability to actively take up P. At present the *Active Uptake Factor* is best determined through calibration.

5.2 MATERIALS AND METHODS

5.2.1 Brief overview of data set used to test the model

Data from a trial conducted in Kenya to determine the effects of N and P deficiency on maize (Probert and Okalebo, 1992) was used to test the model. Briefly, there were five fertilizer rate treatments (Table 5.1) for the ‘short rains’ season in 1989/90 (SR89). Nitrogen and P were applied at sowing; N in the form of calcium ammonium nitrate, and P, in the form of superphosphate as a band placed at a 20 cm depth. For the high N level treatments, a second N fertilizer application was made 27 days after planting (DAP) and a third 37 DAP.

Table 5.1 N and P rates applied in the first season (SR 89)

Treatment	Nitrogen (# applications)	Phosphorus
	kg ha^{-1}	
N1P0	30 (1)	0
N1P1	30 (1)	10
N2P0	90 (3)	0
N2P1	90 (3)	10
N2P2	90 (3)	40

For the ‘long rains’ 1990 season (LR90), the crop was planted on the same ridges as for SR89 with minimal disturbance of the previously banded fertilizer. All plots received the higher rate of N (90 kg ha^{-1}), but P application histories and fresh applications differed between treatments (Table 5.2).

Table 5.2 Rates of banded P applied to modified treatments over the SR89 and LR90 seasons

Treatment	P application (kg ha^{-1})	
	SR 89	**LR 90**
P0	0	0
P10	10	0
P40	40	0
F10	0	10
F40	10	40

Rainfall from planting to harvest was 430 and 379 mm for the SR89 and LR90 seasons, respectively, with good climatic conditions for maize growth being experienced for both seasons (Probert and Okalebo, 1992). The soil is classified as a Haplic Lixisol, with a sandy clay texture, pH (H_2O) 6.1, 0.59% organic C, 0.06% total N and a Bray 2 P value of 4 mg kg^{-1}.

5.2.2 Model set-up and calibration

The soil profile was initialized using the soil parameters reported above and measured soil layer water contents, and the soil was classified as slightly weathered for modelling purposes (Van der Laan et al., in press). For the LR90 treatments, a single simulation over both seasons was used, without any re-initialization at the beginning of the LR90 growth season.

Model calibration was achieved using the treatment N2P2/P40 treatment. As SWB-Sci has been designed as a mechanistic, generic crop model, minimal changes were made to the standard crop N and P parameters. Other crop growth parameters were only adjusted within reasonable ranges as required and are presented in Table 5.3.

Table 5.3 Crop model parameters for maize determined from N2P2 field data, literature and previous SWB research

Parameter	Values	Unit
Canopy extinction coefficient for solar radiation	0.80	-
Dry matter: water ratio	5.5	Pa
Radiation use efficiency	0.0018	kg MJ^{-1}
Base temperature	10	°C
Optimum temperature	25	°C
Maximum temperature	30	°C
Thermal time: emergence	75	d °C
Thermal time: flowering	700	d °C
Thermal time: maturity	1250	d °C
Thermal time: transition (from vegetative to reproductive)	10	d °C
Thermal time: leaf senescence	250	d °C
Leaf water potential at maximum transpiration rate	-1500	kPa
Maximum transpiration rate	9	mm day^{-1}
Specific leaf area	13.5	m^2 kg^{-1}
Leaf stem partitioning factor	1.8	m^2 kg^{-1}
Total dry matter at emergence	0.0029	kg m^{-2}
Root partitioning function	0.2	-
Stem dry matter translocation	0.05	-
Root growth rate	5	m^2 $kg^{-0.5}$
Maximum canopy height	3.2	m
Root N concentration	0.01	kg kg^{-1}
P concentration at emergence	0.0045	kg kg^{-1}
Optimal vegetative growth P concentration	0.001	kg kg^{-1}
Optimal reproductive growth P concentration	0.0008	kg kg^{-1}
Root Active P uptake factor	4.5	-

5.2.3 Statistical criteria for validation

Model performance was evaluated according to reliability criteria as described by De Jager (1994) (Table 5.4). The square of the correlation coefficient (r^2) is used to evaluate the association between measured and predicted values, the mean absolute error (MAE) is an average of absolute errors, and the index of agreement (D) proposed by Wilmot (1982) indicates the relative size of the average differences (Singh et al., 2008). The measured variables used to test model performance were aboveground dry matter and yield, leaf area index (LAI), aboveground N and P mass, N:P ratios, and profile water content.

Table 5.4 Statistical criteria used to judge model performance

Statistical parameter abbreviation	Extended meaning of abbreviation	Reliability criteria
r^2	Square of the correlation coefficient	> 0.80
D	Wilmot (1982) index of agreement	> 0.80
MAE (%)	Mean absolute error (%)	< 20

5.2.4 Nitrogen:Phosphorus Ratios

A review of N:P ratios in cereal crops showed that these ratios ranged from 1 to 20 (Sadras, 2006). This high variability is assumed to be related to variations in the supply of nutrients to crops, and a tendency for crops to absorb and store more P than is immediately required (Bollons and Baraclough, 1990; Greenwood et al., 2008). In a review of maize shoot N:P ratios in a number of trials, Jones (1983) observed N:P shoot ratios ranging from 1-34. N and P concentrations in maize earleaf have also been observed to be highly correlated to nutrient supply in factorial N × P fertilizer rate experiments, with earleaf N:P ratios relatively stable for the high yielding experiments (Escano et al., 1981a, b; Jones 1983). Following a review of N:P ratios in wetland vegetation fertilization studies, Koerselman and Muleman (1996) suggest that N:P ratios could be used to determine whether N or P is limiting and proposed that N:P ratios of less than 14 indicate N is limiting, while ratios higher than 16 indicate that P is limiting. Ratios between 14 and 16 indicate that either N or P is limiting, or growth is co-limited by N and P together. To the best of our knowledge, no similar approach has been proposed for maize, so these guidelines were used in assessing the simulation results of this study.

5.3 RESULTS

5.3.1 Total aboveground dry matter and yield

SR89

The model was able to simulate the production of total dry matter (TDM) relatively well for the first growth season (Table 5.5). The highest MAE of 42% was obtained for the treatment receiving the lowest rates of N and P. For all treatments the r^2 and D values were above 0.80.

Table 5.5 Statistical evaluation of measured and simulated values for total aboveground dry matter (TDM) during the SR 89 season

Treatment	r^2	D	MAE (%)
N1P0	0.98	0.95	42
N1P1	0.88	0.97	23
N2P0	1.00	1.00	10
N2P1	0.97	0.99	14
N2P2*	0.99	0.99	11

*Data used for model calibration

The model also performed well in simulating the limiting effects of different fertilizer N and P application rates on crop growth for the five treatments (Figure 5.1). For treatments N2P2, N2P1 and N1P1 there was a decrease in TDM between the fourth and fifth measurements, which may be an indication of in-field variability for the site. This would have statistical implications. Measured data reflected higher TDM production for the N1P1 treatment than for the N2P0 treatment, except for the final measurement of the season. This would indicate that P was the limiting factor and this was also predicted by the model.

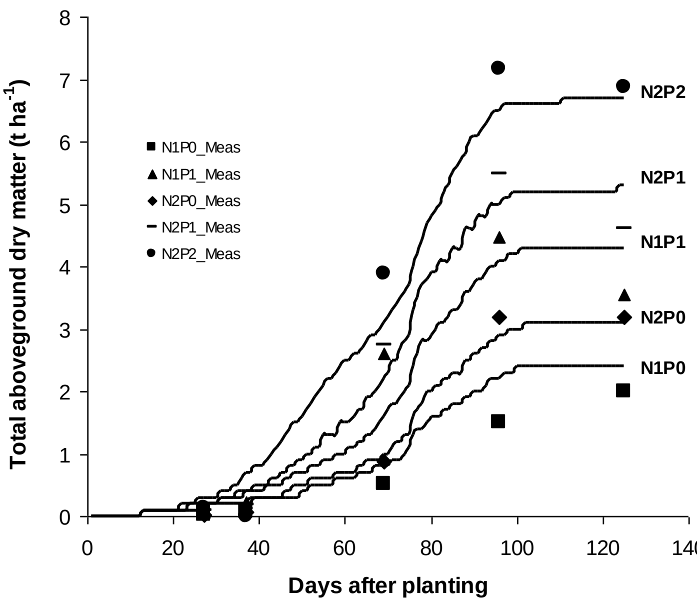

Figure 5.1 Measured and simulated values for total aboveground dry matter (TDM) production for the five treatments for the SR89 growth season

Yield was only measured once for each treatment and is compared with simulated values for the five treatments in Figure 5.2. While the simulated values all lie above the 1:1 line indicating the model over-estimated grain yield consistently, statistical analysis of measured versus simulated values for the five treatments showed that yield was reasonably well simulated according to De Jager's (1994) reliability criteria with r^2=0.88, D=0.86, MAE=28. Very similar yields of around 1.4 t ha^{-1} were measured for treatments N1P1 and N2P0.

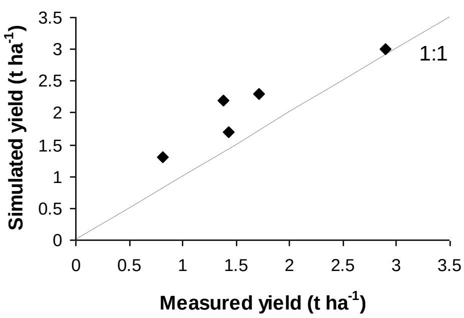

Figure 5.2 Measured versus simulated values for yield for the five treatments for the SR89 growth season

The relative effects of N and P stress on overall crop growth were therefore judged to be adequately predicted by the model for the SR89 season during which different combinations of N and P fertilizer application rates were used.

LR90

TDM was less accurately simulated for the LR90 growth season than for the SR89 growth season. MAE ranged from 26 to 34%, although r^2 and D values were above 0.80 for all treatments (Table 5.6).

Table 5.6 Statistical evaluation of measured and simulated values for total aboveground dry matter (TDM) during the LR90 season

Treatment	r^2	D	MAE (%)
P0	0.99	0.96	34
P10	0.99	0.94	28
P40	0.98	0.94	29
F10	0.92	0.94	25
F40	0.98	0.94	26

Except for the treatment receiving the lowest P application (P0), TDM for all treatments were underestimated in the LR90 season (Figure 5.3). For both the measured and simulated data the P40 treatment achieved a higher TDM than the F10 treatment. Measured TDM values for the F40 and P40 treatments were similar throughout the season. It is therefore plausible that P was not the limiting factor for these two treatments.

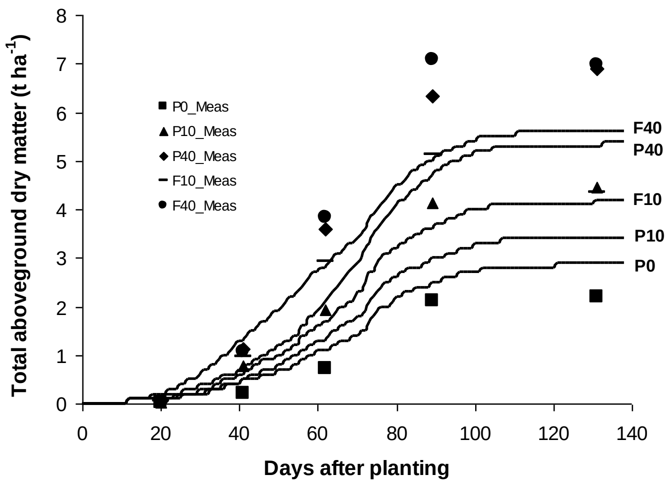

Figure 5.3 Measured and simulated values for total dry matter production for the five treatments for the LR90 growth season

In contrast to the previous season, yield was grossly under-predicted by the model for all treatments except P0 (Figure 5.4). The under prediction was greatest for the high P application treatments P40 and F40. Yield was reasonably well predicted for the F10 treatment. The overall statistics for yield were reasonable (r^2=0.98, D=0.77, MAE=24).

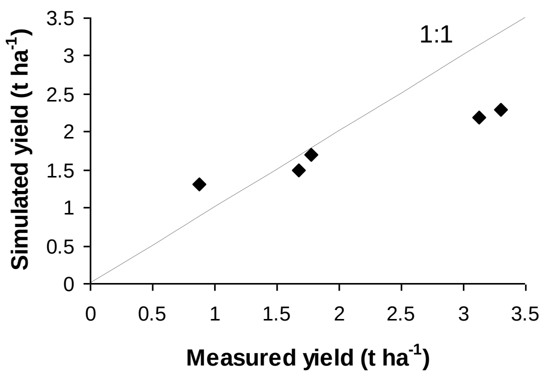

Figure 5.4 Simulated versus measured values for yield for the five treatments for the LR90 growth season

5.3.2 Leaf area index

SR89

LAI was also well simulated in the SR89 season in most cases (Table 5.7). The highest MAE of 31% was obtained for the N2P0 treatment, despite TDM being most accurately simulated for this treatment. The best simulation of LAI was for the N1P0 treatment, while LAI was underestimated for treatments N2P1, N2P0 and N1P1.

Table 5.7 Statistical evaluation of measured and simulated values for leaf area index (LAI)

Treatment	r^2	D	MAE (%)
N1P0	0.85	0.90	17
N1P1	0.77	0.80	26
N2P0	0.76	0.75	31
N2P1	0.86	0.93	16
N2P2*	0.52	0.83	14

*Data used for model calibration

LR90

For the LR90 growth season, despite a low r^2 value, LAI simulations were judged to be reasonable based on De Jager's (1994) reliability criteria (r^2 = 0.61, D = 0.88, MAE = 18) (Figure 5.5). LAI was under-estimated for the P10, P40 and F10 treatments. This underestimation of LAI is associated with the underestimation of TDM for these treatments.

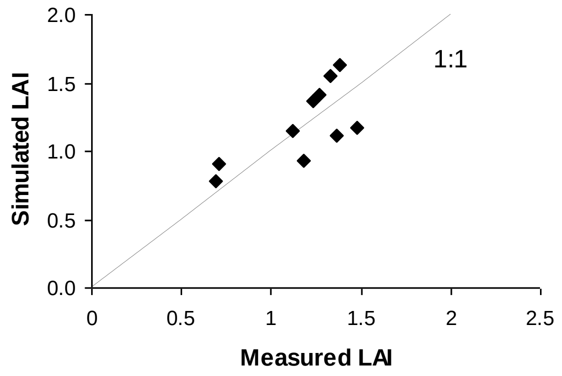

Figure 5.5 Simulated versus measured values for leaf area index (LAI) for the LR 90 growth season

5.3.3 Profile water content and deep drainage

Profile water content for the N2P1/F40 treatment is presented in Figure 5.6. Profile water content was well simulated for all treatments by the model. During the SR89 growth season, treatments N1P0, N1P1, N2P0, N2P1 and N2P2 experienced water stress for 1, 3, 1, 22 and 27 days, respectively, predominantly from early February to early March. During the LR90 season, only a single day of water stress was experienced by all of the treatments.

Modelled drainage below 1.5 m ranged from 275 mm for the treatment receiving the lowest rates of N and P (N1P0) to 9 mm for the treatment receiving the highest rates of N and P (N2P2) for the SR89 season. For the LR90 growth season, 180 mm of drainage was simulated for the treatment receiving the lowest P application rate (P0), while 143 mm of drainage was simulated for the treatment receiving the highest P rate (F40).

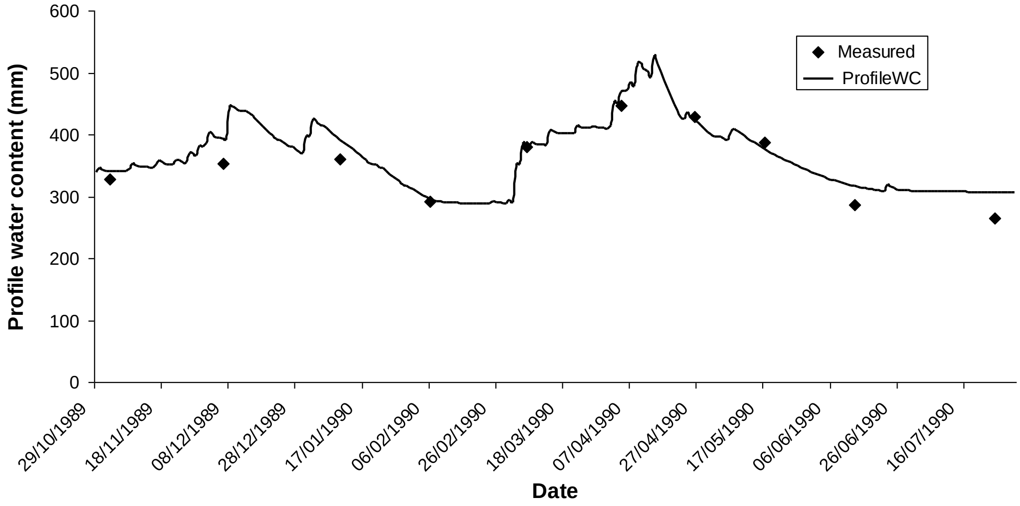

Figure 5.6 Profile water content (PWC) for the SR89 N2P1 treatment and the LR90 F40 treatment

Statistical evaluation was carried out for the five treatments that continued over the two consecutive growth seasons (Table 5.8), and all fell within reliability criteria range (De Jager, 1994).

Table 5.8 Statistical evaluation of measured and simulated values for profile water content (PWC) over consecutive growth seasons for selected treatments

Treatment	r^2	D	MAE (%)
N2P0/P0	0.95	0.96	5
N2P1/P10	0.92	0.99	6
N2P2/P40	0.88	0.96	5
N2P0/F10	0.98	0.89	5
N2P1/F40	0.82	0.97	4

5.3.4 Aboveground N and P mass

SR89

Aboveground N mass was over-predicted for the N1P0 treatment and under-estimated for the N2P2 treatment (Figure 5.7). Aboveground P mass was initially also over-predicted for the N1P0 treatment but not for the final measurement. Aboveground P mass was slightly over-estimated for the N1P1, N2P1 and N2P2 treatments, and under-estimated for the N2P0 treatment.

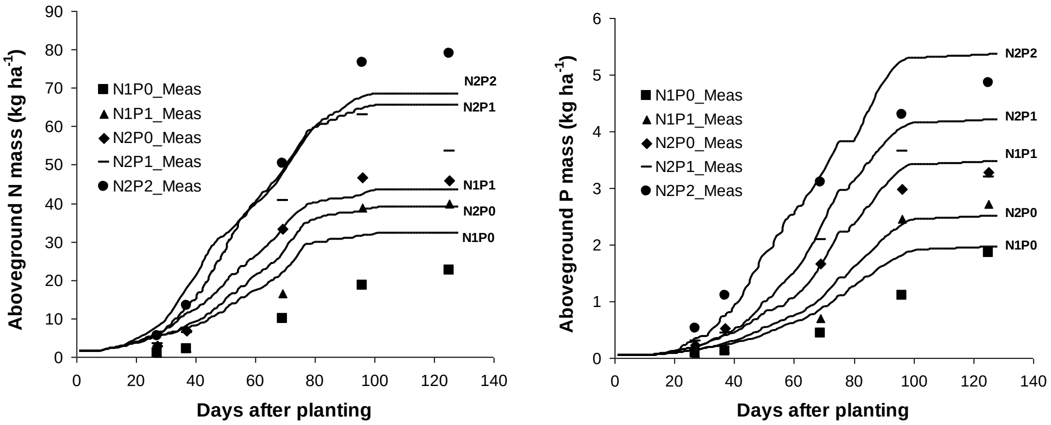

Figure 5.7 Measured and simulated values for aboveground N mass (left) and aboveground P mass (right) for the SR89 growth season

Statistical analysis shows that the model predicted aboveground N and P mass with satisfactory levels of accuracy for the five treatments (Table 5.9). The highest MAE for aboveground N mass (50%) was obtained for the treatment receiving the highest N and lowest P fertilizer rate (N2P0), with N uptake being under-estimated. For P, the highest MAE (38%) was obtained for the N1P0 treatment in which aboveground P mass was over-estimated during the middle of the growth season. For the rest of the treatments, aboveground N and P mass was relatively well simulated according to De Jager's (1994) reliability criteria.

Table 5.9 Statistical evaluation of measured and simulated values for crop nitrogen (N) and phosphorus (P) uptake during the SR89 season

Treatment	r^2		D		MAE (%)	
	N	P	N	P	N	P
N1P0	0.94	0.89	0.97	0.93	15	38
N1P1	0.84	1.00	0.94	1.00	26	8
N2P0	0.95	0.99	0.91	0.99	50	13
N2P1	0.98	0.98	0.99	0.97	8	18
N2P2*	0.96	0.99	0.98	0.98	9	15

*Data used for model calibration

As only a single measurement of grain N and P mass was made for each treatment, measured versus simulated values for the five treatments were plotted in Figure 5.8. Grain N mass (r^2 = 0.89, D = 0.80, MAE = 33) was more accurately simulated than grain P mass (r^2 = 0.90, D = 0.51, MAE = 48), with grain N mass consistently over-estimated by the model while grain P mass was consistently under-estimated by the model.

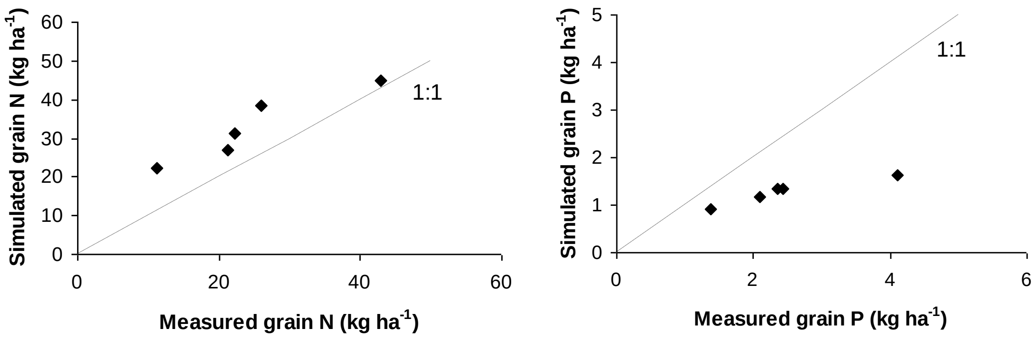

Figure 5.8 Simulated versus measured values for grain N mass (left) and grain P mass (right) for the SR 89 growth season

LR90

Measured values for aboveground P mass for treatments P40 and F40 were very similar at harvest (Figure 5.9). Measured values for aboveground P mass were also consistently higher for the P40 than for the F10 treatment. This indicates high P uptake from the banded fertilizer P applied during the previous growth season. The model simulated that 19.5 kg ha^{-1} of the original 40 kg ha^{-1} banded P application was still available for uptake at planting of the second crop for the P40 treatment. Although aboveground P mass was higher for the F10 than the P10 treatment for the first four measurements as was expected, the opposite was true for the final measurement, and this could reflect a sampling error. The most accurate simulations for final aboveground P mass were obtained for the F40 and F10 treatments.

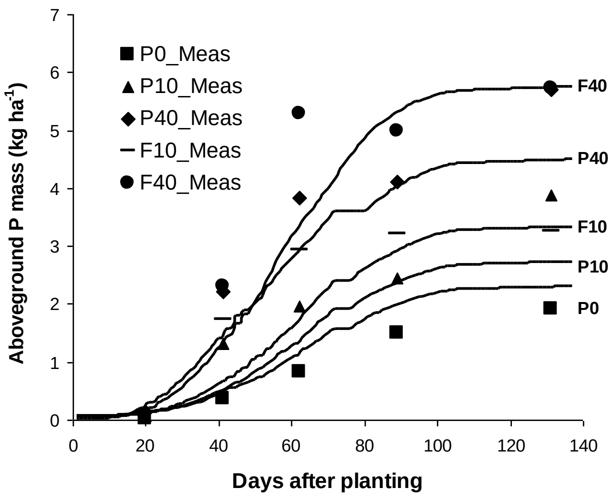

Figure 5.9 Measured and simulated values for aboveground P mass for the LR90 growth season

N uptake was generally better simulated than P uptake, especially for the P10, F10 and F40 treatments (Table 5.10). N uptake was however greatly over-predicted by the model for the P0 treatment.

Table 5.10 Statistical evaluation of measured and simulated values for crop nitrogen (N) and phosphorus (P) uptake for the LR 90 season

Treatment	r^2		D		MAE (%)	
	N	P	N	P	N	P
P0	0.97	0.99	0.67	0.96	132	29
P10	0.94	0.89	0.97	0.91	19	28
P40	0.97	0.90	0.98	0.97	14	17
F10	0.97	0.82	0.99	0.91	11	24
F40	0.93	0.90	0.97	0.89	17	30

Unlike the previous season simulations for the LR90 season did not perform as well, with overall grain P mass (r^2 = 0.55, D= 0.56, MAE = 32) only slightly better simulated than overall grain N mass (r^2 = 0.33, D= 0.52, MAE = 39) for the five treatments (Figure 5.10). Grain N mass was over-predicted for the P0, P10 and F10 treatments. Grain P mass was over-predicted for the P0 treatment, well simulated in the P10 and F10 treatments and under-predicted for the P40 and F40 treatments.

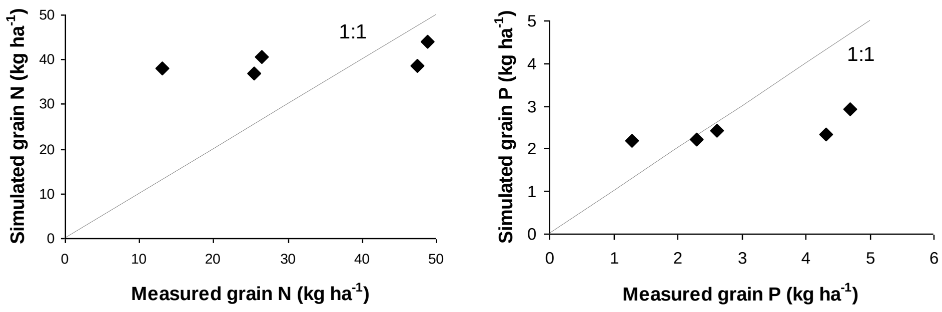

Figure 5.10 Simulated versus measured values for grain N (left) and grain P (right) for the LR90 growth season

5.3.5 Nitrogen:Phosphorus ratios

Nitrogen:Phosphorus ratios from the shoot N and P analyses carried out on 5 February 1990 and N:P ratios for the simulated crop for the same date are presented in Figure 5.11. Based on the approach by Koerselman and Meulen (1996), for the measured data P was limiting for the N1P0, N2P1 and N2P2 treatments, while N and P were limiting for the N1P1 and N2P0 treatments. The simulation results were somewhat different with P limiting for the N1P0 and N2P0 treatments, N limiting for the N1P1 and N2P2 treatments, and N and P limiting for the N2P1 treatment.

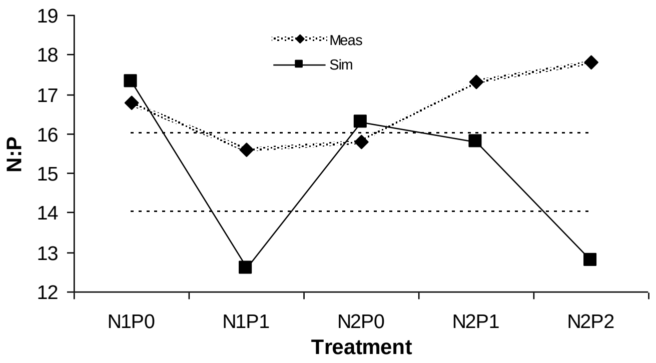

Figure 5.11 Measured and simulated shoot nitrogen:phosphorus ratios for the five treatments in the SR89 growth season. Measured data are based on analyses carried out on 5 February 1990 (before grain filling)

N:P ratios from the shoot N and P analyses carried out on 12 June 1990 (LR90 growth season) and N:P ratios for the simulated crop for the same date are presented in Figure 5.12. The measured P data indicate P was limiting in all treatments except the F40 treatment. The simulations demonstrate similar trends with the largest differences between the measurements and simulations occurring in the P0 and P10 treatments. The high N:P ratios obtained for the simulated P0 (N:P = 30) and P10 (N:P = 26) treatments indicates that the model did not simulate realistic proportions of N and P uptake by the crop. This is attributed to the over-estimation of N uptake rather than an under-estimation of P uptake.

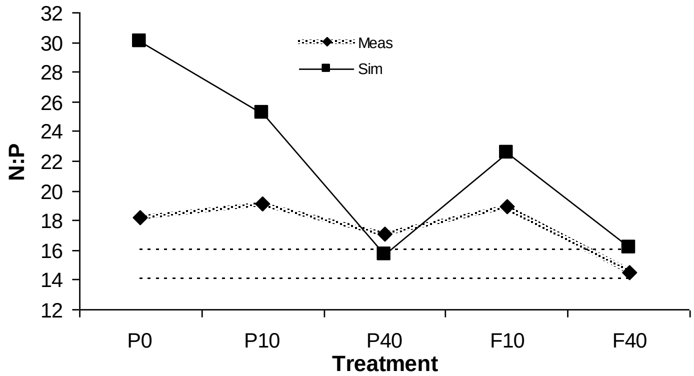

Figure 5.12 Measured and simulated shoot nitrogen:phosphorus ratios for the five treatments in the LR90 growth season for the analyses done on 12 June 1990 (before grain filling)

5.4 GENERAL DISCUSSION

The model performed well according to De Jager's (1994) model reliability criteria in simulating TDM and yield, although TDM for treatments P10, P40 and F40 were under-estimated in the LR90 growth season. Reasons for this under-estimation are not clear. Higher water stress was predicted for the SR89 growth season than for the LR90 season, and PWC was well simulated for all treatments continuously over both growth seasons. Furthermore, updating soil layer water content at planting for the LR90 growth season did not lead to any significant improvements in the simulations. As N and P uptake was also judged to be well simulated, this under-estimation is not attributed to an over-estimation of nutrient stress. The LR90 season was observed to be considerably wetter than the long-term average (Probert and Okalebo, 1992), so model calibration could have been inadequate to cope well with this season.

Leaf Area Index (LAI) was simulated relatively well during the SR89 growth season. LAI was initially underestimated for treatments N1P1 and N2P0 in the SR89 season, and for the treatments P10, P40 and F10 for the LR90 season. Inaccuracies in the simulation of LAI for the LR90 growth season are attributed to underestimation of TDM. Probert and Okalebo (1992) observed that P deficiency decreased the rate of leaf appearance. Jamieson and Semenov (2000) suggest that certain modelling approaches may be inadequate where lack of mechanical description causes inaccuracy. The effect of N and P deficiencies on crop canopy development may therefore require further attention.

The uptake of N was better simulated for the SR89 season than for the LR90 season. The large over-estimation of N uptake for the P0 treatment during the LR90 growth season may be indicative of the important role of the plant P status in the uptake of other nutrients, a feature which is not yet well represented in the model. Crop P uptake is highly complex, with plants often making use of mycorrhizae and root exudates to increase P uptake under seemingly deficient conditions. P uptake using the new approach presented in this paper was judged to be well simulated. Over both seasons, grain P mass was under-estimated for all treatments. This indicates that simulating grain P mass by adding only the P taken up by the crop following the onset of flowering may be inadequate. An alternative approach could be to predict grain P mass by using a crop-specific grain N:P ratio, provided that grain N mass can be adequately simulated. As total aboveground P mass was well simulated the modelling of crop P uptake from fertiliser bands and the simple approach used to estimate dissolution of these bands was also judged to be satisfactory. Further studies on the dissolution of banded P over time, and the effect of factors such as soil type, temperature and water content is suggested to improve our abilities to model banded P dissolution and uptake.

Critical assessment of model performance when comparing measured and simulated data requires careful consideration of field data variability and accuracy. Errors in data can be expected in any extensive dataset from a field trial and this needs to be checked rather than blindly assuming that good correlation between measured and simulated values indicates accurate model simulations. Errors in measurements may be caused by several factors, including spatial variability, sampling error, lab analysis variations in accuracy and others. Several anomalies were observed in the data used in this study that need to be considered when assessing model performance. For example measured TDM decreased between the fourth and fifth sampling events for treatments N2P0, N1P1, N2P1, N2P2, F10 and F40. For treatments N1P1, N2P1 and F10 a reduction in aboveground crop N mass was observed between the fourth and fifth sampling events. Only slight increases in aboveground N mass were observed for the N2P0 and P0 treatments. A similar phenomenon was observed when reviewing a similar dataset for maize (Schmidt, 1993). On the contrary, aboveground crop P mass increased between the fourth and fifth sampling events for all treatments. Whether decreases in TDM or aboveground crop N mass between the fourth and fifth sampling events were due to sampling error, or as a result of a natural phenomenon such respiration or leaf senescence, is unclear. As any natural decreases in dry matter and aboveground N mass are not simulated by SWB-Sci, a decrease in one of these variables will most likely result in less favourable statistics for model performance. Further work on this issue is therefore recommended.

In the mechanistic modelling of crop N and P uptake simultaneously, the comparison of measured and simulated shoot N:P ratios can provide further insights into model performance and potential model weaknesses. Ratios can provide information on which nutrient may be limiting in a particular scenario, or whether unrealistic uptake of one nutrient relative to another is being simulated. For the SR89 season, simulated N:P ratios were observed to fluctuate more widely between treatments than for measured values. Very high simulated N:P ratios were observed for P0 and P10, and this is related to the over-estimation of N uptake for these two treatments. Such high ratios have been recorded in the literature, however, especially for the earlier growth stages in maize when < 75% of plants have silks visible (Jones, 1983). Ratios were observed to reflect expected deficiencies according to N and P fertilization rates in most cases, and measured and simulated values often showed similar trends across seasons. The 14-16 guideline suggested by Koerselman and Meulen (1996) to determine whether N or P is limiting does seem appropriate for maize. This will however require further investigation using data from a wide range of maize trials and other crops to fully explore its applicability and usefulness in crop growth modeling.

Higher drainage was simulated for the treatments receiving lower rates of N and/or P fertilizer application due to related poor crop growth. Higher drainage volumes can result in increased nutrient leaching, and highlights the importance of aligning fertilization strategies with water availability to reduce nutrient leaching from the soil profile.

5.5 CONCLUSIONS

In the first season, the model performed well simulating TDM, yield, LAI and crop N and P uptake considering the complexity of the system. Relative effects of different N and P fertilizer application rates were also well predicted by the model in the SR89 growth season. Simulations were less accurate, but often still met recommended model performance criteria for the second season when the model was run continuously over the two seasons. Errors in measured data could have contributed to some of the differences between measured and simulated values, and highlights the need to check and ensure sufficient effort is invested in obtaining quality measurements.

The newly developed approach to model crop P uptake and stress shows good potential in predicting effects of P stress on dry matter production. Modelling soil P availability and uptake is challenging, and further tests using a variety of soils is recommended. The approach introduced to model banded P was also found to perform well, but further studies on crop availability and persistence of banded fertilizer P is recommended. Additional model refinement and calibration work can be expected to improve the accuracy with which the model simulates nutrient dynamics. Unfortunately soil N and P levels were not measured during the growth season and could therefore not be tested in the model. Far more work has been done by the scientific community to test crop N models than crop P models. SWB-Sci has been designed as a user-friendly, generic-crop model and has to date been successfully applied to a broad range of cropping systems. Successful enhancements to the model, as demonstrated in this paper, highlights its potential as a tool to further improve understanding and management of N and P in cropping systems, and to minimise unwanted impacts of NPS pollution from agriculture.

5.6 ACKNOWLEDGEMENTS

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CHAPTER 6

MONITORING AND MODELLING MOBILE AND IMMOBILE SOIL WATER NITROGEN AND PHOSPHORUS CONCENTRATIONS TO ESTIMATE LEACHING LOSSES

ABSTRACT

Nitrogen (N) and phosphorus (P) leaching losses from cropping systems can lead to a deterioration in water quality and represent an economic loss to farmers. Quantifying N and P losses in deep drainage is highly challenging due to uncertainties associated with estimating drainage fluxes and solute concentrations in the leachate. Active and passive soil water samplers are used to determine solute concentrations and estimate leaching but give limited information on water fluxes. Mechanistic models are also used to estimate leaching, but often require complex calibration with measured data to ensure their reliability. Data from a drainage lysimeter trial under irrigation in which soil profile nitrate (NO_3^-) and P concentrations were monitored using ceramic suction cups (active sampler) and wetting front detectors (passive sampler) was compared to N and P concentrations in immobile and mobile soil water phases as simulated by the SWB-Sci model. SWB-Sci is a daily time-step, cascading soil water and solute balance model, and mobile N and P concentrations were obtained using a simple solute mixing fraction approach. As hypothesized, suction cup concentrations aligned closely with immobile soil water concentrations, while wetting front detector concentrations aligned closely with mobile soil water phase NO_3^- concentrations. Soil P concentrations were adequately monitored using wetting front detectors but were often over-estimated by the model. These results for NO_3^- demonstrate that monitoring and modelling can be used together to estimate NO_3^- leaching losses. Further work on simulating P solubility in soils is needed before such an approach is used for this reactive solute. The monitoring of changes in nutrient concentrations in soil to obtain threshold N and P levels on which to base 'adaptive' fertilization strategies to reduce leaching losses shows high potential.

6.1 INTRODUCTION

Minimizing nitrogen (N) and phosphorus (P) leaching losses from cropping systems requires a good understanding of the key physical, chemical and biological processes impacting on solute movement in soils; and additional uncertainties arise due to the heterogeneous nature of soils (Addiscott, 1996). Predicting the movement of solutes through soil is far more challenging than predicting the soil water status (Flühler et al., 1996), making the quantification of N and P leaching losses difficult. Although physical monitoring provides direct estimates of solute concentrations in soil water, uncertainties regarding the pore volume being sampled and drainage fluxes make an estimation of actual leaching losses difficult. Mechanistic modelling can be used to obtain concentrations as well as fluxes, but such models often require extensive calibration using measured data, and uncertainty remains regarding how well the key processes are represented in the model (Keating et al., 2001). The consideration of mobile and immobile water phases, arising from a spectrum of pore-water velocities associated with the infiltrating water, is widely accepted as important in solute flux modelling (Turner, 1958; Coats and Smith, 1964; Clothier et al., 1995; Ilsemann et al., 2002). The mobile water phase undergoes miscible displacement by incoming precipitation or rainfall water, while the immobile water phase is bypassed (Corwin et al., 1991).

A range of devices have been developed over the years to sample soil water solutions, and are classified as either active or passive samplers, depending on whether action needs to be taken by the operator to obtain a sample (Litaor 1988, Paramasivam et al., 1997). Active samplers, most often ceramic suction cups (SC), are commonly used worldwide. The wetting front detector (WFD), is a funnel shaped passive sampler which is buried in the soil and is able to alert a user by means of a mechanical float when a wetting front has passed a specific depth in the soil, thereby making it a potentially useful irrigation and solute monitoring tool (Stirzaker, 2003). The WFD collects and stores a water sample from a wetting front as long as the suction behind the front is wetter than -3 kPa (Stirzaker, 2008). The funnel shape means that unsaturated flow lines converge towards a small area at its base, and after an irrigation/rainfall event, water is withdrawn from the cavity by capillary action (see www.fullstop.com.au). WFDs have been used successfully to improve understanding of the leaching of salts and NO_3^- in a system to which high rates of municipal sludge were applied (Tesfamariam et al., 2009). Differences in solute concentrations of soil water samples collected by active and passive samplers under temporally and spatially similar conditions can differ markedly, and identifying the reasons for these differences remains challenging (Haines et al., 1982). As passive samplers only collect samples under relatively wet conditions, they are more indicative of the soil water moving through the root zone, as opposed to suction cups which are more indicative of what plants are able to take up (Magid and Christensen, 1993; Simmons and Baker, 1993). As reviewed by Stirzaker and Hutchinson (1999), initial water content together with four principal factors affect the composition of solute collected from an active sampler, namely: (1) the suction applied to the cup, (2) the time period the suction is applied, (3) the porous material used for the suction cup, and (4) the size of the cup. Suction cups can influence soil solution chemistry through the adsorption of ions, the loss of volatile compounds, changes in redox dependent ions, and pH changes (Grobler et al., 2003; Corwin, 2002). Certain advantages and disadvantages exist in the in-field deployment of either active or passive samplers (Silkworth and Grigal, 1981; Barbee and Brown, 1986). Several studies have shown that only a fraction of phosphate was recovered after being passed through a ceramic SC (Hansen and Harris 1975; Tischner et al. 1998), so an additional advantage of WFDs is that these samplers will not adsorb phosphate.

SWB-Sci is a mechanistic, generic crop model which has undergone extensive testing regarding its ability to simulate crop growth and the soil water balance (Jovanovic and Annandale 1999; Jovanovic et al., 1999; Annandale et al., 2000; Jovanovic and Annandale 2000; Jovanovic et al., 2000; Tesfamariam, 2004). Recently, N and P modelling subroutines have been included into the model and tested using several datasets from maize and wheat trials (see Chapters 4 and 5). Soil water is simulated using a multi-layered cascading approach and crop growth is simulated by calculating a daily dry matter increment which is either radiation or water limited. Currently, a wide range of models are available to estimate N and P leaching losses at various scales. The routines used by these models to simulate vertical solute movement in the soil can differ markedly with regards to the approach used to simulate incomplete solute mixing, also referred to as bypass flow, during a drainage event. CropSyst, for example accounts for bypass flow in its cascading soil water balance using an approach developed by Corwin et al. (1991) using Cl^{-1} as a tracer (Stöckle et al. 2003); while the SWIMv2.1 model which uses a finite difference model, makes use of a diffusion coefficient and pore water velocity to estimate solute concentrations in the mobile water phase. This diffusion coefficient is dependent on temperature, concentration of the solute, and the ionic composition of the solute (Verburg et al. 1996). Larger scale models often make use of much simpler approaches. The EPIC model (Williams et al., 1983) for example uses a user defined fraction to reflect the amount of interaction occurring between mobile and immobile soil water NO_3^-. The representation of incomplete solute mixing in a wide range of models highlights that it is an important process. Model testing exercises, especially for N, often compare simulated values with measured crop N uptake data and measured soil inorganic N levels at different depths, but to the best of our knowledge, the mobile and immobile soil water solute concentrations have not yet been compared to measured concentrations from active and passive samplers.

The hypothesis tested in this paper was that simulated immobile soil water phase NO_3^- concentrations align with concentrations measured in SCs, while simulated mobile soil water phase NO_3^- concentrations align with concentrations measured in WFDs. Correspondingly, simulated mobile soil water phase P concentrations and those measured in WFDs will also align closely. The hypothesis that simulating incomplete solute mixing is important, and that it can be represented using a simple algorithm included in SWB-Sci was also tested. These hypotheses were tested using a large drainage lysimeter into which SCs and WFDs were installed to provide measured data with which to test the model.

6.2 MATERIALS AND METHODS

6.2.1 Drainage lysimeter trial

A drainage lysimeter with a volume of 6.1 m^3, a surface area of 4.7 m^2 and a depth of 1.3 m was used to represent a typical rootzone which could be used effectively to study leaching losses at the local scale. The lysimeter was packed with sandy clay loam (18% clay) in mid-2006 and allowed to settle naturally for 17 months. The lysimeter is located at the University of Pretoria Experimental Farm (25°44'S

28°15'E, 1370 m above sea level). A gravel layer was placed at the base of the lysimeter to facilitate drainage. The following instrumentation was installed into each lysimeter: suction cups (SCs) at 15, 30, 45, 60, 80 and 100 cm depths; wetting front detectors (WFDs) at 15, 30, 45 and 60 cm depths; and Decagon ECH_2O-TE sensors at 15, 30, 45, 60 and 80 cm depths (hereafter referred to as capacitance sensors). Data characterizing the initial soil properties were obtained by averaging results from samples collected at 0-15, 15-30, 30-45, 45-60, 60-80 and 80-100 cm depths (Table 6.1).

Table 6.1 Properties for the drainage lysimeter soil

SOIL PROPERTY	VALUE
pH (H_2O)	4.73
Bulk density (kg m^{-3})	1120
Base Saturation (%)	44.52
EC (dS m^{-1})*	1.40
CEC (cmol(c+) kg^{-1})	4.418
C (%)	1.11
Sand (%)	72.3
Silt (%)	9.66
Clay (%)	18
Bray I P (mg kg^{-1})	11

*Saturated paste water extract

The vegetable test crop swiss chard (*Beta vulgaris* ssp. *cicla*) was chosen for this trial due to its ease of cultivation, relatively deep root system (~ 80 cm) and because multiple harvests of the outer leaves can be made without having to re-sow the crop. The crop was planted at an effective spacing of 20 × 30 cm. Harvesting was done by removing all leaves except the middle three from each plant. A representative 1 m^2 plot was harvested and dry mass determined by drying in an oven at 60°C for 4-5 days. Leaf samples were analyzed for N and P content at each harvest, except for the final harvest when samples were spoilt, so an average N and P percentage for the three previous analyses was used.

Suction was applied to the SCs using a 60 ml syringe immediately following irrigation/rainfall. According to the manufacturers, pulling the piston of the syringe back 2-3 times creates a suction of 60-70 kPa. If available, soil water samples were collected from both the WFDs and SCs the day following irrigation or rainfall.

Drainage from the lysimeter was captured in large drums from which the quantity could be measured and a water sample taken for analysis. For each sample, NO_3^- was analyzed using a Merck RQEasy Nitrate Reflectometer, and P was analyzed using a C99 Multiparameter Bench Photometer (Hanna Instruments, Italy). P was only determined for samples collected by WFDs, as ceramic SCs are known to adsorb P from the soil water.

Irrigation was applied with the primary objective of minimising both plant water stress and N leaching. Following planting, small amounts of irrigation water were applied at regular intervals. Thereafter, irrigation was applied to allow the WFD placed at 15 cm to respond, and as daily crop water demand increased, water was increased to allow the WFD placed at 30 cm to respond. Applications were made at weekly intervals, or more often if judged necessary.

Nitrogen fertilizer (as calcium ammonium nitrate) was applied as a top dressing if an average NO_3^- concentration from WFD samples was less than 100 mg l^{-1}. P fertilizer (as single superphosphate) was also applied as a top dressing three times during the growth season. Timing and application rate for N and P fertilization is presented in Table 6.2. The soil was limed and all other nutrients were applied as deemed necessary following a comprehensive soil analysis and assumed to be non-limiting.

Table 6.2 Nitrogen (N) and phosphorus (P) fertilization over the growth season

Days after planting	**N/P applied** **kg ha^{-1}**
0	0 N/49 P
7	10 N/0 P
108	10 N/49 P
132	10 N/0 P
148	30 N/0 P
175	30 N/49 P

6.2.2 Modelling incomplete solute mixing

A simple algorithm was included into SWB-Sci to represent the influence of incomplete solute mixing on solute concentration in the mobile water phase. This was based on the assumption that incomplete mixing takes place when enough water is entering a layer to increase the volumetric water content (VWC) of that layer to above FC (defined as water content at 10 kPa). This is done by using a layer-specific *Solute Mixing Fraction* as follows:

$$[Solute]_{mob} = \frac{SoluteMass_{layer} \times F_{mix}}{\theta_{layer} \times d_{layer} \times \rho_w} \tag{6.1}$$

where $[solute]_{mob}$ = mobile soil water phase solute concentration
$SoluteMass_{layer}$ = mass of solute in layer
F_{mix} = solute mixing fraction
θ_{layer} = volumetric water content of layer
d_{layer} = depth of layer
ρ_w = density of water

An F_{mix} of 0.7 was selected through iteration for the sandy clay loam used in this trial.

Crop growth parameters for swiss chard were obtained from a trial conducted in close proximity to the lysimeter trial in the summer of 1996/1997 (Jovanovic and Annandale, 2000). Further calibration for N and P modelling, involving the estimation of crop N and P uptake factors and optimal P concentrations, was done using data from a preliminary trial conducted during the previous season (2007). Soil analysis results were used as inputs for the model, including organic matter %, texture, soil pH(H2O) and cation exchange capacity. The soil was classified as 'highly weathered' for P modelling purposes (Sharpley et al. 1989; Van der Laan et al. in press), so only clay percentage was required to estimate the P availability index. Soil labile P was initialized using results of the soil Bray I P analyses, while NO_3^- levels were initialized using concentrations obtained from the SCs. Ammonium (NH_4^+) levels were assumed to be 1/8th of NO_3^+ values. Finally, calibration was carried out to match simulated cumulative drainage with end of season measurements through adjustment of the drainage factor (0-1) and drainage rate (mm d^{-1}) values, with the aim of ultimately assessing the ability of the model to simulate dynamic changes in N and P concentrations in the mobile and immobile soil water phases. The calibration yielded a drainage factor of 0.75 and a drainage rate of 55 mm d^{-1}. For a layer, water in excess of FC can potentially drain to the next layer, and the drainage factor determines what fraction of that water will drain each day. The drainage rate (mm d^{-1}) sets an upper limit on the drainage that can take place in one day.

6.3 RESULTS

6.3.1 Rainfall and irrigation

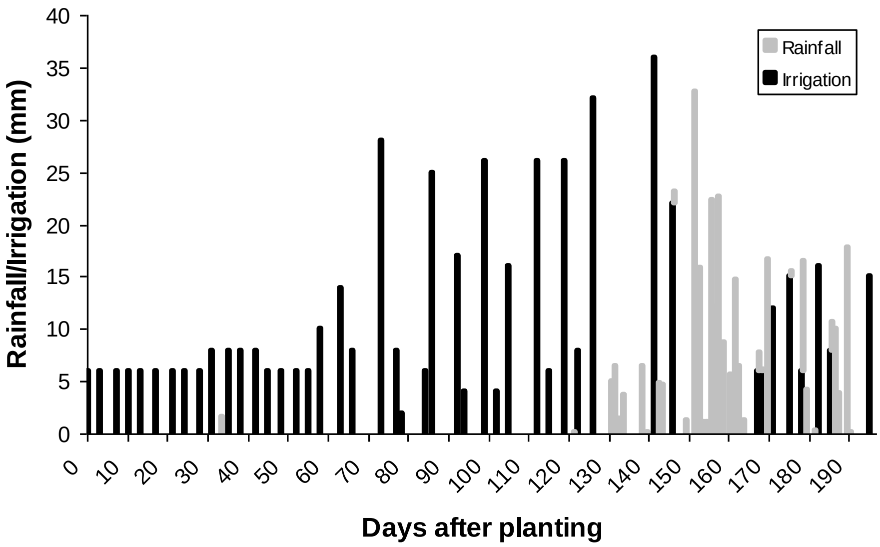

Figure 6.1 Rainfall and irrigation for the growth season

Total water input over the growth season to the lysimeter included 495 mm of irrigation and 251 mm of rain. Most of the rain occurred 130 days after planting (DAP) (Figure 6.1). Depending on antecedent water content, irrigation applications of 14-22 mm were required for the WFD at 15 cm to respond, while irrigation applications of 20-36 mm were required for the WFD at 30 cm to respond.

6.3.2 Soil water content and response of WFDs

Measured versus simulated profile water content data to a depth of 90 cm is presented in Figure 6.2. Lack of agreement between measured and simulated data early in the season is attributed to the sensors still 'settling in' after being installed only a few days before planting. It is also possible that the automated sensor at 15 cm under-estimated soil water content. Thereafter measured and simulated values were in better agreement for the remainder of the growth season.

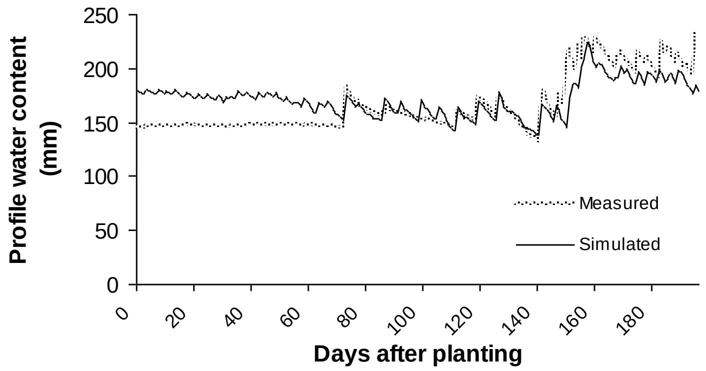

Figure 6.2 Measured and simulated profile water content over the growing season to a depth of 90 cm (measurements are based on data from the capacitance sensors)

Measured and simulated VWC (θ), and WFD response at depths of 15, 30, 45 and 60 cm is presented in Figure 6.3. While there were periods of difference between measured and simulated VWC which could be attributed to soil heterogeneity and variation in sensor sensitivity to changes in water content, the model performed reasonably well in simulating soil layer VWC. The WFDs were clearly observed to respond when increases in VWC were measured by the automatic sensors which coincided with times that high water potentials were simulated (data not shown). These WFDs typically respond to wetting fronts in the range of 0 to -3 kPa (Stirzaker, 2008). The highest water potentials simulated in SWB-Sci ranged from -4 to -9 kPa, and this is attributed to the daily time step used in the model, resulting in a daily water potential lower than for the wetting event itself.

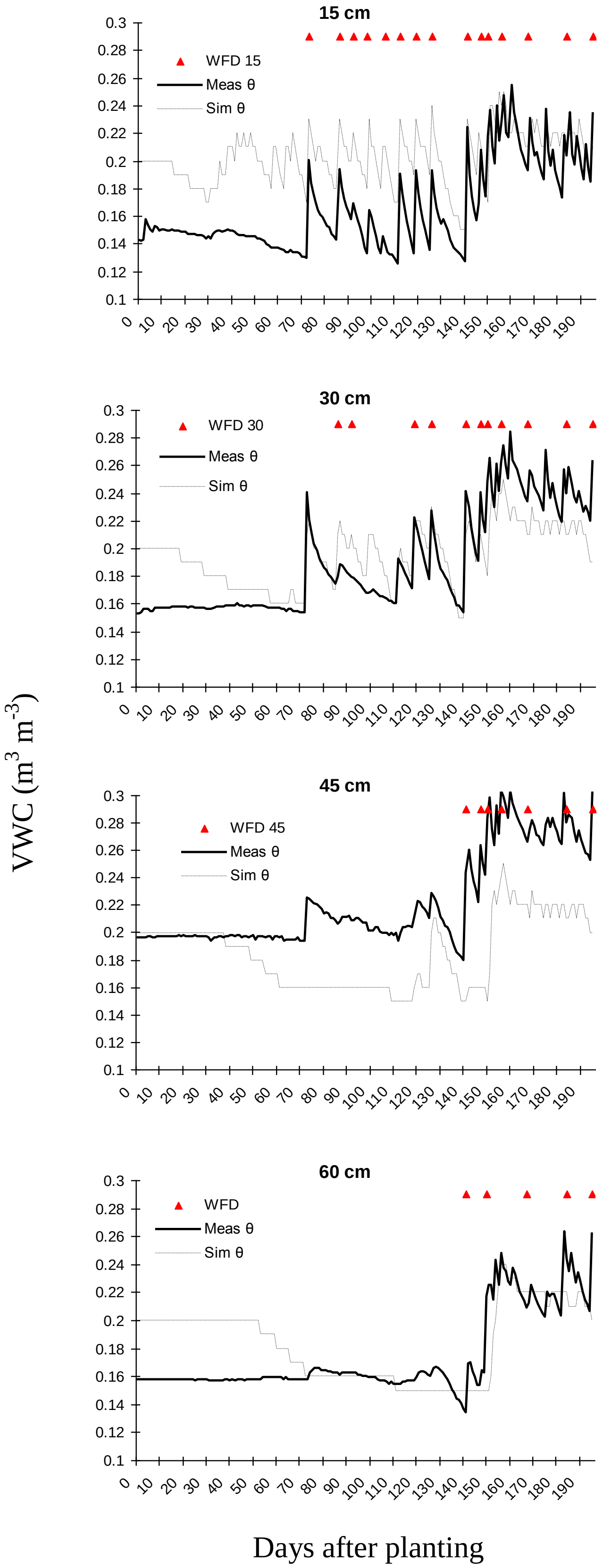

Figure 6.3 Measured and simulated volumetric water content (VWC), and WFD response at depths of 15, 30, 45 and 60 cm

6.3.3 Cumulative aboveground dry matter production and N and P uptake

Total aboveground dry matter (TDM) production ranged from 1600 to 2900 kg ha^{-1} per harvest and was well simulated by the model (Figure 6.4). Aboveground N mass ranged from 51 to 70 kg N ha^{-1} per harvest. Crop N removed was significantly over-estimated for the first harvest by the model, but was accurately simulated for the following three harvests. The amount of P removed ranged from 3 to 40 kg P ha^{-1} per harvest. This was also accurately simulated except for the third harvest when, as with TDM, P mass was under-estimated. Unusually high leaf P concentrations were measured for this third harvest, so this may also be attributed in part to a laboratory analysis error.

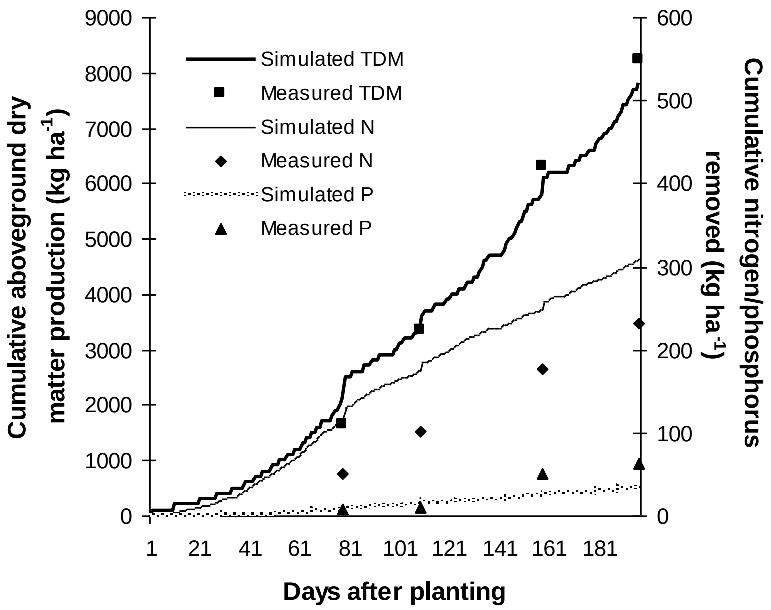

Figure 6.4 Cumulative aboveground dry matter (TDM) production (primary y-axis), and N and P removal (secondary y-axis) over the growth season

6.3.4 Drainage and leaching

Cumulative drainage from the lysimeter over the growth period was measured at 45 mm, with the first appearance of deep drainage occurring from 150 DAP (Figure 6.5). Despite calibrating the model to obtain an equal final volume, the measured and simulated differed significantly through the growth season. The simulated drainage commenced later but then occurred more rapidly in comparison to the measured drainage. This may partly be attributed to the nature of drainage from a lysimeter, in which a saturated lower boundary is required to create free water for drainage.

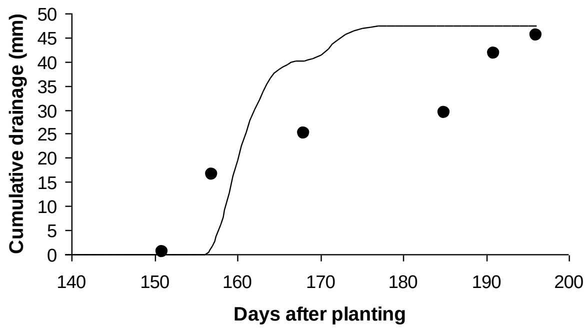

Figure 6.5 Measured and simulated cumulative drainage (mm) over the growth season

A total of 86 kg ha^{-1} NO_3-N was measured to have leached from the 1.3 m soil profile (Figure 6.6). Measured NO_3^- concentrations in the drainage water increased rapidly from 330 mg l^{-1} at 151 DAP to 1008 mg l^{-1} on 168 DAP and thereafter remained relatively constant at around 1000 mg l^{-1}. Similar to drainage, NO_3-N leaching was initially under-estimated, then over-estimated through the mid-season period, with the final end of season simulated cumulative NO_3-N leached (74 kg NO_3-N) in reasonable agreement with the measured value.

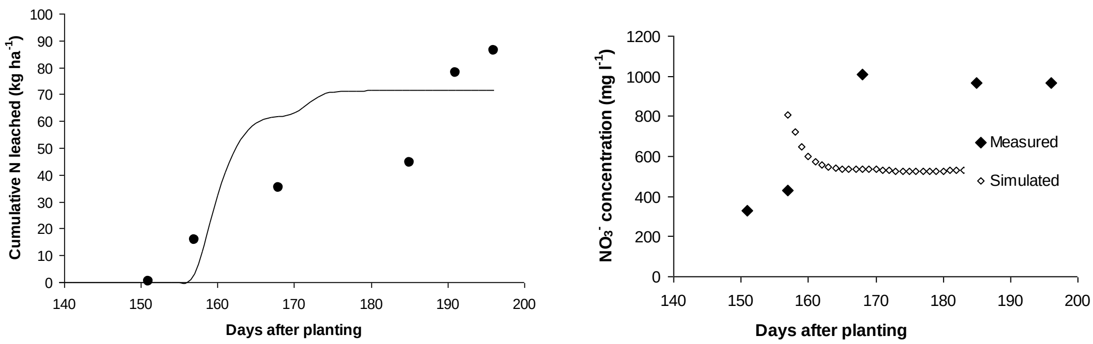

Figure 6.6 Measured and simulated cumulative N leached (left) and drainage water NO_3^- concentrations (right)

For P, a total of 0.44 kg ha^{-1} was measured to have leached from the soil profile, with P concentrations in the drainage water ranging from 0.46 – 1.17 mg P l^{-1} (Figure 6.7). SWB-Sci greatly over-estimated P concentrations and hence cumulative P leached from the profile, by 3-fold.

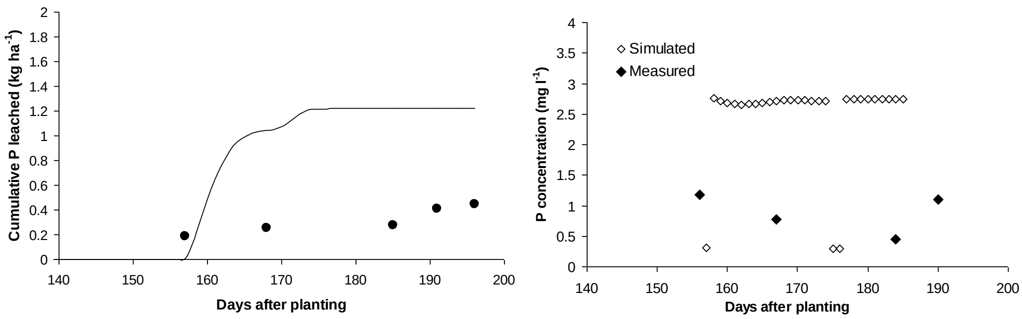

Figure 6.7 Measured and simulated cumulative P leached (left) and drainage water P concentrations (right)

6.3.5 Soil water nitrate and phosphorus concentrations

6.3.5.1 Nitrate

High soil solution NO_3^- concentrations were observed at all depths at planting despite no fertilization having taken place since the previous season (Figure 6.8). These high NO_3^- concentrations are therefore attributed to mineralization occurring over a four month fallow period during which very little drainage took place. After planting, the removal of N from the system by an actively growing crop is observable in the measured data. In almost all cases, measured NO_3^- concentrations from WFDs were less than those measured from SCs. This is consistent with lower solute concentrations found in the mobile soil water phase due to bypass flow or incomplete mixing with the immobile soil water phase as observed in other experiments (Stirzaker and Hutchinson, 1999). Another reason for obtaining higher NO_3^- concentrations from the SCs could be because the SCs are sampling from the smaller pores, and hence sites expected to have higher microbial activity and greater N mineralization. Significant positive correlations ($r^2 > 0.50$) between NO_3^- concentrations measured in SCs and WFDs were only observed at 45 cm ($r^2 = 0.66$).

Lack of correlations at the other depths indicates that different sampling mechanisms are clearly being employed by SCs and WFDs.

The addition of 10 kg N ha^{-1} 7 DAP is observable by an associated increase in NO_3^- concentration as detected by the SCs placed at 15, 30 and 45 cm (Figure 6.8). The effect of a second addition of 10 kg N ha^{-1} 108 DAP is only observable in the SC and WFD at 15 cm. A third addition of 10 kg N ha^{-1} 132 DAP does not result in a clear increase in SC NO_3^- concentration. After an addition of 30 kg N ha^{-1} 148 DAP, a sharp increase in NO_3^- concentration followed by an immediate sharp decrease was observed in the SCs placed at 15 and 30 cm. An increase in NO_3^- concentration for the WFD placed at 15 cm was also observed. The final application of 30 kg N ha^{-1} 175 DAP did not cause clearly observable increases in NO_3^- concentration in either the SCs or WFDs. As additions of fertilizer N were more clearly reflected at the beginning of the season when the crop did not yet have a fully developed root system, this N 'disappearance' is therefore mostly attributed to crop uptake.

The onset of the rainy season clearly moved NO_3^- down the soil profile, as can be observed from both the SC and WFD data. SCs placed at 45 and 60 cm showed an increase in NO_3^- concentration after the onset of rain, and the measurements suggest a pulse of NO_3^- moved down the profile. A large increase in NO_3^- concentration in the WFD placed at 60 cm 185 DAP is also consistent with the movement of a NO_3^- pulse down the profile.

From the simulated data (Figure 6.8) it is clear that the SC concentrations reflect the concentrations in the immobile water phase, while the WFD concentrations reflect those in the mobile water phase. For both sets of comparisons, measured and simulated values showed similar trends to a depth of 60 cm, although simulated values did not fluctuate as much as the measured values. At 60 cm, in comparison to NO_3^- concentrations measured in the WFD, simulated mobile phase concentrations were greatly over-estimated, despite good correlation for the SC NO_3^- concentrations and simulated immobile phase concentrations.

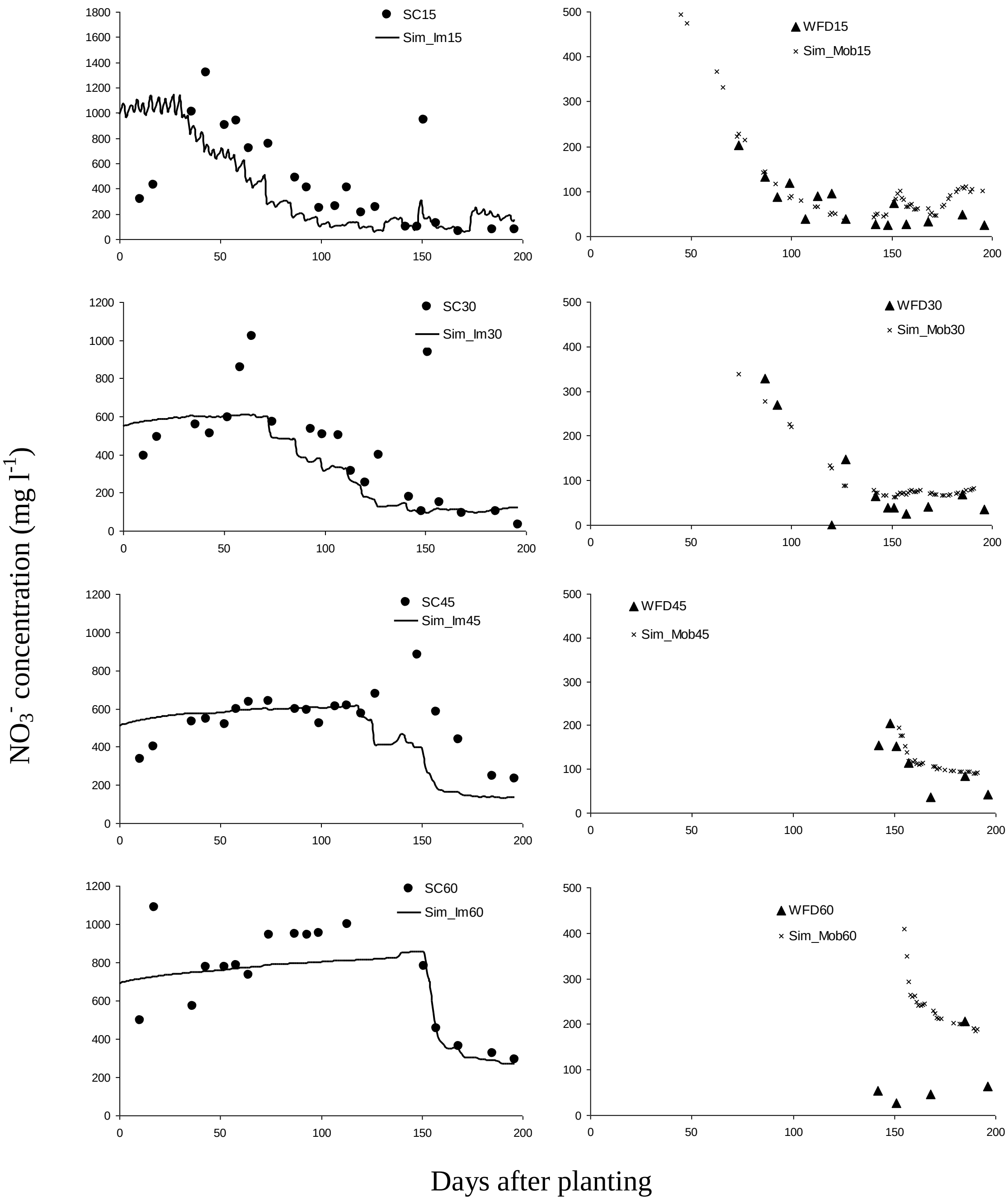

Figure 6.8 Measured NO_3^- concentrations from suction cups compared to simulated immobile soil water phase concentrations (Sim_Im; left) and measured NO_3^- concentrations from wetting front detectors compared to simulated mobile soil water phase concentrations (Sim_Mob; right) at depths of 15, 30, 45 and 60 cm

For the SCs at 80 and 100 cm, a sharp decline in NO_3^- concentration can be observed after the onset of the rainy season. This is after an initial slight increase in NO_3^- concentration prior to 150 DAP. These data indicate that N is also moving past the 80-100 cm depth, as is confirmed by the leachate data collected at the base of the lysimeter.

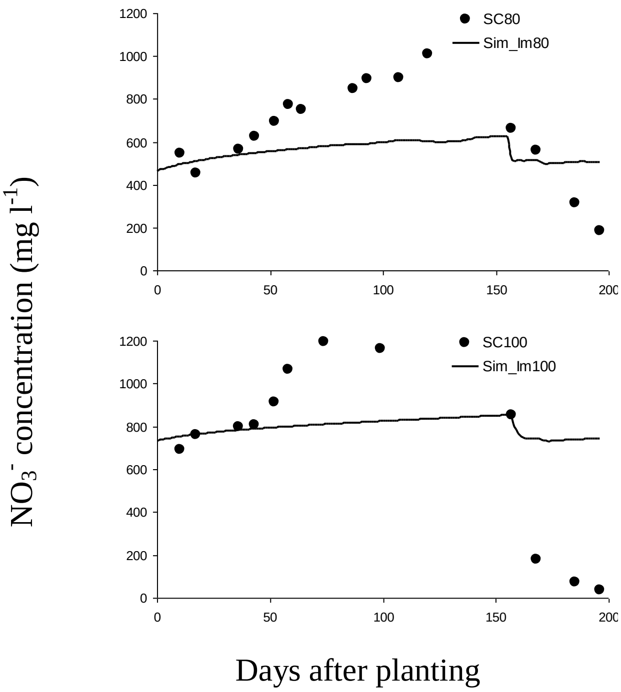

Figure 6.9 Measured NO_3^- concentrations from suction cups compared to simulated immobile soil water phase concentrations at depths of 80 and 100 cm

The initial increase in measured SC NO_3^- concentrations at 80 and 100 cm was under-estimated by SWB-Sci. The rapid decrease in NO_3^- concentration after 150 DAP was also under-estimated by the model, especially at the 100 cm depth. Saturation of the bottom layer, as required for free drainage to occur, may have resulted in increased denitrification and hence an over-estimation in simulated NO_3^- concentrations at the lower depths because of inadequate representation of this process in the model.

6.3.5.2 Phosphorus

P was successfully detected in water samples collected from WFDs. The highest P concentrations were detected in the WFD buried at 15 cm, ranging from 2.8 to 8.7 mg l^{-1}. For the WFDs buried at 30, 45 and 60 cm P concentrations ranged from 0.7 to 2.6 mg l^{-1}. The effect of the first P fertilizer addition of 49 P kg ha^{-1} at planting cannot be observed, as the WFDs did not collect soil water samples over this period (Figure 6.10). The second fertilizer addition of 49 P kg ha^{-1} 108 DAP resulted in an associated increase in P concentration at 15 cm. A third application of 49 kg P ha^{-1} 175 DAP did not cause equivalent increases in P concentration in the WFD at 15 cm. From P concentrations measured in WFDs over the growth season, an overall increase in the soil ‘P status’, most likely as a result of the fertilizer P applied, can be observed. This increase in P concentration was observed down to 60 cm depth, suggesting that fertilizer P was moving vertically down the profile, but this may also be due to natural fluctuations in P occurring in the soil water sampled by the WFD. As expected, P concentrations measured in the WFD at 60 cm were generally higher than those measured in the drainage exiting the lysimeter. The average P concentration measured in the WFD at 60 cm was 1.72 mg l^{-1}, while the average P concentration in the drainage water was 0.8 mg l^{-1}. This is to be expected as some of the soluble P is adsorbed to soil colloids as it moves deeper through the soil.

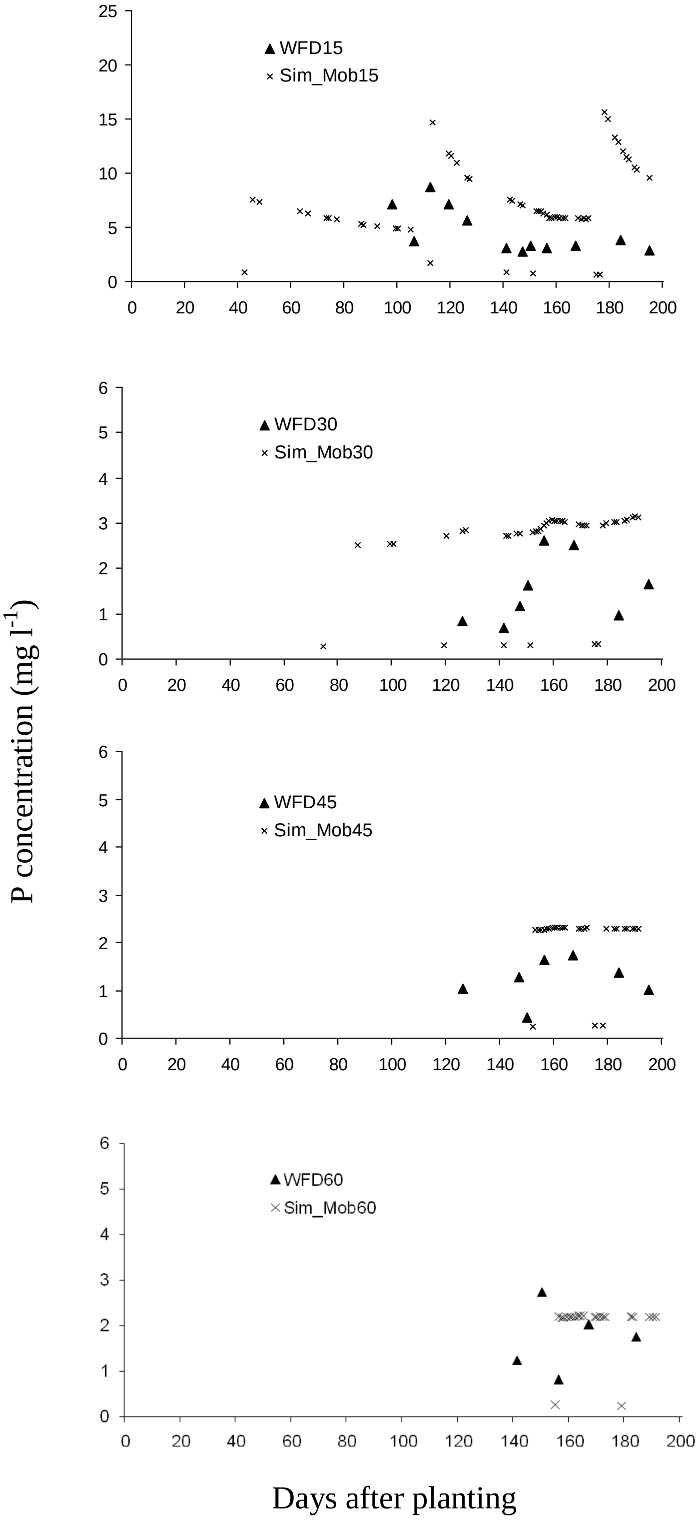

Figure 6.10 Measured P concentrations from wetting front detectors and simulated mobile soil water phase P concentrations at depths of 15, 30, 45 and 60 cm

The P concentrations in the mobile water phase estimated by SWB-Sci were mostly higher than P concentrations measured in WFDs. Reasons for the overall over-estimation by the model could be due to incorrect model initialization, over-estimating the amount of soluble P in the respective layers, or incorrect estimation due to model time-step related errors. When high drainage rates were being simulated, however, simulated mobile phase concentrations were in some cases lower than those measured in WFDs. From 110 DAP, measured and simulated values show a very similar trend at 15 cm.

6.4 GENERAL DISCUSSION

NO_3^- concentrations sampled from SCs were almost always higher than those sampled from WFDs for the soil tested. Good visual correlations between measured NO_3^- concentrations from the SCs and simulated immobile soil water phase concentrations, and measured concentrations from the WFDs and simulated mobile phase NO_3^- concentrations were observed. This indicates that these samplers clearly sample different soil water phases as hypothesized; and that the use of a simple solute mixing fraction approach incorporated in a straightforward cascading soil water balance model with a daily time-step, was effective in modelling the impacts of the mobile and immobile soil water components on solute transport. A major implication of this is that measuring and modelling can be used together to improve estimates of N leaching losses. Two fundamental approaches are proposed. The first involves using a mechanistic crop N model such as SWB-Sci to model N dynamics together with data from WFDs and/or SCs to calibrate and test the model. The second involves using measured N concentrations together with water fluxes obtained from a crop soil water balance model like SWB-Sci to estimate leaching. SC concentrations can be used during ‘slow’ drainage events and WFD concentrations can be used during ‘fast’ drainage events, as indicated by the model. For both approaches, the simultaneous measurement of VWC at different depths will provide additional data to improve accuracy of the simulated leaching.

Relatively high NO_3^- concentrations were measured in this trial. A reason for such relatively high NO_3^- concentrations may have been that during the soil packing stage of the lysimeter set-up, soil disturbance could have resulted in increased exposure of a certain fraction of organic matter, usually occluded from microbial attack in the smaller soil pores, to N mineralization (Hassink, 1994; Strong et al., 1999). Even higher NO_3^- concentrations were, however, measured on a commercial vegetable farm in Tarlton, near Johannesburg (data not shown).

WFDs were used effectively provide estimates of mobile P concentrations down to the deepest depth tested (60 cm). As a result of complex interactions with the soil matrix, interpreting P data is clearly more complex than for NO_3^-. Compared to WFD as well as the drainage water P concentrations, simulated P concentrations within the soil profile were consistently over-estimated by the model, but were still estimated with relative accuracy considering the complexity of the system. The exact reason for this over-estimation is at present still unknown. Algorithms for modelling inorganic P are based on work done by Jones et al. (1984) and Sharpley et al. (1984), and were developed using mostly continental USA soils. An over-estimation of soluble P using this approach may be possible, most likely due to differences in estimations of P sorbed between US soils compared to South African soils using this approach. This requires further investigation using a wider range of soils. Further work on P concentrations obtained from WFDs shows potential in improving our understanding of the dynamics of P in the soil profile, and developing approaches for improved estimation of inorganic P leaching.

In using of this type of mechanistic modelling, it is essential to simulate the various key processes such as crop uptake and mineralization accurately. Unfortunately challenges associated with obtaining relevant data to test these processes individually leaves some uncertainty in the way the current version of SWB-Sci simulates N and P. Although this was not an independent dataset against which the model was tested, the ability of the model to estimate soil water, crop growth, N and P uptake and N and P leaching was judged to be adequate. Using data obtained from devices such as SCs and WFDs which collect samples using the same mechanism in the same location over a time period, assists in reducing data errors associated with soil heterogeneity. The use of a simple algorithm to obtain mobile phase concentrations, which is incorporated into a well-tested crop model, makes this approach easy to apply to other systems without complex parameterization requirements. Further work, based on the approaches proposed in this paper, is recommended for a wide range of cropping systems on a range of different soil textures to further enhance the robustness and effectiveness of these approaches to support improved understanding and reduction of NPS nutrient pollution.

In addition to using SCs and WFDs to estimate leaching, basing adaptive management fertilization strategies on measured concentrations shows excellent potential. In this study, using a threshold value of 100 mg NO_3^- l^{-1}, was not very effective in reducing N leaching losses from the bottom of the profile. Another strategy could have been to not apply any further N fertilizer and force the crop to use N deeper in the soil profile. This may have impacted crop yield ultimately but would be a trade-off to reduce leaching losses. Establishing such thresholds for different crops is challenging, but a start could be to use predicted total crop transpiration and N uptake to calculate the passive NO_3^- concentration required in the soil water. Such an approach would help reduce over-fertilization, thereby reducing N concentrations in the deep drainage leaving the rootzone. Due to complex P adsorption/desorption reactions in the soil, such an approach would be less straightforward for P, but could still provide farmers with valuable information on the P status of their soil, especially if P is monitored routinely.

6.5 CONCLUSIONS

Nitrogen and P leaching from agriculture can pose a serious threat to receiving water bodies, but simple and effective ways of estimating these leaching losses are lacking. A diversity of approaches, ranging widely in levels of complexity, have been proposed to model solute concentrations in soil water. The relatively straightforward approach proposed in this paper was found to simulate 'mobile' and 'immobile' soil water NO_3^- concentrations that reflect the concentrations measured with WFDs and SCs, respectively. This work reinforces the value of using monitoring and modelling together to estimate solute leaching and proposes a pragmatic approach for doing so. Simulated mobile phase P concentrations and concentrations measured in WFDs were less well related than for NO_3^- suggesting we have not yet fully captured the complex sorption/desorption processes that control soil P behaviour. More work is therefore needed to further improve our understanding of the interaction of reactive solutes with soil water. In addition to estimating leaching losses, mechanistic modelling and sampling devices such as WFDs and SCs can be play an important role in guiding development and application of fertilization strategies to help reduce the unwanted impact of crop production on the environment.

6.6 ACKNOWLEDGEMENTS

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