Development, testing and application of a crop nitrogen and phosphorus model to investigate leaching losses at the local scale

by

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DECLARATION

I, Michael van der Laan, hereby declare that this dissertation for the degree PhD (Agronomy) at the University of Pretoria is my own work and has never been submitted by myself at any other University. The research work reported is the result of my own investigation, except where acknowledged.

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ABSTRACT

The leaching of nitrogen (N) and phosphorus (P) from the rootzone of cropping systems is a major contributor of non-point source pollution resulting in deterioration of fresh water supplies. An escalating world population is forcing further intensification of agricultural production practices and the identification of suitable and effective management practices to reduce N and P leaching losses is becoming ever more important. Such leaching losses are, however, extremely challenging to measure and quantify due to uncertainties associated with the estimation of deep drainage and N and P concentrations in this drainage water. SWB-Sci is a locally developed, mechanistic crop model to which N and P subroutines have been added to enable analysis of leaching losses at the local scale. This involved novel approaches to estimate the effects of N deficiencies on yield; to simulate crop P demand, uptake and stress effects; to simulate banded P fertilizer applications; and to estimate incomplete solute mixing. New equations to estimate the size of the *Labile P* pool from soil P tests commonly used in South Africa, and guidelines on the classification of South African soils as calcareous, slightly weathered or highly weathered which is required to simulate P, were also developed. The upgraded more versatile model was tested using historical datasets from the Netherlands, Kenya and South Africa, and performed well in simulating N and P dynamics in maize and wheat cropping systems. Variables tested included aboveground dry matter production, yield, leaf area index, aboveground crop N and P mass, grain N and P mass, soil water content and soil inorganic N levels. A study was also conducted on a large drainage lysimeter into which suction cups and wetting front detectors were installed, and data from this experiment together with the SWB-Sci model was used to study vertical solute movement more closely. As hypothesized, wetting front detector nitrate (NO_3^-) and P concentrations were observed to align closely with simulated mobile phase concentrations, and suction cup NO_3^- concentrations were observed to align closely with simulated immobile phase concentrations. These results confirm that monitoring and modelling can be used together to improve understanding and obtain more accurate estimates of N and P leaching losses, and further work on this approach is recommended for a wide range of soils and cropping systems. Finally, long-term modelling with the SWB-Sci model was used to analyse and compare N and P leaching losses from a dryland versus an irrigated monoculture maize production system. Over a 30 year simulation period, irrigated maize was estimated to leach considerably higher loads of N and P (~ 4-fold higher). For dryland production, zero leaching was observed for consecutive years on several occasions, with major leaching losses associated with high rainfall events. A 'room for rain' irrigation scheduling management practice was estimated to reduce N leaching by 12% and P leaching by 14%, while a crop rotation system which incorporated wheat grown over the winter months was estimated to reduce N leaching by 23% and P leaching by 24%. From this study, long-term modelling was confirmed as an effective approach to investigate N and P leaching losses, to assist with the planning and design of field trials, and to assess the effectiveness of best management practices. It is envisaged that SWB-Sci will continue to evolve as a valuable tool for analysing and reducing N and P leaching losses from cropping systems to further reduce non-point source pollution.

CHAPTER 1
INTRODUCTION

1.1 Rationale

Increased eutrophication of inland water bodies resulting in the deterioration of fresh water quality requires a better understanding of the sources and pathways of nutrient pollutants. Nitrogen (N) and phosphorus (P) are most frequently the limiting nutrients for algal growth and are therefore implicated as the primary nutrients leading to eutrophication. In addition to the many negative consequences of eutrophication (Toerien, 1974; Dunst et al., 1974), high nitrate (NO_3^-) levels in drinking water can also be hazardous to infants and livestock (Tredoux, 1993). Although point sources are usually the major contributors of N and P pollutants into receiving water bodies, agriculture has also been implicated as a significant non-point source (NPS) contributor to this type of pollution. Matson et al. (1997) observed that NO_3^- contamination is common in agricultural regions throughout the world, and Isermann (1990) calculated that agriculture was responsible for about 60% of the N and 25% of the P emissions into the North Sea.

In South Africa, Cullis et al. (2005) observed that reliable pollution data was limited for assessing the contribution of agriculture to pollution loads. In studying several catchments (the Breede, Middle Vaal and Mgeni catchments) representative of different agricultural practices, the authors concluded that while agriculture can have a major impact on salinity loads, nutrient loads were most often dominated by point sources. Nonetheless, for a Breede sub-catchment the agricultural NPS N load was observed to be 7 kg ha^{-1} a^{-1}, and for a Mgeni sub catchment the agricultural NPS P load was observed to be 0.12 kg ha^{-1} a^{-1}. NPS nutrient loads were observed to be greater in the wet season and in some cases a ‘first flush’ impact was observed at the beginning of the wet season. Cullis et al. (2005) also suggested that estimates of N and P loads from agriculture may have been larger if the natural removal of nutrients from point sources along flow paths was accounted for. Reducing the contribution of point sources has received much attention since the late 1960’s due to the ease of identification and treatment of these sources, with more attention now being directed at NPS pollution (Heathwaite et al., 2000). High P levels are generally low in South

African groundwater, but certain regions in South Africa do contain groundwater that is NO_3^- enriched (Annandale and Du Preez, 2005).

According to the FAO, between the years 1960 and 2000, nitrogenous fertilizer consumption increased 7-fold and phosphate fertilizer consumption increased 3-fold (Tilman et al. 2002). Total crop uptake for the two nutrients can be as low as 50% of applied N (Smil, 1999) and 45% of applied P (Smil, 2000). The fate of the other 50% and 55% of added N and P, respectively, is often unknown. Tilman et al. (2001) used past global trends and their dependence on population and GDP to obtain trajectories for N and P fertilizer consumption and global irrigated area in 2020 and 2050 (Figure 1.1).

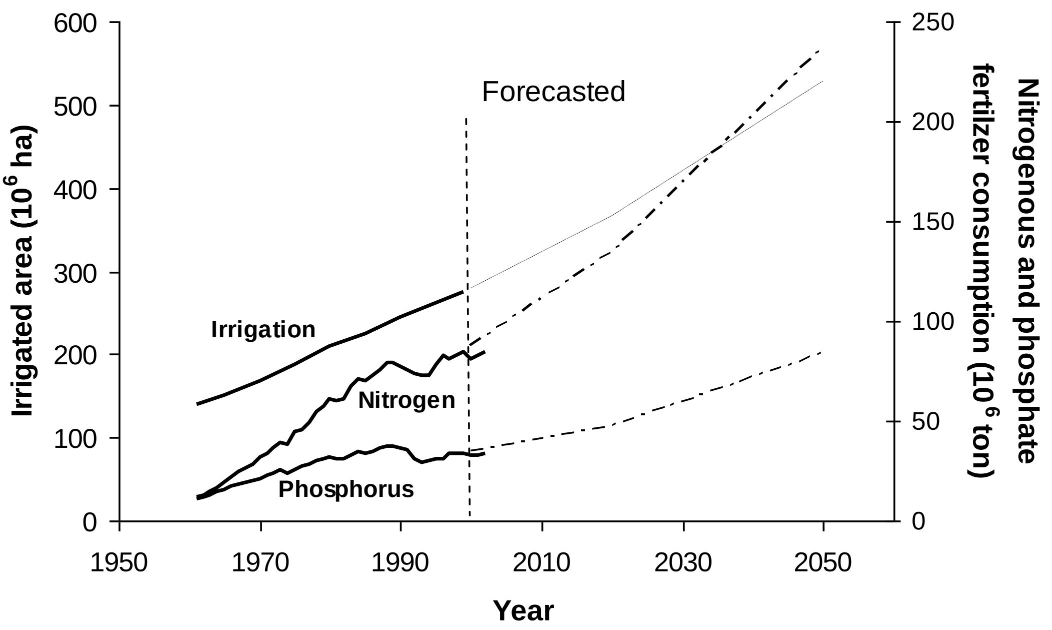

Figure 1.1 Total global increase in irrigated area and nitrogenous and phosphate fertilizer since the 1960's (www.worldwater.org; http://faostat.fao.org) and forecasted increase in irrigated area and nitrogenous and phosphate fertilizer consumption until 2050 (from Tilman et al., 2001)

The authors estimate that from 2000 values, global N fertilization would increase 1.6-fold by 2020 and 1.9-fold by 2050, and global P fertilization would increase 2.7-fold by 2020 and 2.4-fold by 2050. Furthermore, total irrigated area doubled between 1960 and 1999, and the authors predicted this area will increase 1.3-fold by 2020 and 1.9-

fold by 2050, with most increases occurring in Latin America and sub-Saharan Africa. These large projected increases could have significant environmental impacts (Tilman et al., 2001) and exacerbate NPS N and P pollution from cropping systems.

The contribution of agriculture to NPS nutrient pollution is technically difficult and challenging to monitor and estimate. In estimating leaching losses, difficulties arise in obtaining N and P concentrations in the drainage water as well as estimating drainage fluxes, both of which are difficult to measure. Both inorganic and organic forms of N and P present in the drainage water must be considered. Understanding the fate of N and P once it has leached from the vadose zone and entered the groundwater is an equally perplexing issue. In considering runoff losses, soluble inorganic and organic forms of N and P must be considered in addition to the losses of P and ammonium (NH_4^+) attached to sediment. Due to this complexity involved in monitoring NPS N and P pollution, modelling has been identified as a valuable tool to help improve our understanding of the sources and pathways of pollutants and hence our estimates of NPS pollution from agriculture.

In 2005, the Water Research Commission (WRC) of South Africa initiated a project titled ‘Development of an integrated modelling approach to prediction of agricultural non-point source (NPS) pollution from field to catchment scale for selected agricultural NPS pollutants’. The pollutants selected were sediments, pesticides and nutrients, specifically N and P. Although two experimental catchments were established to collect data for model development and testing at the catchment scale, intensive measurements were not made at the local scale. A second WRC project, titled ‘Adapting the wetting front detector to the needs of small-scale furrow irrigators and providing a basis for the interpretation of salt and nutrient measurements from the water sample’ was also initiated at this time. An aspect of this project involved measuring solute concentrations in soil water collected by wetting front detectors and suction cups to improve our understanding of the nutrient status of soils and salt and nutrient leaching in the soil profile. The research presented in this thesis on N and P leaching in cropping systems was carried out within the context of these two projects.

1.2 NITROGEN LEACHING FROM CROPPING SYSTEMS

Nitrogen can occur in the soil in organic form as part of plant residues and organic matter, and in inorganic form as NO_3^-, NH_4^+, and urea [$(NH_2)_2CO$]. It can also occur in soil in gaseous form as nitrogen gas (N_2), nitrous oxides (N_2O, NO_x) and ammonia (NH_3) (Shaffer and Ma, 2001). Over 90% of soil N is in the form of organic N. In addition to N loss in the form of NO_3^-, N can also be transported into waterways in the form of soluble NH_4^+ or NH_4^+ attached to sediment. Goulding (2000) reports that recent findings indicate small but significant amounts of N can also be lost as soluble organic N in drainage water. Leaching is also more predominant in coarse than fine textured soils. Other N losses include denitrification and ammonia volatilization (Romkens et al., 1973). The pathway and quantity of N loss from agricultural systems can be highly variable and because it is determined by prevailing conditions (Shaffer and Ma, 2001), significant changes can occur within just a few hours or days (Shaffer et al., 1994).

Various methods are used to measure NO_3^- leaching, including routine soil sampling, active and passive samplers, drainage lysimeters and field scale drainage facilities; with no one technique being suitable for all situations (Goulding, 2000). Different studies investigating NO_3^- leaching have produced a wide range of results depending on experimental conditions, with the amount of NO_3^- leached usually being well related to the amount of fertilizer N applied and the percolation volume (Timmons and Dyla, 1981). Sexton et al. (1996) observed that the majority of NO_3^- leaching in a season occurred during only two major rainfall periods. Rainfall and irrigation events following fertilizer application can therefore be regarded as high risk periods. Intensively managed horticulture cropping systems under irrigation may be highly vulnerable to NO_3^- leaching due to the shallow root systems and low N use efficiency requiring high N inputs (Hanson and Trout, 2001). ‘Leaky’ cropping systems involving for example potatoes, oilseed rape and sugarbeet which leave large amounts of residual N available for mineralization and leaching may also be high risk (Goulding, 2000). High NO_3^- leaching potential is often expected in relatively arid areas where intensively managed fruit and vegetable crops are common, as mild winters permit crop residue decomposition, and heavy rainfall can occur within a few winter months, promoting leaching (Coppock and Meyer, 1980). Similarly, although cover crops can play an important role in retaining N in the system, when the crop senesces, the N is returned to the soil and can contribute to NO_3^- leaching (Goulding, 2000). Therefore as periods of crop absence and lack of N uptake from the soil may coincide with high NO_3^- losses, irrigation allows farmers to grow crops during the dry period, reducing the duration of this risky period. Artificial drainage systems may also increase NO_3^- leaching as it will shorten the distance that NO_3^- must move through the soil to be leached and higher rates of mineralization can be expected due to the increased aeration status of these soils (Di and Cameron, 2002).

1.3 PHOSPHORUS LEACHING FROM CROPPING SYSTEMS

Inorganic P is relatively immobile in soil and adheres strongly to soil particles and organic material. Although soils often contain high levels of bound mineral P, low concentrations of plant available P often necessitate fertilization to achieve optimum yields (Hart et al., 2004). P loss can occur via runoff or leaching. Annual P losses in surface runoff have been observed to be 1.5 to 10 times higher than for leaching below the root zone (Carter et al., 1973; Alberts and Spomer 1985). Runoff losses are therefore thought to be the dominant form of P export from watersheds (Sharpley and Rekolainen, 1997; Sharpley et al., 1999). Soil slope and surface conditions, as well as water quality, may influence runoff P losses (Aase et al., 2001). P runoff loss can further be influenced by rate and timing of fertilizer application, method of application, form of fertilizer used, slope, temperature, soil type, tillage practice and vegetation (McDowell et al., 2001). P can be transported in runoff in the form of soluble P, often referred to as dissolved reactive P (DRP), or attached to sediment and referred to as particulate P (PP). Sediment losses from near zero up to over 100 Mg ha^{-1} have been observed under surface irrigation, and this sediment can take as much as 900 to 1200 mg kg^{-1} of total P (TP) with it (Carter, 1990). Shigaki et al. (2006) observed that P loss in runoff was strongly influenced by water solubility of the P sources and concluded that this characteristic may be considered as an indicator of DRP loss potential.

Movement of P through the soil profile is less well documented than P movement in surface runoff (Bush and Austin, 2001), but recently more attention is being given to P leaching. P dynamics within the soil are highly complex and understanding the mechanisms and pathways of subsurface P transport are limited or under-investigated (Sharpley et al., 2002; Hart et al., 2004). According to Bond (1998), P leaching is only likely to occur on very sandy soils receiving high P loading, but Toor et al. (2005) caution that significant amounts of P can be lost shortly after P fertilizer applications when preferential transport takes place through cracks, root holes and worm borings in the soil. P leaching is usually minimal in soils through which water moves very slowly and there is prolonged contact with the soil particles (Djodjic et al., 2004). Higher P leaching can also be expected in soils saturated with P, but Djodjic et al. (2004) concluded that soil test P (STP) values from topsoil should not be used alone for obtaining P leaching risk assessments, as other important soil factors also need to be considered. Toor et al. (2005) measured P leaching to a depth of 70 cm in a silt loam soil under permanent irrigated grassland. P losses below the root zone from treatments to which superphosphate had been applied at a rate of 45 kg P ha^{-1} together with dairy effluent at a rate of 40 kg P ha^{-1} or 80 kg P ha^{-1} were 1.6 to 2.3 kg ha^{-1}. Sixty percent of the total P lost was during the first eight drainage events after effluent application, while the remaining 40% was lost in the subsequent 43 drainage events. This was calculated to be 3.5 to 4.3% of the P applied in the effluent. P leaching losses for the mineral P fertilizer only treatments were 0.3 kg P ha^{-1}. In studying seasonal fluctuations of P leaching from soils to which dairy farm effluent had been applied, Toor et al. (2004) observed that PP losses were higher in the irrigation season, while DRP losses were higher in the non-irrigation season (natural rainfall only). The authors attribute this to increased dislocation of particles in the soil profile by the high intensity flood irrigation, and rapid transport of this PP through the macropores.

1.4 MITIGATION MEASURES

Laws and regulations to control NPS N and P pollution are often inadequate or non-existent. Best management practice (BMP) effectiveness can be rated in terms of impact on pollutant load, farmer acceptability, cost-effectiveness and ease of implementation and maintenance (Logan, 1990). According to Heathwaite et al. (2000), differences in chemistry and pathways between N and P means that mitigation efforts aimed at only a single nutrient can negatively impact on the other. Increasing artificial drainage may for example reduce P runoff losses, but may also increase NO_3^-

leaching losses (Turtola and Paajanen, 1995). Heathwaite et al. (2000) therefore encourage an integrated approach to nutrient management targeted at critical areas that contribute the highest N and P loads in a watershed. The leaching required for sustainable irrigation moves salts from soils into rivers and lakes (Wichelns and Oster, 2006). Losses of N and P to waterways will therefore also occur during this salt leaching if not carefully managed. A comprehensive approach which also accounts for salinity management is therefore required to manage the system.

1.4.1 Reducing N leaching in cropping systems

Irrigation scheduling, system uniformity, and N fertilizer application type, rate and timing are all interacting factors affecting crop yield and NO_3^- leaching (Pang et al., 1997). The primary objective of BMPs is to limit the movement of agricultural chemicals out of the root zone while still maintaining crop yields (Nguyen et al., 1996) and profitability. Schneekloth et al. (1996) warn that strategies to reduce N leaching can often only be accomplished at an economic loss to the grower.

Applying split applications of fertilizer N can potentially reduce N leaching regardless of irrigation method (Nakamura et al., 2004), as can the application of less soluble forms of N or slow-release N fertilizers (Paramasivam et al., 2001). Additional N added in the form of NO_3^- in the irrigation water should be accounted for when determining fertilization rates. Irrigating 20 ML ha^{-1} yr^{-1} of water with a nitrate concentration of 10 mg NO_3-N will add 200 kg N ha^{-1} yr^{-1}, and it could be beneficial to extract water from the upper parts of an aquifer if large amounts of N are reaching the groundwater (Bristow, 2004). During the growing season, the average amount of N mineralized under irrigated conditions may be higher than under comparative dryland conditions, allowing the required amount of fertilizer to optimize yield to be reduced for relative target yield (Ferguson et al., 1991).

Irrigation scheduling and uniformity can play a major role in reducing NO_3^- leaching, especially on permeable soils which otherwise require frequent nutrient applications because of leaching (Follet and Hatfield, 2004). Moreno et al. (1996) found that the highest NO_3^- leaching occurred during heavy rainfall when the soil was already wet from irrigation, and the authors were able to reduce NO_3^- leaching in a full replenishment treatment by 11% by periodically applying liquid N through the irrigation system as opposed to granular N. Ferguson et al. (1991) observed that the inability of furrow irrigation systems to apply water uniformly can play a significant role in increasing NO_3^- leaching. Performing simulation studies using the CERES-maize model, Pang et al. (1997) observed that decreased irrigation uniformity increased NO_3^- leaching and that higher N rates must be applied for a given yield for systems with lower irrigation uniformity. Improving irrigation system uniformity can therefore be expected to reduce NO_3^- leaching from the soil profile.

Irrigating to supplement rainfall in the soil profile has been observed to be effective in reducing NO_3^- leaching compared to full irrigation. Soil texture and soil moisture status will play a determining role in the amount of rain that can be stored in the soil profile, with lighter soils permitting less room for rain, and the risk to crop yield must be considered (Klocke et al., 1996). Timmons and Dylla (1981) found that application of a partial replenishment as opposed to a full replenishment irrigation strategy reduced NO_3^- leaching loss by 31% without a significant reduction in yield. Trials conducted in Mexico showed that altering irrigation scheduling and N application could reduce inputs by almost 30% and reduce NO_3^- leaching by 49 to 70 kg ha^{-1}, while maintaining equal yields (Follet and Hatfield, 2004). High leaching losses can be common during the fallow period when there is not an actively growing crop. End of season irrigation management to increase precipitation storage capacity during the non-growing season can also reduce nitrate leaching (Schneekloth et al., 1996). In a field trial studying N leaching on a sandy soil, Aronsson and Torstensson (1998) observed that N leaching could be reduced by 40-50% when using a catch crop.

Micro-irrigation can be advantageous in reducing leaching as these systems are able to apply water and nutrients to where crop roots are concentrated, and this can be an efficient strategy in maintaining additional pore space for rain in the soil section that is not irrigated (Waddell et al., 2000). Systems such as trickle irrigation often do not have clear design and management guidelines and are therefore often designed to achieve economic optimum in terms of engineering with less attention paid to environmental outcomes (Cote et al., 2003). Improved fertigation practices can also play a role in reducing NO_3^- leaching. It is generally accepted that applying fertigation at the end of an irrigation cycle will limit NO_3^- leaching. Using the simulation model

HYDRUS2D Gärdenäs et al. (2005) observed that, with the exception of surface drip irrigation on clayey soils, fertigation at the end of an irrigation cycle using micro-irrigation generally reduced NO_3^- leaching. In a similar study, Cote et al. (2003) observed that in permeable soils, fertigating at the beginning of an irrigation cycle reduced the risk of NO_3^- leaching compared to fertigating at the end of an irrigation cycle. The reason for this is that more NO_3^- can be expected to collect closer to the surface due to capillary movement of the water applied initially, while water movement at the end of an irrigation cycle will be dominated by downward gravitational forces, and more NO_3^- can be expected to collect below the root zone as a result. The important role of specific soil hydraulic properties and soil structure in influencing the shape and dimensions of the wetting patterns and solute movement should therefore be considered in determining an optimal fertigation strategy (Cote et al., 2003). Fertigation at the beginning of a long irrigation event should generally be avoided for surface drip systems, while fertigation strategy is less of a factor for subsurface drip (Gärdenäs et al., 2005). In a similar study, Gärdenäs et al. (2005) found that using a urea-ammonium-nitrate fertilizer as opposed to a nitrate-only fertilizer increased the nitrate concentration near the drip line. The urea-ammonium-nitrate fertilizer further resulted in slightly smaller percentages of nitrate leaching than for the nitrate-only fertilizer. As mentioned earlier, artificial drainage systems – often required for salinity and water logging management – can lead to increased NO_3^- leaching, in which case specific management practices should be implemented to deal with this drainage water.

1.4.2 Reducing P leaching in cropping systems

All of the mitigation measures mentioned above that reduce the amount of unwanted drainage occurring can be expected to also reduce P leaching. Two approaches to P fertilization are generally followed in South African and other developed countries. The first involves P application in excess of seasonal crop demand to build up the P status of soils (Farina and Channon, 1987), while the second alters fertilizer application according to anticipated or target yields for the season (Henry and Smith, 2004). Advantages of the first strategy include the positive effect of a good soil P reserve on yield and protection from the negative effects of inflation on production costs (Henry and Smith, 2004). A disadvantage will be increasing the P leaching potential of the soil. Henry and Smith (2004) observe that it is important to understand the kinetics of sorption for a particular soil when choosing a P fertilization strategy. The degree of soil saturation with P (DSSP) can potentially be used to assess the P loss risk for a soil, and is calculated using the P, iron (Fe) and aluminium (Al) contents (mmol kg^{-1}, extracted with acidified ammonium oxalate-oxalic acid) as follows (Hooda et al., 2001):

$$DSSP(\%) = \frac{[P] \times 100}{[Fe + Al]} \tag{1.1}$$

In the Netherlands for example, a DSSP of 25% is considered unacceptable as P losses will potentially be high enough to contaminate water (Breeuwsma and Silva, 1992), and no further P fertilizer application is permitted. Sims et al. (1998) suggest that crop and soil management practices that reduce preferential flow through macropores can potentially reduce P leaching, but caution that such practices can increase erosion losses from the system.

1.5 MODELLING N AND P DYNAMICS IN AGRO-ECOCSYSTEMS

1.5.1 Overview

Technological advances and an increase in computer availability have to lead to a widespread use of mathematical models that simulate nutrient dynamics in cropping systems. Despite this, ‘examples of real impacts of these modelling efforts on current farming practices are rare’ (Carberry et al., 2002). Mechanistic crop models have played a role in greatly enhancing our understanding of nutrient dynamics, and according to McCown et al. (1992), such models can asses fertilizer use in a way not possible using long-term trial data on its own. Carberry et al. (2002) discussed four case studies where models were used to improve understanding in nutrient use efficiency and found evidence that models can be utilized to contribute to significant changes in management practices for commercial farmers. In applying the Agricultural Production Systems Simulator (APSIM) model to maize/legume systems in Africa, Whitebread et al. 2009 identified four distinct modes of use: (1) to add value to experimentation, (2) to facilitate direct engagement with farmers, (3) to explore system constraints and opportunities with researchers and extension offices, and (4) to generate information for policy makers and financial institutions.

Modelling NPS N and P pollution is practiced at different spatial scales. Some confusion exists in the literature on the dimensions of different scales, but point (~1 m^2), plot (~25 m^2), hillslope (~1 ha), field (broadly defined), small catchment (~1 km^2), and large catchment (~1000 km^2) scales are often referred to (Quin, 2004). In this thesis, local scale is referred to as a scale between the plot and field scales which can be adequately simulated by a one dimensional model. Local scale, mechanistic models with high user-input requirements which have been used to study the export of N and/or P from cropping systems include APSIM (Keating et al., 2003), CropSyst (Stöckle et al., 2003) and the DSSAT models CERES and CROPGRO (Daroub et al., 2003). For the field to catchment scales, models such as EPIC (Williams et al., 1983), GLEAMS (Muller and Gregory, 2003), SWAT (Neitsch et al., 2002) and ACRU-NP (Campbell et al., 2001) can be used to predict NPS N and P pollution from agriculture. This modelling of larger areas often requires the aggregation of input parameters and the use of more empirical algorithms to capture important N and P processes in the simulation.

Shaffer et al. (2001) produced an extensive publication on approaches used to model N, and Lewis and McGechan (2002) did a comprehensive review of field scale P models, including the GLEAMS model. Models often use approaches that can differ vastly in complexity to simulate N and P in cropping systems. This leads to various strengths and weaknesses for a particular model. For a model to be considered mechanistic, the cropping system being described at one level must be described by processes operating at a lower level (Sinclair and Seligman, 2000). In reviewing 14 N simulation models, De Willigen (1991) observed that aboveground variables (yield, grain N mass) were better simulated than belowground variables (soil water and mineral N content) and concluded that simulating soil biological processes is the most problematic. This most likely also applies for P. Despite an improved understanding of P sources and transfer pathways since early work done by Jones et al. (1984) and Sharpley et al. (1984), models are often not updated adequately to reflect these new insights (Sharpley et al., 2002; Vadas et al., 2006). Radcliffe and Carberra (2007) suggested that with recent research showing that leaching can be an important subsurface pathway for P losses, improved description of P leaching in models is required. A wide range of approaches have been developed to model solute movement in soils with differences in purpose, complexity, flexibility, transferability and usefulness for field soils (Addiscott and Wagenet, 1985).

A problem with a BMP approach to reduce N and P leaching is the lack of a sufficient research base with which to judge the effectiveness of these BMPs, and modelling approaches are increasingly being used to assess BMP effectiveness (Gitau and Veith, 2007). According to Gitau and Veith (2007) advantages in using modelling to assess the effectiveness of BMPs are (1) several BMPs can be studied simultaneously, (2) the effectiveness of a single BMP as well as the combined effect of several BMPs can be studied, and (3) BMP effects can be simulated for varying location-specific conditions. The authors list disadvantages as uncertainty in model prediction due to parameterization uncertainties and lack of data for calibration and validation exercises. Mechanistic crop N and P models can be coupled with economic models to address environmental and financial implications simultaneously. When N and P export and potential BMPs are being modelled at the local scale, it is important to consider hydrological flow pathways in order to assess whether nutrients are likely to leave the local area of interest and become pollutants at the larger scale. Some type of upscaling approach will therefore be required, and most popularly large scale models which have simpler crop and nutrient routines but simulate hydrological flow pathways more comprehensively are employed.

1.5.2 Background to SWB-Sci

SWB-Sci is a mechanistic, generic crop model originally developed as a real time irrigation scheduling tool (Annandale et al., 1999a). The commercially available version is called SWB. Evapotranspiration is calculated according to the Penman-Monteith grass reference method as recommended by the Food and Agricultural Organization (FAO) (Smith et al., 1996). The soil water balance can be modelled using either a cascading soil water balance or a finite difference model (Annandale et al., 1999a). Crop dry matter accumulation per day is the lesser of radiation limited growth (Monteith, 1977) and dry matter accumulation in direct proportion to transpiration corrected for vapour pressure deficit (Tanner and Sinclair, 1983).

Thermal time is used to calculate phenology and partitioning and the effect of water stress is accounted for through the use of a stress factor. The crop and soil water components of the model have undergone extensive testing for a wide range of crops and judged to adequately simulate the soil-plant-atmosphere continuum (Jovanovic and Annandale 1999; Jovanovic et al., 1999; Annandale et al., 2000; Jovanovic and Annandale 2000; Jovanovic et al., 2000; Tesfamariam, 2004). The chemical equilibrium routine of Robbins (1991) has been included into SWB-Sci to enable salt simulations and it has been used extensively to study the feasibility of irrigating crops with gypsiferous mine water (Annandale et al. 1999b; Annandale et al., 2001; Annandale et al., 2002).

1.6 THESIS OBJECTIVES

The overall objective of this study was to better our understanding of N and P dynamics in cropping systems with a view to address leaching losses at the local scale through the improvement of management practices. The approach used to achieve this objective is described below. In order to facilitate the publishing of the research done in this study, the chapters involving novel research (Chapters 3 to 7) are presented in the form of scientific papers.

1.6.1 Model development

The first component of this study was to include N and P subroutines into the existing SWB-Sci model. Whenever possible, algorithms from well established existing models were used. Despite the identification of similar models, ultimately the decision to include N and P into SWB-Sci was made for several reasons. Having an in-house model allows for the complex calibration and crucial code modifications often required when modelling different cropping systems and doing long-term simulations. The model also needed to be applied by the same research group in the assessment of the sustainability of biosolid applications to croplands as a disposal strategy, and was projected to ultimately lead to developing capacity in NPS N and P pollution modelling in South Africa. Finally, our interest in wetting front detectors and suction cups required an in-house model to further test fine scale processes involved in vertical solute movement. A large amount of crop parameterization work has been done locally for SWB-Sci, and testing exercises have shown that the model favourably simulates the soil water balance and crop growth (Jovanovic et al., 1999; Annandale et al., 2000; Jovanovic et al., 2000), making it an ideal model for the inclusion of N and P simulating capabilities.

The lack of detailed parameterization data is a common limitation to model application (Sharpley, 2007). During the development phase it became clear that obtaining P initialization soil parameters for South African soils was highly challenging because the algorithms to model P were originally developed by Jones et al. (1984) and Sharpley et al. (1984) mostly using soils from the USA. Two fundamental difficulties were identified: the first was categorizing South African soils as slightly weathered, highly weathered or calcareous according to the guidelines supplied which were more appropriate for soils classified according to the USDA taxonomic system. The second was the estimation of soil labile P using soil P tests popularly used in South Africa (Ambic, Bray 2, ISFEI method) but which were not included in the original work done by Sharpley et al. (1984). These issues were addressed in this study. As NO_3^- is a non-reactive solute, and a simple algorithm using clay % is used to calculate NH_4^+ sorption, similar guidelines for the parameterization of South African soils for N were not required.

1.6.2 Model testing

In order to gain confidence that the model is robust, extensive testing of the model using measured data was required. Three historical datasets collected in the Netherlands (Groot and Verbene, 1991), Kenya (Probert and Okalebo, 1992) and South Africa (Schmidt, 1993) were selected for this purpose. Datasets were selected according to suitability, primarily based on the scale at which the data was collected and the variables that could be tested. The Netherlands and South African datasets involved the testing of N subroutines exclusively, while the dataset from Kenya included both N and P. A dataset that was collected as part of work for this study involving a drainage lysimeter trial was further used to test certain aspects of the model. Where appropriate, correlation between measured and simulated values was assessed using standard statistical criteria (De Jager, 1990).

1.6.3 Model application

The final objective of this study was to investigate how the model could be applied practically to address problems associated with N and P leaching from cropping systems. This objective was approached by assessing how such a model can enhance our understanding of leaching losses, be used to improve our estimation of N and P leaching, and finally to address the effectiveness of mitigation measures. Due to the complexity of such systems and the influence of weather variables on crop growth and percolation volumes, simulating single seasons often provide only limited information of N and P dynamics and the effectiveness of mitigation measures. For this reason long-term modelling was utilized to provide further insight and demonstrate the application of the SWB-Sci model to investigate N and P leaching losses from different cropping systems.

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CHAPTER 2
DEVELOPMENT OF A LOCAL SCALE NITROGEN AND PHOSPHORUS CROP MODEL

2.1 INTRODUCTION

The Soil Water Balance (SWB) model is a mechanistic, generic crop model originally developed for real-time irrigation scheduling (Annandale et al., 1999a). This model is based on a simple cascading soil water balance approach (Campbell and Diaz, 1988) although a 2-D finite difference model was also subsequently developed. A daily crop dry matter increment is calculated as being either water supply (Tanner and Sinclair, 1983) or solar radiation (Monteith, 1977) limited. Additionally, crop growth and water use can be simulated using the simpler FAO crop factor approach (Annandale et al., 1999b). Since development, the model has undergone extensive testing for a wide range of different cropping systems (Jovanovic et al., 1999; Jovanovic and Annandale, 2000; Steyn, 1997; Jovanovic et al., 2002; Annandale et al., 2003; Tesfamariam 2004). The chemical equilibrium routine of Robbins (1991) and a weather generator were later included into SWB to investigate the long-term sustainability of irrigating crops with gypsiferous mine water (Annandale et al., 2002; Beletse, 2008). Currently there are two forms of the model, the simpler version that can be easily used for applications such as irrigation scheduling, water use estimates and yield predictions referred to as SWB, and the more complex research version called SWB-Sci, which now contains salt and nutrient simulation capabilities, and is the focus of this chapter.

2.1.1 Source models from which algorithms were obtained

Nitrogen (N) and phosphorus (P) simulation approaches and algorithms are based largely on those used in CropSyst (Cropping Systems Simulation Model) (Stöckle et al., 2003) for N, and GLEAMS (Groundwater Loading Effects of Agricultural Management Systems) (Muller and Gregory, 2003) for P. SWAT (Soil Water Assessment Tool) (Neitsch et al., 2002) was also used, but to a more limited extent. CropSyst was developed by C. Stockle and R. Nelson from Washington State University and M. Donatelli from ISCI, Italy. It is described by Stöckle et al. (2003)

as a multi-year, multi-crop, daily time-step crop simulation model; and was designed to draw from the conceptual strengths of EPIC (Erosion Productivity Impact Calculator), but with a more process orientated approach. GLEAMS was developed by S. Muller and J. Gregory at the University of Florida. The model is based on CREAMS (Chemicals, Runoff and Erosion From Agricultural Management Systems), which was developed by the U.S. Department of Agriculture's Research Service to evaluate agricultural NPS pollution from field-scale catchment areas (Knisel, 1980). CropSyst is written in the Visual Basic programming language, GLEAMS in the Fortran programming language, while SWB is written in Delphi.

2.2 MODEL DESCRIPTION

2.2.1 N and P simulation initialization

2.2.1.1 Model interface

Five new interface screens have been included into SWB-Sci, as numerous additional inputs are required to simulate N and P processes at the local scale (Appendix 2.1). Additional inputs, together with how these inputs are used in processes in the model are discussed below.

2.2.1.2 Soil initialization

As for the soil water balance, 11 soil layers are simulated for nutrients. Table 2.1 contains the inputs required to initialize a soil profile.

Table 2.1 Soil inputs required to initialize a simulation for N and P

Input	Units	Per layer	Comment
Sand	%	Yes	
Clay	%	Yes	
Organic matter	%	Yes	
Soil pH (H_2O)	-	Yes	
CEC	mmol(+) $100g^{-1}$	Yes	
Base saturation	%	Yes	P simulations only
$CaCO_3$	%	Yes	P simulations only
Soil test P	mg kg^{-1}	Yes	P simulations only Bray I, Bray II, Ambic, ISFEI, Citric Acid, Olsen
Nitrate	mg kg^{-1}	Yes	
Ammonium	mg kg^{-1}	Yes	
Root residues	kg ha^{-1}	Yes	
Soil P test type	-	No	
Soil group		No	Highly weathered, slightly weathered, calcareous
Standing stubble mass	kg ha^{-1}	No	
Surface stubble mass	kg ha^{-1}	No	
Cultivation depth	m	No	
Annual average air temperature	ºC	No	
Annual temperature amplitude	ºC	No	
Phase of temperature sine function	Days	No	
Bypass coefficient	0-1	No	
Microbial biomass C fraction	0-1	No	Must be specified for soil depths ≤ 0.3 m and > 0.3 m
Active labile SOM C fraction			
Active metastable SOM C fraction			
Passive SOM C fraction			

Simulations for N only can be done, but P must be modelled together with N. Certain inputs are therefore only required to model P. Furthermore, when modelling P, base saturation is only required for a 'slightly weathered' soil, while $CaCO_3$ percentage is only required for 'calcareous' soils. Guidelines on whether a soil is classified as 'slightly weathered', 'highly weathered' or 'calcareous' are presented in Chapter 3. Organic N and P values are calculated from the organic matter (OM) percentage value using input C:N and C:P ratios for the various OM pools.

2.2.1.3 Estimation of *Labile P*

Labile P was defined by Sharpley et al. (1984) as the P that can be extracted from soil using an anion exchange resin saturated with bicarbonate ions. The size of the *Labile P* pool is calculated from the soil test P value, and can be estimated using results from the following P tests: Bray 1, Bray 2, Olsen, Double Acid, Ambic, Mehlich and Truog (the last two can only be used for highly weathered soils). The calculation of Labile P from the Ambic and Bray 2 tests, tests popularly used in South Africa, were included using conversion equations from the literature and is discussed further in Chapter 3. The following equations are used in the model to determine the size of the *Labile P* pool (mg kg^{-1}):

Slightly weathered	**Highly weathered**	**Calcareous**
Labile P = 0.56BP1 + 5.1	*Labile P* = 0.14BP1 + 4.2	*Labile P* = 0.55BP1 + 6.1
= 1.07OP + 4.1	= 0.55OP + 2.1	= 1.09OP + 3.2
= 0.13MP1 + 11.4	= 0.24MP1 + 2.9	= 0.10MP1 + 10.2
= 0.69AP + 7.2	= 0.17AP + 4.7	= 0.68AP + 8.2
= 0.24BP2 + 5.9	= 0.059BP2 + 4.4	= 0.23BP2 + 6.89
= 0.38IP+ 4.69	= 0.09IP + 4.1	= 0.37IP + 5.70

where BP1 = Bray I P test
OP = Olsen's P test
MP1 = Mehlich I P test
AP = Ambic P test
BP2 = Bray II P test
IP = ISFEI P test

2.2.1.4 Estimation of phosphorus availability index (PAI)

The PAI is used to determine the amount of P available for crop uptake and influences P concentrations in runoff and drainage water. Different equations are used depending on the soil group classification, as follows:

Slightly weathered: $PAI = 0.0054 \times BaseSat\% + 0.116 \times pH(H_2O) - 0.73$ (2.1)

Highly weathered: $PAI = 0.46 - 0.0916 \times \ln(Clay\%)$ (2.2)

Calcareous soils: $PAI = 0.58 - 0.061 \times [CaCO_3]$ (2.3)

2.2.1.5 Estimation of *Active P* and *Stable P* pools

The *Active P* pool (slowly available P) can be calculated from *Labile P* and the PAI values using the following equation:

$$Active\_P = Labile\_P \times \frac{1 - PAI}{PAI} \quad (2.4)$$

The *Stable P* pool (unavailable P) is four times larger than the *Active P* pool. The units for the three inorganic P pools are in kg m^{-2}.

2.2.1.6 Crop residues

The model differentiates between amounts of standing stubble and surface residues of the previous crop. The type of crop from which the stubble originated must also be entered to obtain the relevant C:N and N:P ratios. The relevant fractions of fast-cycling, slow-cycling and lignified fractions for the above ground and root residues as well as the half-life for these fractions must also be specified.

2.2.1.7 Inputs that can be estimated by the model

If certain 'Initial N & P' inputs are not entered, they will be estimated by the model using the OM% of the soil. Algorithms to estimate initial soil nutrients are taken from SWAT. This will be helpful to users who do not have all the input values. If NO_3-N concentrations are not inserted, the model uses the following equation to estimate NO_3-N concentration (mg kg^{-1}):

$$NO_3\text{-}N = 7e^{-d} \quad (2.5)$$

where d = layer lower boundary depth (m)

If NH_4-N concentrations are not entered, a default value of 2 mg kg^{-1} for all soil layers is set. This value is then converted from a concentration to a mass value.

2.2.1.8 Nutrient related crop parameters

In addition to the original crop parameters required to simulate water and radiation limited growth (Annandale et al., 1999a), additional crop parameters required for N and P simulations are presented in Table 2.2.

Table 2.2 Crop parameters required for N and P simulations

Parameter	**Units**
C3/C4	-
N fixation	Yes/No
Grain N partitioning coefficient	1 – small grains and cereals -0.5 – maize and sorghum
Photoperiod sensitive	Yes/No
Critical photoperiod	Hours
N: P ratio	-
Root N concentration	kg N kg^{-1} DM
Maximum grain N concentration	kg N kg^{-1} DM
Slope	-
Increased root activity biomass	kg m^{-2}
P conc. at emergence	kg P kg^{-1} DM
Optimal P conc.: Vegetative	kg P kg^{-1} DM
Optimal P conc.: Reproductive	kg P kg^{-1} DM
Crop P uptake factor	-

Crop P uptake can be estimated using a crop N:P ratio, in which case the final four input parameters listed in Table 2.2 are not required. Further information on the use of these parameters is given in Section 4.4.

2.2.2 Fertilization

The model accounts for both organic and inorganic fertilizer applications. A wide range of predefined organic and inorganic fertilizers with respective N and P concentrations are provided, including various South African biosolids. If a predefined fertilizer is selected, the user is only required to enter the amount being applied and application method. Users are also able to specify user defined values for the fertilizer being applied. In some cases, values can be entered as concentrations and the model will convert to kg ha^{-1} of the specific nutrient to increase user-friendliness. The user must specify if the fertilizer is either broadcast or incorporated. When fertilizer is broadcast, the inorganic N and P remains on the soil surface until a rainfall/irrigation or tillage event, after which it is added to the surface layer.

2.2.2.1 Banded P applications

Banded P applications can be simulated in SWB-Sci. Users indicate the amount of the banded P application and depth of placement. The banded P fertilizer is then placed in the layer corresponding to placement depth. A simple banded P dissolution algorithm has been included in the model, in which a set daily fraction of the band is subject to dissolution and this fraction is then added to the *Labile P* pool. Further information on this approach is provided in Chapter 5.

2.2.2.2 Addition of N and P via rainfall and irrigation

The model accounts for N and P additions through rainfall and irrigation. This is done by entering the concentrations of N and P in rainfall/irrigation. Different concentrations can be entered for each rainfall/irrigation event, otherwise the model will use the most recent concentration entered. This method is used to account for fertigation nutrient inputs as well.

2.2.3 Tillage management

Tillage is simulated using the GLEAMS approach. Depth of tillage must be specified by the user. Different tillage implements are assigned different *Incorporation Efficiency* and *Mixing Efficiency* factors (Appendix 2.2). Unfortunately no mention is made of the operation of the tillage implement using this approach. Users are therefore advised to take this into account when selecting these factors. The *Incorporation Efficiency* factor influences the amount of crop residues and surface applied manure that is incorporated into the soil, while the *Mixing Efficiency* factor influences the extent of mixing and redistribution of the various organic matter pools and inorganic N and P pools between the soil layers. Water is currently not re-distributed between the layers during a tillage event. Any effects of tillage on infiltration and bulk density are also not currently simulated. In the event of burning, 95% of N and 5% of P is removed from the surface residues. This is a modification of the GLEAMS approach, which removes 95% of both N and P. These values might need to be re-visited and refined at a future stage. User defined inputs for incorporation and mixing efficiencies are also permitted.

Based on the CropSyst approach, a *Tillage Intensity Factor* is also required and influences the rate of incorporated residue decomposition. The factor ranges from 0 to 1 according to the following guidelines:

1.0 - Inversion with some mixing
0.8 - Mixing with some inversion
0.7 - Mixing only
0.4 - Lifting and fracturing
0.15 – Compression

This factor is then used to calculate a *Tillage Decomposition Adjustment Factor* which ranges from 1 - 2 and increases the rate of residue decomposition according to the intensity of the tillage practice.

2.2.4 Soil temperature, water and pH functions

2.2.4.1 Soil temperature function

Soil temperature for the various soil layers is calculated using the method used for SWAT. This method requires a value for the previous day's soil temperature for all layers. In order to estimate this value for the very first time, a method from CropSyst was used. This method requires the annual average temperature, the yearly sine function temperature phase, and half the yearly air temperature amplitude. Annual average air temperature can be entered by the user, or can be calculated before a simulation run using the weather data the user has selected. Care should be taken to ensure that there is suitable data to obtain an accurate annual average temperature when using this method.

The following temperature parameters are hard-coded into the model:

T_Minimum = -5ºC
T_Optimum = 35 ºC
T_Maximum = 50 ºC

If soil temperature is T, the *Temperature Function* is then calculated in the following way:

$$Temperature\_Fucntion = \frac{(T[i] - T\_Minimum)^{Q} \times (T\_Maximum - T[i])}{(T\_Optimum - T\_Minimum)^{Q} \times (T\_Maximum - T\_Optimum)} \qquad (2.6)$$

where T = layer soil temperature

$$Q = \frac{T\_Minimum - T\_Optimum}{T\_Optimum - T\_Maximum} \qquad (2.7)$$

If t is greater than *T Maximum* or less than *T Minimum* then the *Temperature Function* is set to zero.

2.2.4.2 Soil water function

The CropSyst equation used to calculate the influence of moisture levels on various soil processes is used. Values for a water-filled porosity (WFP) for zero response (WFPmin = 0.1), a WFP low threshold value for maximum response (WFPlow = 0.5) and a WFP high threshold value for maximum response (WFPhigh = 0.7) are hard-coded into the model. If WFP is between WFPmin and WFPlow, the *Soil Water Function* is calculated using Equation 2.8:

$$Soil\_Water\_Function = \frac{WFP - WFP\min}{WFPlow - WFP\min} \qquad (2.8)$$

where $WFP = \frac{\theta}{\theta s}$ (2.9)

If WFP is between WFPlow and WFPhigh, the *Soil Water Function* is equal to one. If WFP is greater than WFPhigh but less than or equal to 1, the *Soil Water Function* is calculated using Equation 2.10:

$$Soil\_Water\_Function = WCsat + (1 - WCsat) \times \sqrt{\frac{1 - WFP}{1 - WFPhigh}} \qquad (2.10)$$

2.2.4.3 Soil pH Function

Minimum (pHmin) and maximum pH (pHmax) function values are hard-coded into the model as 3.5 and 6.5, respectively. The pH function is then calculated using Equation 2.11:

$$pH\_Function = \frac{pH - pH\min}{pH\max - pH\min} \qquad (2.11)$$

2.2.5 Processes simulated

2.2.5.1 Mineralization and immobilization

Mineralization of crop residues and soil organic matter (SOM) closely follows the approach used by CropSyst. For standing and surface stubble crop residue, a *Contact Fraction* is used to account for surface residue contact with the soil during decomposition. Residue material is divided into three groups, fast-cycling, slow-cycling and lignified material. Each pool has its own half-life and C to CO_2 fraction which is hard-coded (Appendix 2.3). Potential C decomposition is calculated as follows:

$$Potential\_C\_Decomposed = C\_Mass\_Org\_\mathrm{Re}sidue \times Contact\_Fraction$$
$$\times (1 - e^{(-Decomp\_Cons\tan t \times Temperature\_Function)}) \times Mositure\_Function \qquad (2.12)$$

where Decomp_Constant is a pool specific constant (d^{-1}), converted from half-life in the case of crop residues

Decomposed fast- and slow-cycling residue is transformed into microbial biomass and CO_2 whilst decomposed lignified crop residue is converted to metastable SOM and CO_2.

SOM is divided into microbial biomass, labile SOM, metastable SOM and passive SOM. Each pool has its own *Decomp Constant* that has been hard-coded into the model (Appendix 2.3). The C fraction in all organic matter pools has a constant value of 0.58. Equation 2.12 is also used to simulate decomposition of the SOM with the Contact_Fraction always equal to one for these pools.

The C:N ratio of the decomposing pool and the pool(s) to which organic matter is being transferred will determine whether N mineralization or immobilization occurs. Net N mineralization is calculated first. If N mineralization does take place from a pool then the N immobilization demand is assumed to be zero. If the calculated mineralization amount is negative, however, then the absolute value of this amount becomes the N immobilization demand and net N mineralization is set to zero. This is done for each SOM pool and accumulated to form a total N immobilization demand. N immobilization firstly takes place from the NH_4^+ pool. If there is not enough NH_4^+ to satisfy the total immobilization demand, N from the NO_3^- pool will also be immobilized. If there is not enough N from both pools to satisfy demand, this deficit will carry over to the next day. This deficit will further contribute to decreasing the decomposition rate through its effect on the decomposition reduction factor which is calculated as follows:

$$Decomp\_Reduc\_Fact = \frac{N\_Immob\_Demand - Defecit\_For\_Immob}{N\_Immob\_Demand} \qquad (2.13)$$

As CropSyst does not simulate crop residue and SOM mineralization/immobilization of P, new code was written for this purpose. C:P ratios of the various organic matter pools are used to obtain the quantity of P mineralized directly from the amount of C mineralized for SOM. P immobilization by the microbial biomass is related directly to

N immobilization using the C:N and C:P ratios. A C:P ratio of 106 is currently being used for all SOM pools. In the same way, P mineralization from crop residue is directly proportional to N mineralization quantities using crop N:P ratios. Modifications to the code to model P in the same mechanistic way as organic N is modelled should be considered in future refinements to the model.

2.2.5.2 Inorganic N transformation processes

2.2.5.2.1 Ammonia volatilization

Whether the applied NH_4^+ fertilizer is broadcast or incorporated has a primary role in the amount of volatilization that takes place. Soil pH and cation exchange capacity (CEC) further influence the fraction of applied NH_4^+ fertilizer which is available for volatilization. A turbulent transfer coefficient value is calculated making use of wind speed at 2 m and soil, residue and/or crop friction velocities, as well as the leaf area index (LAI) of the crop.

2.2.5.2.2 Nitrification

If climatic conditions are favourable, nitrification will take place if the soil layer *NO_3 NH_4 Ratio* is less than the hard-coded constant value of 8, and is calculated using Equation 2.14:

$$Layer\_N\_Nitrified = (NH4[i] - \frac{NO3[i]}{NO3\_NH4\_Ratio}) \times (1 - e^{(-Nitrification\_Constant \times pH\_Function \times Soil\_Temperature\_Function)}) \times Nitrification\_Moisture\_Function \quad (2.14)$$

where Nitrification_Constant = 0.2

Nitrification_Moisture_Function is the same as the Soil_Water_Function (Equation 2.8)

2.2.5.2.3 Denitrification

Denitrification mostly occurs when N is lost to the atmosphere in the form of a gas, but can also be leached in the drainage water. Only N lost to the atmosphere is simulated in the model. Firstly the model calculates whether the quantity of water entering a layer is greater than the current air filled porosity of the layer. If this condition is met, denitrification does occur in that layer for that day. Whether a denitrification event occurs the next day is dependant on the sand fraction of the layer, which is related to how quickly water will drain from the layer. If the sand fraction is greater than 0.5, dentrification is not assumed to occur on the following day. The Potential_Denitrification constant is hard-coded as 0.000032 kg N kg soil^{-1} d^{-1}, and the *Denitrification Half Rate* is hard-coded as 0.00006 kg N kg soil^{-1} d^{-1}. When a denitrification event does occur, Equation 2.15 is used to estimate the amount of NO_3^- lost through dentrification:

$$Layer\_N\_Denitrified = \frac{Potential\_Denitrification}{Soil\_Mass \times Denitrification\_Factor} \quad (2.15)$$

where the Denitrification_Factor is the minimum of:

$$\mathrm{Re}\,spiration\_\mathrm{Re}\,sponse\_Function = \frac{CO_2\_Loss\_Per\_Unit\_Soil\_Mass}{CO_2\_\mathrm{Re}\,spiration\_Threshold} \quad (2.16)$$

$$Nitrate\_\mathrm{Re}\,sponse\_Function = \frac{NO3\_Conc\_Dry\_Soil}{NO3\_Conc\_Dry\_Soil + Denitrification\_Half\_Rate} \quad (2.17)$$

Denitrification_Moisture_Function = 1 (1st day), 0.5 (2nd day) (2.18)

2.2.5.2.4 Nitrogen fixation

Certain crops are able to fix N and this capability has been included into the model, based on the approach by Bouniols et al. (1991). Daily N fixation is calculated as follows:

$$Nitrogen\_Fixation = Minimum[Crop\_N\_Demand \times N\_Fixation\_Factor, Min\_Daily\_N\_Fixation\_Mass] \quad (2.19)$$

where Min_Daily_N_Fixation_Mass = 6 kg N ha^{-1} d^{-1}

N_Fixation_Factor is the minimum of the following factors:

N_Fix_Temp Factor: 1 for temperatures > 36°C

0.7 for temperatures between 0-36°C

0 for temperatures < 0°C

Soil_N_Factor: 0 for root zone N masses > 300 kg ha^{-1}

1 for root zone N masses < 100 kg ha^{-1}

$1 - \frac{Root\_Zone\_N\_Mass - 100}{300}$ for root zone N masses between 100-300 kg ha^{-1} (2.20)

$$N\_Fix\_Moisture\_Function = \frac{PAW\_Top\_30 - 0.5}{0.5} \quad (2.21)$$

where PAW_Top_30 is the plant available water in the top 30 cm of the soil profile

For crops that are able to fix N, the N demand of the crop is reduced by an amount that can be supplied by N_2-fixing bacteria.

2.2.5.3 Inorganic P transformation processes

The modelling of P processes in soil is generally accepted to be highly challenging involving complex interactions. The approach used to model soil inorganic P is based on the approach originally developed by Jones et al. (1984) and Sharpley et al. (1984).

2.2.5.3.1 Soil inorganic P

Movement of inorganic P between the *Labile P* and *Active P* pools is determined by the following equation:

$$Labile\_Active\_P\_Flux = 0.1 \times Moisture\_Function \times e^{(0.115 \times Soil\_Temp - 2.88)}$$
$$\times (Labile\_P - Active\_P \times \frac{PAI}{1 - PAI}) \qquad (2.22)$$

As can be seen from the above equation soil water content and temperature will influence the flux. If the flux is positive it indicates P adsorption (*Labile P* → *Active P*), while if the flux is negative, it indicates soil P desorption (*Active P* → *Labile P*). Vadas et al. (2006) subsequently observed that a constant of 0.1 underestimated soil P desorption and suggested a constant of 0.6 be used instead when the flux is moving in this direction. This modified approach has been included into SWB-Sci.

As previously mentioned, the *Stable P* pool is always four times larger than the *Active P* pool, and movement between these two pools will be determined by the following equation:

$$\text{Active\_Stable\_P\_Flux} = \text{P\_Flux\_Coeff} \times (4 \times \text{Active\_P} - \text{Stable\_P}) \qquad (2.23)$$

where PFluxCoeff = 0.00076 for calcareous soils

or PFluxCoeff = $e^{(-1.77 \times PAI - 7.05)}$ for weathered soils (2.24)

2.2.5.4 Crop N and P uptake

2.2.5.4.1 Crop N uptake and stress effects

N uptake is based on CropSyst algorithms which are based on the approach by Godwin and Jones (1991). N uptake is determined as the minimum between crop N demand and potential N uptake. Total potential N uptake is calculated according to the amount of available N in the soil, and using adsorption coefficients of 0 for NO_3^- and 5.6 for NH_4^+. N demand requires the calculation of reference plant N concentration, and critical, minimum and maximum N concentration parameters for different growth stages are hard-coded for C3 and C4 plants (Appendix 2.4).

When the crop biomass is below a user defined value (*Biomass For Increased Root Activity*), a *Root Activity Factor*, which begins at 3 and approaches 1 as the crop grows, is used to account for higher N uptake than simple passive uptake. The root activity factor is calculated using the following equation:

$$Root\_Activity\_Factor = 1 + 2 \times (1 - (\frac{Cumulative\_Biomass}{Biomass\_For\_Increased\_Root\_Activity})^3) \quad (2.25)$$

This *Root Activity Factor* is multiplied by potential NO_3^- and NH_4^+ uptake to account for increased root activity and active uptake during the earlier growth stages. When N supply does not meet crop N requirement, crop growth is reduced using an N-limited growth factor. The N taken up is first assigned to the roots. If not enough N is available a *Root N Stress Factor* is calculated as follows:

$$Root\_N\_Stress\_Factor = \frac{Available\_N}{Root\_N\_Demand} \quad (2.26)$$

Thereafter N is assigned to the aboveground biomass. If not enough N is available for aboveground biomass growth, a *Top N Stress Factor* is calculated as follows:

$$Top\_N\_Stress\_Factor = 1 - (Top\_N\_Stress\_Index)^2 \quad (2.27)$$

where

$$Top\_N\_Stress\_Index = \frac{Top\_N\_Conc - Top\_Minimum\_N\_Conc}{Top\_Critical\_N\_Conc - Top\_Minimum\_N\_Conc} \quad (2.28)$$

If the *Top N Stress Factor* is less than 0.3, the leaf area index is reduced using a *N Canopy Reduction Factor* which is calculated as follows:

$$N\_Canopy\_Reduction\_Factor = 1 - \frac{1 - Top\_N\_Stress\_Factor}{0.7} \quad (2.29)$$

In contrast to CropSyst in which grain yield is calculated using a harvest index, in SWB-Sci yield is updated daily after flowering has occurred using a harvestable dry matter increment and estimating daily crop N partitioning. Using this approach, a modified approach to account for stress after flowering was required. Grain N stress is calculated using Equation 2.30:

$$Grain\_N\_Stress\_Factor = \frac{N\_Available\_For\_Distribution}{Grain\_N\_Demand} \tag{2.30}$$

As with pre-flowering crop growth, nutrient stress on grain development is considered the minimum of N and P stress.

2.2.5.4.2 Crop P uptake and stress effects

P uptake is also determined as the minimum between crop demand and potential uptake. A crop specific *Active Uptake Factor* must be specified by the user, and using this factor, the amount of plant available P in the soil layer and the *Moist Function*, a daily *Crop P Uptake Factor* is determined:

$$\text{Crop\_P\_Uptake\_Factor} = (\text{Labile\_P}+\text{Banded\_P})\times\text{Active\_Upake\_Factor}\times\text{Moist\_Function} \tag{2.31}$$

High active P uptake as observed in reality and mechanisms such as plant acid secretions and mycorrhizae interactions enhance P uptake, are therefore assumed to be accounted for through the *Crop P Uptake Factor*.

Potential P uptake for each layer is then calculated using Equation 2.32:

$$\text{Potenital\_P\_Uptake} = \text{Avail\_P\_Conc}\times\text{Layer\_Transpiration}\times\text{Crop\_P\_Uptake\_Factor} \tag{2.32}$$

where Avail_P_Conc = plant avail P concentration (mg l^{-1})

Two options are currently available to estimate crop P demand:

Option 1

In this simpler approach, crop uptake of P is linked to crop N uptake and is determined using N:P ratios for various crops (Appendix 2.5). The effects of P deficiencies on the crop are therefore not simulated when using this option.

Option 2

For this approach, users specify the crop P concentration at emergence, as well as optimal P concentrations for the vegetative and reproductive growth phases. Root P concentration can also be specified or else is taken as 1/6 of root N concentration. The model then uses these concentrations to calculate daily crop P demand. P that has been taken up is firstly assigned to the roots. If available P does not meet root/aboveground P demand, stress effects on crop growth are determined from Equation 2.33 (Daroub et al. 2003):

$$Top/Root\_P\_Stress\_Factor = 1 - [1 - (\frac{Potential\_P\_Uptake}{P\_Demand})]^4 \quad (2.33)$$

The *P Stress Factor* ranges from 0 – 1, and is not directly proportional to the ratio of potential uptake to demand, but is 1 even for values just below 1. Grain P mass is simulated as all the P taken up by the crop after the commencement of flowering. This new approach to modelling P uptake, stress effects and grain filling will benefit from further testing and refinement as researchers gain more experience in modeling P under field conditions.

2.2.5.5 Nutrient runoff losses

2.2.5.5.1 Phosphorus

Soluble P runoff losses are determined by volume of runoff and adsorption/desorption coefficients. In order to determine P partitioning between the soil and water phases, a partitioning coefficient is calculated using the following equation:

$$PPartitionCoeff = 100 + 2.5 \times Clay\% \quad (2.34)$$

Using this partitioning coefficient, the concentration of *Labile P* available for runoff can then be calculated:

$$LabileP\_Avail = \frac{LabilePConcSL \times e^{(-(SurfaceInfiltration - InitialAbstraction))}}{PPartitionCoeff \times BulkDensity + SL\_SaturatedWC} \quad (2.35)$$

where SurfaceInfiltration is the amount of rainfall/irrigation after runoff is calculated

SL_SaturatedWC is the saturated water content of the surface layer

InitialAbstraction = 0.2×(SL_SaturatedWC-SurfaceLayerWC) (2.36)

Soluble P runoff concentration is then determined by the following equation:

$$RunoffLabilePConc = \frac{LabileP\_Avail \times PExtractionCoeff}{1 + PExtractionCoff \times PPartitionCoeff} \quad (2.37)$$

where PExtractionCoeff $= 0.598 \times e^{(-0.179 \times LabilePPartitionCoeff)}$ (2.38)

Finally actual soluble P runoff loss is calculated as follows:

RunoffLabileP= RunoffLabilePConc×RunOff (2.39)

2.2.5.5.2 Nitrogen

NH_4^+ runoff losses are calculated as for P, except the partitioning coefficient is calculated using Equation 2.40:

NH4PartitionCoeff = 1.34 + 0.083×Clay% (2.40)

In the case of NO_3^-, no soil adsorption is considered to take place.

Sediment N and P losses are currently not simulated in SWB-Sci but will be in the future. N and P runoff losses from surface manure and other organic fertilizers are also intended to be included at a later stage.

2.2.5.6 Vertical solute movement

The downward movement of solutes through the vadose zone is based on a simple approach that controls solute concentrations in the mobile soil water phase by making use of a *Solute Mixing Fraction*. This value represents the fraction of solute in a layer that interacts with water that is passing. When the quantity of water entering a layer is greater than the quantity required to take the VWC of that layer above FC, Equation 2.41 is used to calculate the solute concentration in the mobile water phase for the next layer:

$$Mobile\_Solute\_Concentration = \frac{Layer\_Solute\_Mass \times Solute\_Mixing\_Fraction}{Layer\_VWC \times Layer\_Depth \times WaterDensity} \tag{2.41}$$

After N or P has entered a layer from the layer above, instantaneous mixing is assumed to take place across the entire layer. If less water than required to fill the layer to or above FC enters a layer, the concentration of the water leaving that layer is considered to be the same as the immobile water concentration for that layer.

A more mechanistic approach to simulate incomplete solute mixing based on the approach developed by Corwin et al. 1991 has also been included. This approach utilizes a mobility coefficient (γ) which represents the fraction of the liquid phase that is subject to piston-type displacement, with the fraction 1- γ therefore representing the liquid phase that is bypassed.

2.2.6 Mass balances

Several 'mass balances' have been built into the model and form part of the outputs. These will alert the user if matter (water, salt, N, P) has been 'created' or 'destroyed', indicating an error in the simulation.

2.3 CONCLUSIONS

SWB-Sci can now be used to mechanistically simulate N and P in cropping systems. Most of the algorithms to simulate N and P are based on well established and tested existing models. Modifications to algorithms were required in some cases so the model will benefit from further testing and refinement as researchers gain more experience in modelling N and P under field. A strength of SWB-Sci is that considerable work has already been invested locally to test the crop growth and soil water balance simulation capabilities of the model and in obtaining input parameters for a wide range of soils and crops. The mechanistic structure of the model also means that it can be applied to a wide variety of problems and scenarios. A primary objective of this model is to improve our understanding of the effects of fertilization and irrigation strategies on crop growth, and the source of N and P pollutants from agriculture at the local scale. The model was developed with the intention that it not only be used for research, but that it will ultimately also be useful to consultants, extension officers, economists and even farmers to improve nutrient management in order to reduce non point source pollution.

2.4 REFERENCES

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CHAPTER 3

OBTAINING THE PARAMETERS REQUIRED TO MODEL LABILE PHOSPHORUS FOR SOUTH AFRICAN SOILS*

ABSTRACT

Modelling phosphorus (P) in the environment can increase our understanding of potential transfer pathways into receiving water bodies as well as the plant availability of this nutrient in soil. Many current models make use of algorithms originally developed for the EPIC model over two decades ago. These algorithms were developed primarily using continental USA soils. Obtaining the required input parameters can therefore be challenging when applying this approach to soils not classified according to the USA system, and for soils for which similar parameters are not available. In this paper, new equations for the estimation of labile P from Ambic P, Bray 2 P and the modified ISFEI method are proposed. Guidelines for the classification of South African soils as calcareous, slightly weathered and highly weathered are further suggested, and we propose that only topsoil properties be used for this purpose. Depending on the amount of soil information available, this classification can be achieved using the clay fraction SiO_2:Al_2O_3 *molecular ratio, the sum of exchangeable Ca, Mg, K and Na, or a newly proposed categorization system for South African soil forms. It is clear that the above approaches should be thoroughly tested and relevant local research carried out to improve our ability to model P in South African soils.*

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3.1 INTRODUCTION

Loss of phosphorus (P) from agricultural land to waterways is a major concern, as P is often the limiting factor for eutrophication. Increased P fertilizer prices, deficient levels of plant available P in many sub-Saharan African soils and the recognition of P as a finite resource globally, further necessitates the careful management of this nutrient (Buresh et al., 1997; Mengel, 1997). In soils, P exists as organic P associated with soil organic matter and residues, and inorganically, as mineral P with varying degrees of solubility. Plant P uptake occurs in the form of soluble and weakly adsorbed phosphates (HPO_4^{2-}, $H_2PO_4^-$). Sequential chemical extraction is often used to divide total soil P into different organic P and inorganic P fractions (Chang and Jackson, 1957; Buehler et al., 2002). These fractions are not discrete entities, however, as intergrades and dynamic transformations continuously occur towards maintaining steady state conditions.

Models can be utilized to improve our understanding of P dynamics in the environment, identify zones within a catchment with high P export potential, and explore mitigation measures. Although models used to predict P export from land include process-based models, export coefficient models and statistical or empirical models (Sharpley, 2007), only process-based models are the subject of this paper. These models often have technical guidelines for estimating hydrology and sediment parameters, but similar technical notes for selecting P parameters are mostly absent (Radcliffe and Cabrera, 2007). A drawback of process-based P models is the difficult-to-obtain inputs required to run the model (Karpinets et al., 2004), especially at catchment scale when limited soil information is available and model inputs must often be estimated. Acquiring the required parameters can also be challenging for soils different to those from which the original modelling algorithms were developed. The objective of this paper is to guide the user through the parameterization of a P model for South African soils. New equations were required to estimate *Labile P* from soil P tests commonly used in South Africa and are presented here. Additionally, the approach to categorize soils as slightly weathered, highly weathered or calcareous is reviewed. A newly developed approach to categorize soil forms into one of these three groups using information available in land type maps is further proposed to facilitate P modelling at the local and catchment scales.

3.2 REVIEW OF INORGANIC PHOSPHORUS MODELLING

A wide range of models are currently available to model phosphorus in soil-crop systems. To the best of our knowledge, P modelling is practised on a limited scale in South Africa, and models that are currently being used include SWAT (Soil Water Assessment Tool) (Arnold et al., 1998), APSIM (Agricultural Production Systems Simulator) (Keating et al., 2003), ACRU-NP (Campbell et al., 2001) and the newly developed SWB-Sci described in a review by Singels et al. (*in press*). ACRU-NP and SWAT have simple crop routines and were developed to be run at the catchment scale, while SWB-Sci and APSIM were developed to be run on the field scale and are more reflective of management practice interventions. The P modelling routines of all four of these models can be traced back to work done by Jones et al. (1984) and Sharpley et al. (1984) to develop the model EPIC (Erosion Productivity Impact Calculator) (Williams et al., 1983).

In the EPIC approach three inorganic P pools are simulated, namely, *Labile P*, *Active P* and *Stable P* (Figure 3.1). The *Labile P* pool refers to a pool from which plants are able to take up P from the soil, and consists of both soluble P and weakly sorbed P. Phosphorus which is increasingly more strongly adsorbed and not immediately available to the plant is represented by the *Active P* followed by the *Stable P* pools. Phosphorus flux can occur between the *Labile P* and *Active P* pools, and between the *Active P* and *Stable P* pools. For all models, the various P pools are subject to a rate-defined equilibrium. Typically, no attempt is made to equate the *Active* and *Stable P* pools to the soil P fractions obtained through sequential chemical extraction (Probert 2004). Instead, these three pools are used to represent the fast sorption, slower sorption and very slow precipitation processes which P undergoes in soils (McGechan and Lewis, 2002). Phosphorus is also transferred between the *Labile P* and *Organic P* pools as a result of mineralization and immobilization processes occurring in the soil. The size of the *Labile P* pool is further used to determine the concentration of P in runoff and drainage water.

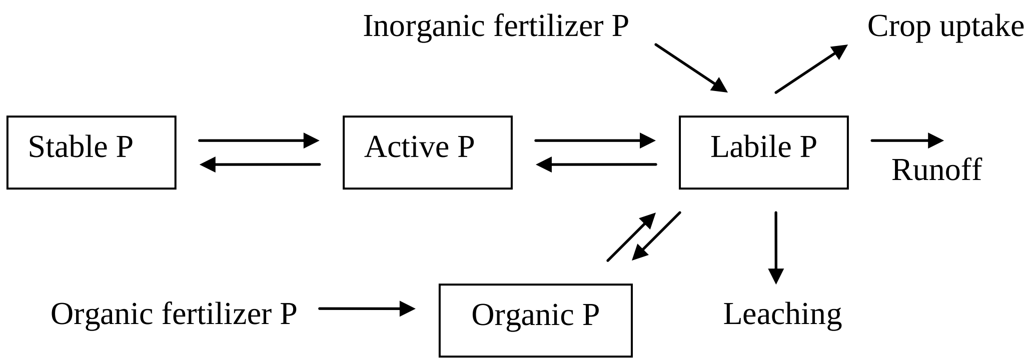

Figure 3.1 Structural diagram of the various P pools simulated using the EPIC approach

Originally, Jones et al. (1984) and Sharpley et al. (1984) used 78 continental USA and Puerto Rican soils to develop their plant and soil P model. Calcareous and non-calcareous soils which have undergone different degrees of weathering can be expected to undergo greatly differing soil-P reactions (Sharpley et al., 1989), and Sharpley et al. (1984) observed that the most accurate estimation of Labile P, was achieved when soils were divided into calcareous, slightly weathered or highly weathered groups based on the presence of calcium carbonate ($CaCO_3$) and degree of weathering. Strict definitions of these soil groups were not provided, however, making this a challenging exercise. The discussion below is provided to inform model users of the issues involved in categorizing a soil into one of these three groups.

3.3 CALCAREOUS, SLIGHTLY WEATHERED AND HIGHLY WEATHERED SOILS

Sharpley et al. (1984) defined calcareous soils as soils with free $CaCO_3$, and according to Thomas (1996), soils with pH (H_2O) values of 7.6 to 8.3 are normally found to be calcareous. According to the South African taxonomic classification system, soils containing sufficient free calcium carbonate or calcium magnesium carbonate to effervesce visibly when exposed to a cold 10% HCl solution are considered to be calcareous (Soil Classification Working Group, 1991).

The degree of weathering that a non-calcareous soil has undergone can be judged by the presence of specific minerals associated with weathering stages (Jackson and Sherman, 1953). Early weathering stages are associated with the presence of gypsum, calcite, olivine-hornblende, biotite and albite; intermediate weathering stages by quartz, muscovite, 2:1 layer silicates and montmorillonite; and advanced weathering stages by kaolonite, gibbsite, hematite and anatase. Sharpley et al. (1984) defined highly weathered USA soils as Oxisols, Ultisols, Quartzipsamments, Ultic subgroups of Alfisols and acidic Ochrepts, while all other soils fell into the slightly weathered group. Not all soils containing < 10 % clay – the definition for Quartzipsamments – should automatically be considered highly weathered, however. In a later study representing eight major soil orders from all regions of the United States, Puerto Rico, Indonesia, Malaysia, Papua New Guinea, Philippines and Sudan, Quartzipsamments were not considered as highly weathered (Sharpley et al., 1987). According to the Soil Classification Working Group (1991), highly weathered or 'ferrallitic' soils are characterized by a clay fraction SiO_2:Al_2O_3 molecular ratio of less than 1.3, whereas slightly weathered or 'ferrisol' soils have a ratio of between 1.3 and 2 and a base saturation of less than 50%. In South Africa, some non-calcareous soil forms are divided into eutrophic, mesotrophic and dystrophic soil families based on the degree of leaching which is an indication of the weathering status; and classification is determined by the sum of exchangeable Ca, Mg, K and Na expressed as cmol(+) kg^{-1} clay (Soil Classification Working Group, 1991). Dystrophic soils (highly weathered) have a value of less than 5, mesotrophic soils (moderately weathered) have a value between 5 and 15, and eutrophic soils (slightly weathered) have a value greater than 15 cmol(+) kg^{-1} clay in their B1 horizons.

Sharpley et al. (1984) originally used weathering and soil taxonomic information to group soils, and although the United States Department of Agriculture mostly uses subsoil parameters to determine classification, for South African soils we suggest that the properties of the top horizon only should be considered for categorization as this is the diagnostic horizon used in the South African Classification system (Soil Classification Working Group, 1991). Furthermore, only surface samples (0-10 cm) were used by Jones et al. (1984) and Sharpley et al. (1984) to develop the various algorithms used.

Grouping of South African soils in the abovementioned groups when only soil form and series (MacVicar et al., 1977) are known from the land-type survey (Land Type Survey Staff, 2001), as is often the case when modelling at the catchment scale, is discussed later in this paper.

3.4 ESTIMATION OF INORGANIC P POOL SIZES

Labile P

The *Labile P* pool is measured using an anion exchange resin, but this is a time consuming and expensive procedure. In order to estimate the size of inorganic P pools, APSIM and SWAT require a direct input of a labile P value (mg kg^{-1}). ACRU-NP and SWB-Sci require a soil test P (STP) result, for which algorithms have been developed to quantify the *Labile P* pool. This approach is based on work by Sharpley et al. (1984) to relate labile P to Bray 1 P (BP1), Olsen P (OP) and Mehlich-1 P (MP1) for slightly weathered, highly weathered and calcareous soils. Sharpley et al. (1989) later added additional equations using BP1 and OP for highly basic calcareous soils (free $CaCO_3$ > 50 g kg^{-1}), and additional BP1, OP, Colwell P (CoP), Truog P (TP) and Mehlich-3 P (MP3) soil P test values for highly weathered acid tropical soils (Al saturation > 30%). Sharpley et al. (1989) caution that the application of these equations is limited to soils having physical and chemical properties within the range covered by the regression analyses. A summary of soil properties for the soils tested is provided in Table 3.1.

The most commonly used extraction methods in South Africa are BP1 (Fertilizer industry) and Ambic 1 (AP) (ARC Institutions and Departments of Agriculture). However, in the Western Cape the Citric acid method (CiP) and in KwaZulu-Natal the TP method, are also used. The OP method is mainly restricted to the Free State Department of Agriculture and the University of the Free State. The Bray 2 P (BP2) is also sometimes used in South Africa. In addition, a modified version of the ISFEI (IP) method was used to determine the 'P status' of modal profiles during the compiling of land type maps (Land Type Survey Staff, 1985). Although much work has been done locally and internationally to compare various P extraction methods, much of this work has been restricted to unpublished reports (Schmidt et al., 2004)

Table 3.1 Ranges of soil properties for five soil groups tested by Sharpley et al. (1984) and Sharpley et al. (1989)

Soil Group	**pH (H_2O)**	**Sand (%)**	**Silt (%)**	**Clay (%)**	**$CaCO_3$ (%)**	**Base sat (%)**	**CEC (cmol kg^{-1})**	**Org C (%)**	**BrayI P**	**Olsen P (µgP g^{-1})**	**Labile P***
Calcareous (N=20)											
Mean	7.7	35	41	24	9.1	100	20	1.4	20	13	17
Median	7.7	35	42	23	0.8	100	17	1.4	11	9	13
Range	7.1-8.4	4-71	17-62	10-67	0.5-54	100	8-55	0.4-3.2	1-77	3-38	6-56
Slightly weathered (N=35)											
Mean	6.4	27	51	22	-	89	17	1.7	24	13	19
Median	6.3	18	53	22	-	95	16	1.7	21	12	16
Range	5.2-8.3	1-87	6-85	6-62	-	40-100	5-43	0.2-3.5	4-79	3-42	4-53
Highly weathered (N=23)											
Mean	5.6	55	30	5	-	58	8.2	1.6	66	20	13
Median	5.6	59	28	10	-	77	7.6	1.4	47	19	11
Range	4.4-6.8	6-96	1-76	0.4-76	-	11-100	1.3-20.5	0.4-3.8	3-222	2-50	3-43
Highly basic calcareous (N=23)											
Mean	8.2	-	-	27.1	34	-	17.6	0.81	2.5	5.7	6.2
Median	8.1	-	-	26.1	22	-	13.4	0.36	0.2	4.9	6.2
Range	7.4-9.1	-	-	2.8-56.3	6-74	-	1.3-34.6	0.04-4.66	0.1-18.1	0.9-15.6	0.6-14.8
Highly weathered acid tropical (N=32)					**Al sat. (%)**						
Mean	4.6	-	-	28.7	68	-	13.8	3.2	17.7	-	12.8
Median	4.6	-	-	15.2	74	-	11.1	2.54	9.4	-	10.6
Range	3.9-5.2	-	-	7.0-76.3	30-96	-	4.4-36.8	1.07-7.77	3.1-72.8	-	3.9-35.9

*Measured using anion exchange resin method (Sharpley et al., 1984)

Equations for the estimation of *Labile P* using the locally popular AP, BP2 and IP test results were not derived for the original work done by Sharpley et al. (1984) in the U.S., but are essential for modelling P dynamics in South African soils. After a study comparing BP1 and AP results from 12 localities in South Africa, Schmidt et al. (2004) reported the following relationship using linear regression analysis:

$$BP1 = 1.23 \times AP + 3.82 \qquad (3.1)$$

An R^2-value of 0.91 was obtained where clay contents of the soils ranged from 8.4 to 47%. Buys and Venter (1980) reviewed correlations between BP1 and BP2 from several studies done by the Fertilizer Society of South Africa and observed greater correlation for acid soils than for alkaline soils and soils treated with rock phosphate. The authors reported the following relationship between BP1 and BP2 for a wide range of South African soils (R^2 not reported):

$$BP1 = 0.42 \times BP2 + 1.44 \qquad (3.2)$$

Buys and Venter (1980) also reported the following relationship between IP and BP1 for a range of 36 South African soils for which an R^2 of 0.95 was obtained:

$$IP = 1.49 \times BP1 + 1.07 \qquad (3.3)$$

Using these correlations, the equations in Table 3.2 are developed for the estimation of *Labile P* in South African soils.

Table 3.2 Current and suggested equations for the estimation of labile P pool size for South African soils*

Soil Group	Number of observations	R^2	Soil Group	Number of observations	R^2
Slightly weathered	35		**Highly weathered acid tropical**		
P_{lab} = 0.56BP1 + 5.1§		0.79	(> 30% Al saturation)	32	
= 1.07OP + 4.1§		0.77	P_{lab} = 0.41BP1 + 5.55†		0.86
= 0.13MP1 + 11.4§		0.39	= 0.20TP + 5.62†		0.80
= 0.69AP + 7.2 ʅ	n/a		= 0.43CP + 4.21†		0.84
= 0.24BP2 + 5.9 ʅ	n/a		= 0.64MP3 + 5.72 †		0.71
= 0.38IP* + 4.69 ʅ	n/a		= 0.50AP + 7.12 ʅ	n/a	
			= 0.17BP2 + 6.14 ʅ	n/a	
Highly weathered	20		= 0.28IP + 5.25 ʅ	n/a	
P_{lab} = 0.14BP1 + 4.2§		0.83			
= 0.55OP + 2.1§		0.74	**Highly basic calcareous**		
= 0.24MP1 + 2.9§		0.51	(> 50 g kg^{-1} $CaCO_3$)	23	
= 0.17AP + 4.7 ʅ	n/a		P_{lab} = 0.69BP1 – 1.76†		0.35
= 0.059BP2 + 4.4 ʅ	n/a		= 0.96OP – 0.19†		0.90
= 0.09IP + 4.1 ʅ	n/a				
Calcareous	23				
P_{lab} = 0.55BP1 + 6.1§		0.76			
= 1.09OP + 3.2§		0.61			
= 0.10MP1 + 10.2§		0.84			
= 0.68AP + 8.2 ʅ	n/a				
= 0.23BP2 + 6.89 ʅ	n/a				
= 0.37IP + 5.70 ʅ	n/a				

* All P tests on a mass basis (mg kg^{-1}), except the IP test which is on a volume basis (mg l^{-1})

§ Sharpley *et al*. (1984)

† Sharpley *et al*. (1989)

ʅ Equations derived for South African soils

A disadvantage of using chemical extractants to determine available P is that these tests are not equally reliable over all soil types, and the relative extractants may dissolve non-labile P tightly bound to Al, Fe and Ca complexes (Myers et al., 2005). The BP1, MP1 and MP3 tests were designed to extract P from non-calcareous soils dominated by Fe and Al-P complexes, while the OP test was designed to extract P from calcareous soils (Bray and Kurtz, 1945; Watanabe and Olsen, 1965; Mehlich, 1984; Myers et al., 2005). This is evident in the low R^2 of 0.35 for BP1 for the highly basic calcareous soil group, while OP has an R^2 of 0.90 for the same soil group. BP2 and AP conversions were therefore not done for the highly basic calcareous group. It should also be noted that at low STP levels the equations can give *Labile P* values higher than the STP value in some cases. Care should therefore be taken when estimating *Labile P* using very low STP values. A standardized extraction method using anion exchange resin membranes, which are more representative of plant available soil P, is suggested by Myers et al. (2005) for widespread adoption.

Active and Stable P pools

The P Availability Index (PAI) of a soil is used to determine the direction and magnitude of fluxes between the *Labile*, *Active* and *Stable P* pools. Additionally, the PAI also influences the amount of *Labile P* that is available for plant uptake as well as P runoff and leaching losses. Algorithms to estimate PAI were first suggested by Sharpley et al. (1984) and later modified by Sharpley and Williams (1990). For calcareous soils, the calcium carbonate ($CaCO_3$) percentage is required to calculate the PAI (Equation 3.4), for slightly weathered soils the base saturation percentage and soil pH(H_2O) is required (Equation 3.5), and for highly weathered soils the clay percentage is required (Equation 3.6):

Calcareous: $PAI = 0.58 - 0.0061 \times CaCO_3$ (3.4)

Slightly weathered: $PAI = 0.0054 \times BaseSat\% + 0.116 \times pH(H_2O) - 0.73$ (3.5)

Highly weathered: $PAI = 0.46 - 0.0916 \times \ln(Clay\%)$ (3.6)

Depending on soil grouping, the abovementioned input parameters will therefore also be required to model inorganic P.

According to the approach of Jones et al. (1984), the initial size of the *Active P* pool is calculated using a P Availability Index (PAI), with Equation (3.7):

$$Active\ P = \frac{Labile\ P}{\left(\frac{PAI}{1 - PAI}\right)} \tag{3.7}$$

ACRU-NP and SWB-*Sci* are also able to estimate the size of the *Active* and *Stable P* pools by subtracting organic P and *Labile P* from total soil P, if these values have been provided by the user. Initial *Stable P* is assumed to be four times larger than *Active P*.

3.5 OBTAINING INPUTS AT CATCHMENT SCALE

When large areas such as catchments are modelled it is often impractical to perform soil analyses for the entire area. At this scale, limited soil information also often means that input data needs to be aggregated. Land type maps are available for the whole of South Africa at a scale of 1:250 000. Each land type map is accompanied by a memoir, from which the soil forms and series of a specific area can be obtained. Profile descriptions of representative soils and analytical data for particle size distribution, water retentivity, modulus of rupture, air-water permeability ratio, mineralogy, cation exchange properties, soluble salts, acidity, CBD-extractable Fe, micronutrients, P status and P sorption are also given in the memoirs (Land Type Survey Staff, 1985).

In Table 3.3, related soil forms (MacVicar et al., 1977) used for land type mapping are placed in four groups in a way that allows the formation of a guideline for each group to enable categorization.

Table 3.3 Grouping of soil forms used for Land-type mapping to facilitate categorization as slightly weathered, highly weathered or calcareous

Soil form			
Group 1	**Group 2**	**Group 3**	**Group 4**
Kranskop	Arcadia	Katspruit	Champagne
Magwa	Inhoek	Fernwood	Nomanci
Inanda	Milkwood		Sterkspruit
Avalon	Mispah		Estcourt
Pinedene	Rensburg		Kroonstad
Glencoe	Willowbrook		Constantia
Griffin	Bonheim		Shepstone
Clovelly	Tambankulu		Houwhoek
Bainsvlei	Mayo		Lamotte
Hutton	Swartland		Cartref
Shortlands	Valsrivier		Wasbank
	Vilafontes		Longlands
	Oakleaf		Westleigh
	Glenrosa		Dundee

After identifying the group to which a specific soil form belongs, the following guidelines are suggested to categorize South African soils as slightly weathered, highly weathered or calcareous.

Group 1: Soil forms in this group are divided into calcareous, eutrophic, mesotrophic or dystrophic soil series. For the purposes of P modelling, we propose that dystrophic soil series are regarded as 'highly weathered', meso- and eutrophic soil series as 'slightly weathered', and calcareous soil series as 'calcareous'.

Group 2: Soil forms in this group are divided into calcareous and non-calcareous soil series. We propose that non-calcareous soil series are regarded as 'slightly weathered' and calcareous soil series as 'calcareous'.

Group 3: Soil forms in this group are divided into acid, neutral or alkaline soil series. We propose that alkaline and neutral soil series are regarded as 'slightly weathered' and acid soil series as 'highly weathered'.

Group 4: Soil forms in this group are not divided into soil series that suit the above categorization procedure. We propose that these soil forms are therefore categorized according to mean annual precipitation, namely 500-750 mm being 'slightly weathered' and >750 mm being 'highly weathered'.

The nearest relevant modal profile to the area of interest should then be used to obtain clay content, 'P status' (IP), as well as pH, base saturation and $CaCO_3$ content of the soil. For the large catchment scale model, SWAT, the *Labile P* pool size is initialized at 25 mg kg^{-1} for the plough layer in cultivated land, and at 5 mg kg^{-1} for all other layers and uncultivated land (Cope et al., 1981; Neitsch et al., 2002). This is recommended for use when no other information is available.

3.6 GENERAL DISCUSSION

The use of the MP, BP2 and the IP tests to accurately estimate *Labile P* using the equations presented in this paper is based on the assumption that good correlation exists for the equations to convert one of the tests mentioned above to Bray 1 P for the soil being simulated. Unfortunately the range of properties for the soils used to obtain the original conversion equations was not reported. The suitability of the equations to estimate the PAI of South African soils requires further investigation. Improved understanding of P reactions in different soils, possibly including the role of various ions in P precipitation as insoluble phosphates (Johnston et al., 1991), is essential to improve our ability to model P solubility in soils. In weathered soils, Fe and Al oxides can reduce P solubility to extremely low levels, while in alkaline soils, especially calcareous ones, the precipitation of Ca and Mg as insoluble phosphates can also drastically reduce plant available P levels (Johnston et al., 1991). Johnston et al. (1991) noted that highly weathered Oxisols and Ultisols which have high Fe and Al contents generally have much higher P fixation capabilities than soils with crystalline mineralogy, and it is generally observed that P fixation is proportionally related to the clay content of soils. Highly weathered soils can often contain larger amounts of Fe and Al than slightly weathered soils. Certain models, including the model ANIMO

(Groenendijk and Kroes, 1999) utilize either Freundlich or Langmuir isotherms to determine P sorption. This approach is, however, often deemed too mechanistic, and inputs too difficult to obtain for inclusion in field to catchment scale models. Numerous studies have been done in South Africa on P sorption kinetics (Johnston et al., 1991; Henry and Smith, 2003; Henry and Smith, 2004). This work can potentially be adapted for local modelling purposes. Local research, similar to the work done by Jones et al. (1984) is ultimately required to develop P modelling algorithms more suited to South African soils.

The approach proposed in this paper to categorize South African soils as 'slightly weathered', 'highly weathered' or 'calcareous' at the catchment scale is open to further discussion and debate. While it is acknowledged that topsoil characteristics such as sum of bases, presence of $CaCO_3$ and acidity can easily be modified through fertilizer or lime applications to cultivated land, in South Africa only 10% of land is under cultivation. In most cases, modal profiles were in native land and soil characteristics would not have been expected to be modified by past agricultural practices. An uncertainty using this approach is whether small cultivated areas with high soil P in a catchment contribute comparable pollutant loads to larger areas with lower soil P. Therefore although by no means a faultless suggestion, it is meant to be a pragmatic approach considering the lack of detailed soil information at catchment scale, and the urgent need to estimate the impacts of land use and management strategies on eutrophication of inland waterways and impoundments.

3.7 CONCLUSIONS

Increased environmental and financial pressures associated with P require the careful management of this widely used agricultural nutrient. Modelling has a major role to play in improving our understanding of the various P processes and determining P management practices. P modelling still closely follows the approach developed over two decades ago by Jones et al. (1984) and Sharpley et al. (1984). It is crucial that these equations only be used to model soils with properties within the range of those used for the establishment of the original regression equations. The lack of detailed input information can often hamper P modelling at all scales. Several guidelines have been provided in this paper to simplify the application of these algorithms to South

African soils. These guidelines are aimed at reducing the effort required to obtain the inputs to model P in South African soils, and should be subjected to ongoing testing and refinement. A lack of suitable and complete P datasets makes validation exercises very difficult. The use of soil analyses to determine modelling inputs such as resin extractable P and sorption isotherms will theoretically give the best results for P modelling. Experienced pedologists and soil mineralogists should be consulted whenever possible for assistance in obtaining soil parameters. It is also hoped that an ability to compare different STPs, and to estimate plant available P and the PAI of soils will facilitate dialogue between modellers, government institutions, consultants and farmers on the P status and optimal management practices for various soils.

3.8 ACKNOWLEDGEMENTS

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CHAPTER 4

ASSESSMENT OF THE ABILITY OF SWB-SCI TO SIMULATE NITROGEN DYANAMICS IN AGRONOMIC CROPPING SYSTEMS

ABSTRACT

Enhanced understanding of nitrogen (N) dynamics in cropping systems through modelling can lead to more sustainable management strategies and reduce unwanted environmental impacts. N simulating capabilities have recently been included into SWB-Sci, mostly using well tested approaches from existing models. When required, certain modifications have also been made. The ability of SWB-Sci to mechanistically simulate N dynamics is tested in this paper using two historical datasets. The model was observed to adequately estimate total aboveground dry matter production, yield, soil water content as well as aboveground and grain N mass in wheat and maize. Soil inorganic N was less accurately simulated, and was often observed to be over-predicted. This is partly attributed to high spatial variability in soils, and data reliability should always be scrutinized during model testing exercises. In its current form, SWB-Sci can be used to investigate the impact of different irrigation and fertilization management practices on N dynamics and in fate of N pollution studies.

4.1 INTRODUCTION

Knowledge on the nitrogen (N) balance in cropping systems is essential in achieving high N fertilizer use efficiency and limiting the export of this nutrient to downstream water systems as a pollutant. Measurement of the various N gains and losses from a system can be highly challenging, even under well controlled experimental conditions. Mechanistic crop N models can be used to estimate these N additions/losses and this information can be used to inform better management practices. In intensive crop production, N fertilizer is, in many cases, applied in excess of crop requirements, often leading to N use efficiency in the region of 30 to 50%. In less-intensive systems, such as rainfed production, N is frequently under-applied, resulting in a ‘mining’ of soil N made available through the mineralization of organic matter (Annandale and Du Preez, 2005). Although the amount of N being applied in the form of fertilizer and the amount of N being removed by the crop is easily measurable, less is known about the quantities of N lost via mechanisms such as leaching, runoff, volatilization and denitrification. Accurate simulations of crop growth, water dynamics, N transformations and the movement of N in drainage and runoff water is required to fill these ‘information gaps’ and improve the understanding of N balances in cropping systems.

SWB-Sci is a daily time-step, mechanistic, generic crop model originally developed for irrigation scheduling (Annandale et al., 1999a) and now includes salt (Annandale et al., 1999b), carbon, nitrogen and phosphorus subroutines (see Chapter 2). Extensive crop parameterization work has been done locally for the model; and the crop, soil and water modules have been extensively tested for vegetable (Javonovic et al. 1999), cereal (Annandale et al., 2002) and pasture crops (Beletse, 2004). SWB-Sci has also been validated for maize N and P uptake and stress effects using field data from Kenya (see Chapter 5). The nutrient subroutines were adapted using algorithms primarily from the CropSyst (Stöckle et al., 2003), GLEAMS (Muller and Gregory, 2003), SWAT (Neitsch et al., 2002) and APSIM (Keating et al., 2003) models. A daily crop dry matter increment is firstly calculated as being either solar radiation or water supply limited, after which N deficiency effects on crop growth are accounted for. As CropSyst uses a different approach to estimate yield, several modifications were required to adapt the N uptake and stress effect algorithms for SWB-Sci. Briefly, in CropSyst, yield is calculated as a fraction of total dry matter production using a harvest index, and N stress effects on yield are only calculated at harvest. In SWB-Sci, after flowering has commenced, a daily harvestable dry matter increment is calculated. Crop N available for translocation to the grain, as well as a yield stress factor based on a supply:demand ratio, is therefore calculated daily in SWB-Sci until physiological maturity.

In this paper the N subroutines in SWB-Sci were further tested using two historical datasets. The first dataset was collected over two growth seasons in the Netherlands and was the subject of a workshop for which several N models were run against the data and a comparison made of these models (De Willigen, 1991). The second dataset was collected in the Free State province of South Africa. Both datasets are characterized by intensive soil water, crop biomass accumulation, aboveground and grain N mass, and soil mineral N measurements over the growth season. The objectives of this paper are therefore to asses the accuracy of SWB-Sci in simulating N dynamics in agronomic cropping systems.

4.2 MATERIALS AND METHODS

4.2.1 *Bouwing* field trial

4.2.1.1 Trial description

A field trial with *Triticum aestivum* (wheat cv. Arminda) was conducted for the 1982/83 and 1983/84 growing seasons at Bouwing near Wageningen in the Netherlands. Soil water content, crop growth, N uptake and inorganic soil N levels were monitored over the growing season. These measurements were only made for the wheat crop which was grown in rotation with potatoes on a naturally drained silty clay loam soil with organic matter ranging from 2.8 to 1.2%. For each season, N was applied at three different rates in three split applications (Table 4.1). Applications were made 116, 204 and 244 days after planting (DAP) in the 1982/83 season, and 113, 195 and 223 DAP in the 1983/84 season. All other nutrients were assumed to be non-limiting.

Table 4.1 N fertilizer application rates applied to the Bouwing trial for the 1982/83 and 1983/84 growing seasons

Treatment	1982/83*			1983/84†		
	N application (kg ha^{-1})					
N1	0	0	0	70	0	0
N2	0	60	0	70	60	40
N3	0	120	40	70	120	40

*Applied 116, 204 and 244 days after planting during the 1982/83 season
†Applied 113, 195 and 223 days after planting during the 1983/84 season

In the first growing season total inorganic N and volumetric water content (θ) was measured for the 0-30, 30-60 and 60-100 cm soil layers, while in the second growing season NO_3^-, NH_4^+ and θ were determined separately for the 0-20, 20-30, 30-40, 40-60, 60-80 and 80-100 cm layer depths. All experimental plots were naturally drained.

A more thorough description of the trial is given by Groot and Verbene (1991).

4.2.1.2 Model set-up

Crop and soil parameters were obtained from Groot and Verbene (1991) and through calibration using the highest N application treatment (N3) for the 1982/83 growth season. Initial soil N levels were estimated using the first measured values for the N1 treatment.

4.2.2 *Glen* field trial

4.2.2.1 Trial description

This trial was conducted near Glen, North-East of Bloemfontein, South Africa; where average rainfall for the area is 553 mm per annum, falling predominantly in the summer months, and average temperature is 16°C. The soil ranges from a sandy loam to a sandy clay loam and is well-drained. For the trial, *Zea mays* (maize cv. PNR473) was grown during the 1990/91 season. Routine soil water content monitoring was done at different depths using a neutron water meter. Soil samples from depths of 0-

20, 20-30, 30-60, 60-90, 90-120, 120-150 and 150-180 cm were taken and analyzed for NO_3^-, NH_4^+ and total N content. Readers are referred to Schmidt (1993) for a comprehensive description of the trial.

Before planting in December 1990, the soil was ploughed to a depth of 0.3 m. The trial consisted of three treatments receiving 0 (Treatment N1), 20 (Treatment N2) and 40 kg N ha^{-1} (Treatment N3) applied in the form of limestone ammonium nitrate in a single application at planting. In comparing the weather data for the growth season to long-term data (1921-1991), Schmidt (1993) observed that the season received more monthly rainfall and A-pan evaporation was lower than the long-term average.

4.2.2.2 Model set-up

Crop parameters for maize were obtained from the SWB-Sci database as well as through calibration using the N3 treatment. Although θ measurements were taken to a depth of 2.7 m, soil sample for N analysis were only taken to a depth of 1.8 m. For this reason comparisons between measured and simulated values are only made to a depth of 1.8 m.

4.2.3 Testing model performance

Model performance was judged using the square of the correlation coefficient (r^2), the mean absolute error (MAE), and the index of agreement (D) proposed by Wilmot (1982) (De Jager, 1994). Statistical criteria for an accurate simulation are r^2 and D values above 0.80, and MAE below 20%. The aim of comparing measured and simulated values statistically when testing a model is to objectively determine what proportion of treatment error, excluding experimental error, is accounted for by the model (Yang et al., 2000). Total aboveground dry matter (TDM), yield, aboveground and grain N mass, soil mineral N and soil water content were the variables used to assess model performance. Soil mineral N levels were not subjected to statistical validation, however, but goodness-of-fit was judged visually. Simulation of total soil N was not tested due to extremely high in-field spatial variability.

4.3 RESULTS

4.3.1 *Bouwing* field trial

4.3.1.1 Total aboveground dry matter and yield

1982/83 season

Total aboveground dry matter (TDM) and yield were well simulated for the 1982/83 growth season. For the N1 treatment, both TDM and yield were slightly under-estimated. For treatments N2 and N3 there was good agreement between measured and simulated values (Figure 4.1). Measured values for TDM and yield were very similar for treatments N2 and N3, with final TDM and yield being even greater for the N2 treatment. Despite this, all three simulations met the set statistical criteria (Table 4.2).

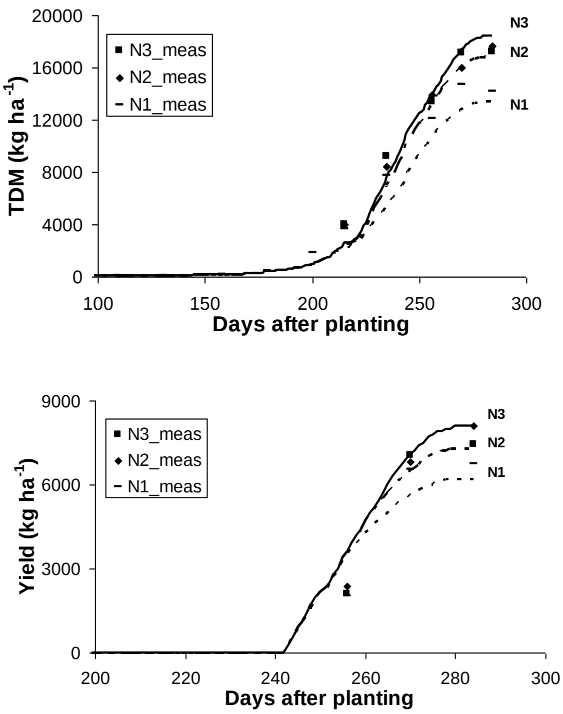

Figure 4.1 Total aboveground dry matter (TDM) and wheat grain yield for treatments N1, N2 and N3 for the 1983/83 growth season

Table 4.2 Statistical evaluation of measured and simulated values for total aboveground dry matter (TDM) and yield during the 1982/83 season

Treatment	TDM			Yield		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.99	0.99	16	0.97	0.97	19
N2	1.00	0.99	8	1.00	0.99	13
N3	0.99	0.99	8	0.99	0.99	13

1983/84 season

For the second growth season, TDM and yield were less accurately simulated than for the previous season by the model (Figure 4.2). TDM was still well simulated for treatments N2 and N3, however (Table 4.3). For all three treatments, TDM at the beginning of the growth season and final yield were under-estimated and this may have been due to the onset of germination and flowering occurring sooner in the field than simulated by the model. Simulated yields for treatments N2 and N3 were almost identical and are superimposed on the graph.

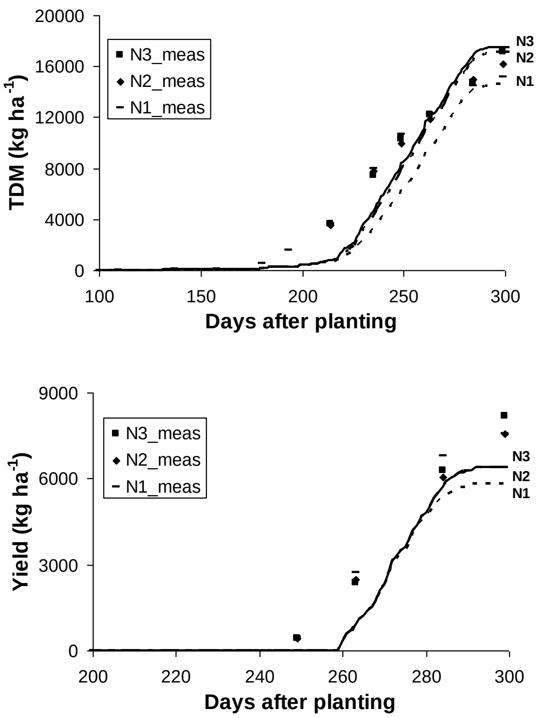

Figure 4.2 Total aboveground dry matter (TDM) and yield for treatments N1, N2 and N3 for the 1983/84 growth season

Table 4.3 Statistical evaluation of measured and simulated values for total aboveground dry matter (TDM) and yield during the 1983/84 season

Treatment	TDM			Yield		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.92	0.96	26	0.98	0.96	42
N2	0.98	0.96	17	0.97	0.98	28
N3	0.98	0.96	16	0.97	0.97	33

4.3.1.2 Profile water content and deep drainage

The model was able to predict profile soil water content adequately for both growth seasons (Table 4.4). Treatment N1 was the least accurately simulated over both growth seasons. While no water stress was predicted for the 1982/83 growth season, water stress was simulated for the final two weeks of the 1983/84 growth season. Drainage did not differ greatly between treatments and 100 mm and 142 mm of drainage was simulated for the 1982/83 and 1983/84 growth seasons, respectively.

Table 4.4 Statistical evaluation of measured and simulated values for profile water content during the 1982/83 and 1983/84 seasons

Treatment	1982/83			1983/84		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.87	0.84	13	0.77	0.71	15
N2	1.00	0.97	7	0.94	0.67	10
N3	0.87	0.89	10	0.92	0.68	10

4.3.1.3 Crop N uptake

1982/83 season

Despite MAE values being above 20% for all treatments except aboveground N mass for treatment N3, aboveground N and grain N mass were still generally well simulated for the three treatments (Table 4.5). Final aboveground N mass was under-estimated for all treatments, and grain N mass was under-estimated for treatments N2 and N3.

Table 4.5 Statistical evaluation of measured and simulated values for top N mass and grain N during the 1982/83 season

Treatment	Aboveground N mass			Grain N		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.89	0.95	26	0.96	0.92	34
N2	0.91	0.79	22	0.99	0.96	22
N3	0.79	0.85	19	0.94	0.95	28

The model was clearly able to reflect differences in N uptake between the different N application rate treatments (Figure 4.3). Grain N mass was over-predicted by the model for the first measurement taken 256 days after planting, but simulated values and measured values taken 284 days after planting were in closer agreement. This may indicate that the model simulates too much N translocation shortly after flowering has taken place.

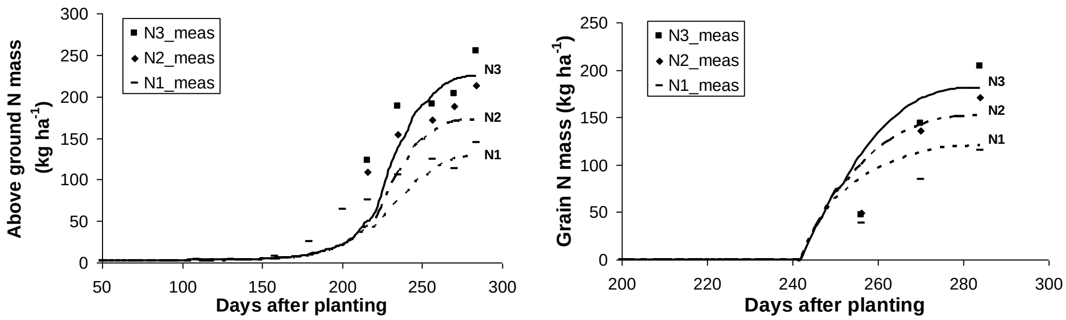

Figure 4.3 Aboveground N mass (left) and grain N mass (right) for the 1982/83 growth season

1983/84 season

Once again, despite all statistical criteria not always being met, aboveground N and grain N mass were relatively well predicted by the model (Table 4.6). For treatment N2 a slight decrease in aboveground N mass was observed between 235 and 264 days after planting, and for treatment N3 a slight decrease in aboveground N mass was observed between 235 and 249 days after planting, and only a slight increase was observed between 263 and 284 days after planting (Figure 4.4). This would have contributed to r^2 values below 0.80 for these two treatments, as the current N model cannot simulate a drop in crop N during this active growth period.

Table 4.6 Statistical evaluation of measured and simulated values for aboveground N and grain N during the 1983/84 season

Treatment	Aboveground N mass			Grain N mass		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.89	0.91	35	0.95	0.98	20
N2	0.70	0.81	25	0.88	0.98	27
N3	0.71	0.83	24	0.80	0.96	34

Aboveground N mass was consistently under-estimated for the N1 treatment. In contrast to the 1982/83 season, grain N was over-estimated by the model for the first measurement taken 249 days after planting, but similar to the previous season, and final grain N mass was again under-estimated for all treatments. This under-estimation of grain N mass is attributed to an under-estimation of yield for the season.

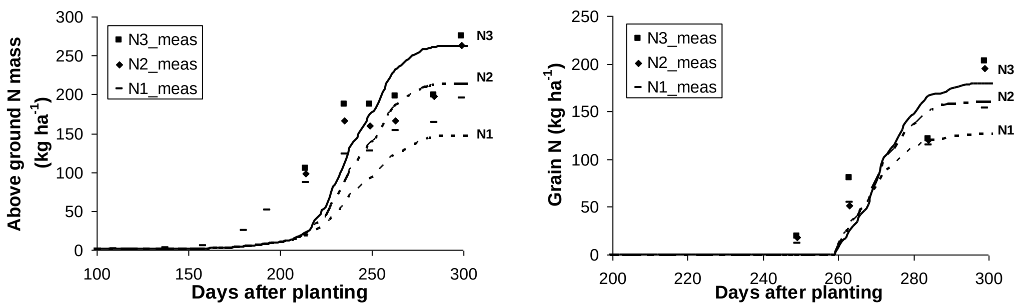

Figure 4.4 Aboveground N mass (left) and grain N mass (right) for the 1983/84 growth season

4.3.1.4 Soil inorganic N

1982/83 season

Soil inorganic N (NO_3^- + NH_4^+) was moderately well simulated for the 1982/83 growth season (Figure 4.5). Inorganic N appeared to be best simulated for the N1 treatment to which no N fertilizer was applied. For all treatments, there was a tendency to over-estimate soil mineral N. Similar trends between measured and simulated values could be observed, however.

The bottom layer (60-100 cm) of the N1 treatment showed a sharp decline in soil mineral N from 73 kg N at 179 days after planting to 5.6 kg N at 235 days after planting. Over the same period, 69 kg N was taken up by the crop from the entire profile and 3.5 kg N was simulated to have leached. This decline in soil mineral N is therefore largely attributed to crop uptake. As more early-season measurements were taken for the N1 treatment, such a decline in soil mineral N would also be expected for treatments N2 and N3.

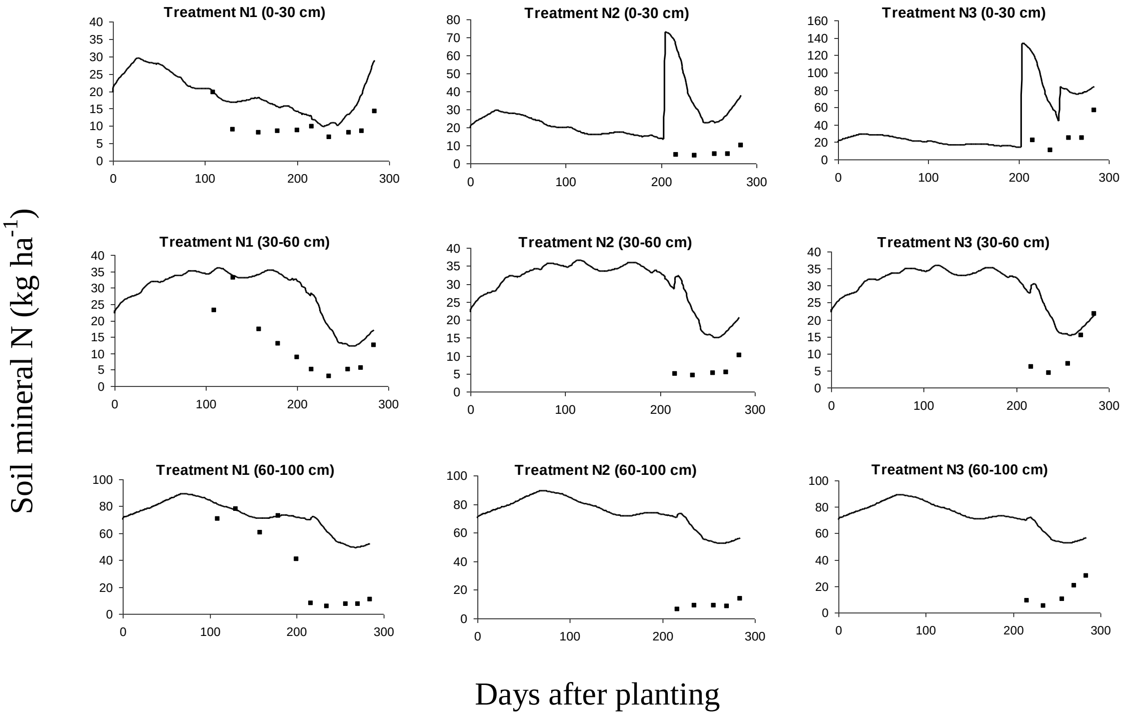

Figure 4.5 Soil mineral N content for the 1982/1983 growth season for treatments N1, N2 and N3 at depths of 0-30, 60-30 and 60-100cm

For treatments N2 and N3, addition of 60 and 120 kg N ha^{-1}, respectively, 204 days after planting was not reflected in the measured data. Thereafter slight increases in soil mineral N were observed, but mineralization likely contributed to this as the same increase was observed for the N1 treatment to which no fertilizer was added.

1983/84 season

Following fertilization 113 days after planting, measured NO_3^- values in the top 0-30 cm layer declined at a faster rate than simulated by the model for the N1 treatment. For treatments N2 and N3, the application of N fertilizer was again not reflected in the measured soil mineral N values (Figures 4.6 and 4.7). For treatment N1, possible movement of NO_3^- down the profile can be observed by an increase in NO_3^- measured data in the 30-60 and 60-100 cm layers. This increase in NO_3^- for the 30-60 cm and 60-100 cm layers was not simulated by the model. As for the 0-30 cm layer, no increase in NO_3^- mass is observable for treatments N2 and N3 in the 30-60 and 60-100 cm layers after the first fertilizer N application.

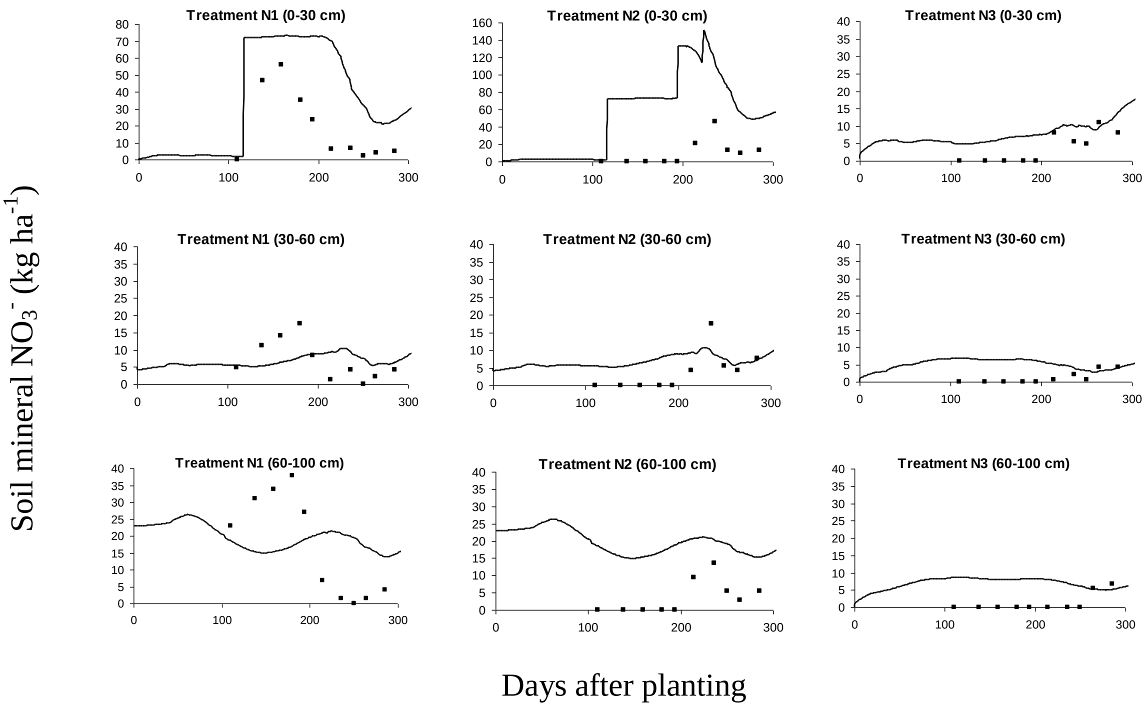

Figure 4.6 Soil NO_3^- content for the 1983/84 growth season for treatments N1, N2 and N3 at depths of 0-30 cm, 60-30 cm and 60-100cm

For the second fertilizer application 195 days after planting of 60 and 120 kg N ha^{-1} for treatments N2 and N3, respectively, and for the third fertilizer application of 40 kg N ha^{-1} for these treatments 223 days after planting, only a slight increase in soil mineral N was observed in the measured data. For treatment N1 following the first fertilization event, and for treatments N2 and N3 following the second fertilization event, an increase in NO_3^- can be observed in the two lower soil layers (30-60, 60-100 cm). A similar increase is not estimated and may be due to a leaching mechanism not simulated by the model. This unaccountable loss of fertilizer was also observed in other similar trials (De Willigen, 1991).

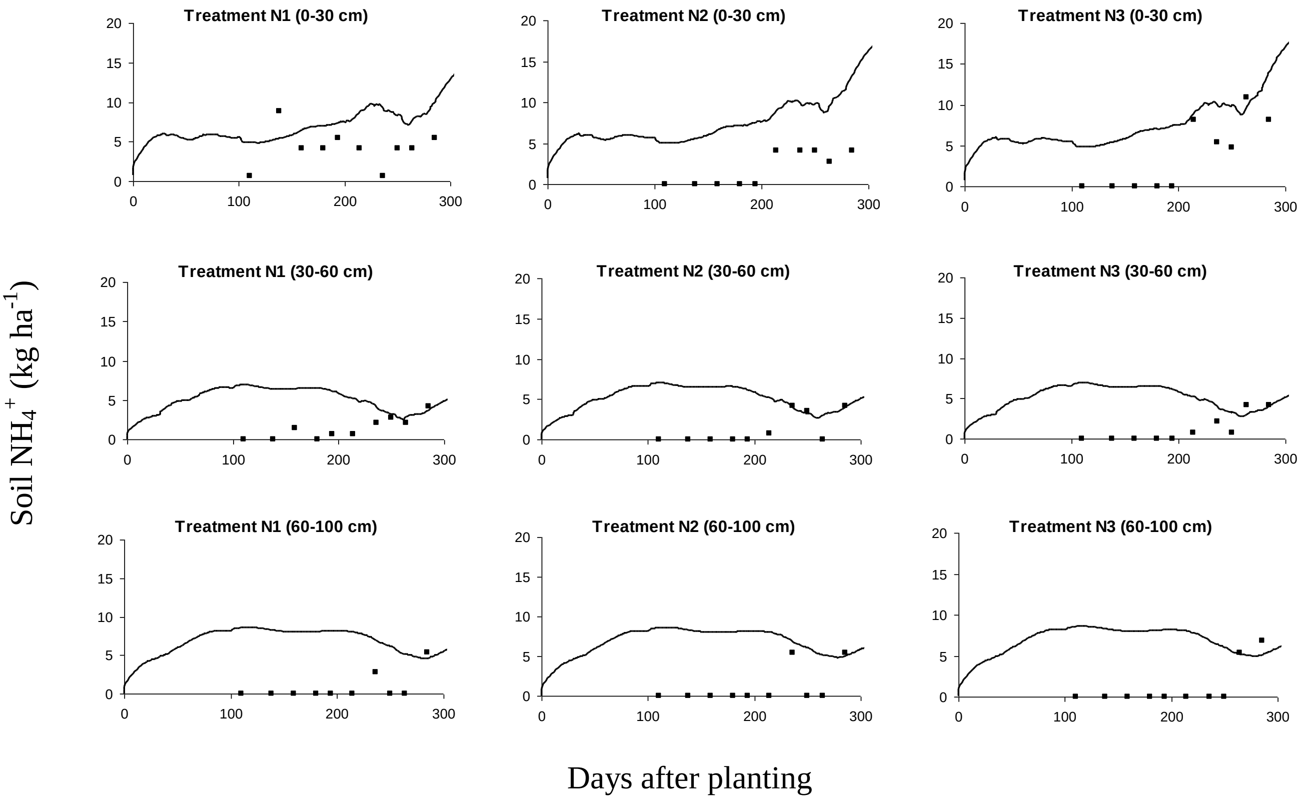

Figure 4.7 Soil NH_4^+ levels for the 1983/1984 growth season for treatments N1, N2 and N3 at depths of 0-30, 60-30 and 60-100 cm

Soil NH_4^+ levels were generally over-estimated but were in better agreement with the measured data towards the end of the growth season (Figure 4.7). This may have been due to an over-estimation of mineralization from soil organic matter in the lower soil layers.

4.3.2 *Glen* field trial

4.3.2.1 Total aboveground dry matter and yield

Despite different N fertilizer application rates of 0, 20 and 40 kg N ha^{-1} for treatments N1, N2 and N3, respectively, all three treatments achieved very similar dry matter production and yield (Figure 4.8).

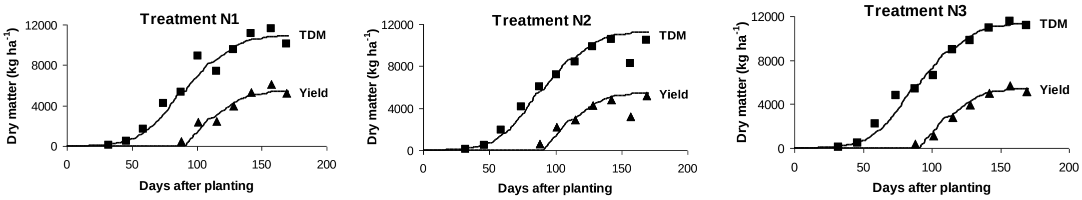

Figure 4.8 Total aboveground dry matter (TDM) and yield for treatments N1, N2 and N3

The model also predicted very similar TDM and yield values for the three treatments, and was able to simulate TDM and yield well (Table 4.7). A slightly higher MAE of 18% for treatment N2 was likely caused by a significant drop in TDM (and HDM) for the second last measurement (Figure 4.8) which is attributed to sampling error or in-field variability.

Table 4.7 Statistical evaluation of measured and simulated values for total aboveground dry matter (TDM) and yield during the 1982/83 season

Treatment	TDM			Yield		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.96	0.99	10	0.93	0.98	14
N2	0.96	0.99	8	0.82	0.93	18
N3	0.98	0.99	6	0.98	0.99	7

4.3.2.2 Profile water content and deep drainage

SWB-Sci adequately simulated soil water content for the layers 0-60 and 60-180 cm (Table 4.8). Drainage of 39 mm was simulated for all three treatments and water stress was predicted to occur on 50 days for treatment N1 and on 51 days for treatments N2 and N3.

Table 4.8 Statistical evaluation of measured and simulated values for profile water content for soil layers 0-60 and 60-180 cm

Treatment	0-60 cm			60-180 cm		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.80	0.87	11	0.93	0.85	8
N2	0.78	0.87	11	0.92	0.84	9
N3	0.87	0.90	13	0.83	0.78	11

4.3.2.3 Nitrogen uptake

Aboveground N mass and grain N mass was also very similar for all three treatments (Figure 4.9). The model estimated similar aboveground N masses of 130, 139 and 150, and grain N masses of 87, 91 and 96 kg N ha^{-1} for treatments N1, N2 and N3, respectively. For all treatments, more N was taken up in the harvestable parts of the crop than applied as fertilizer, indicating an overall 'mining' of soil N.

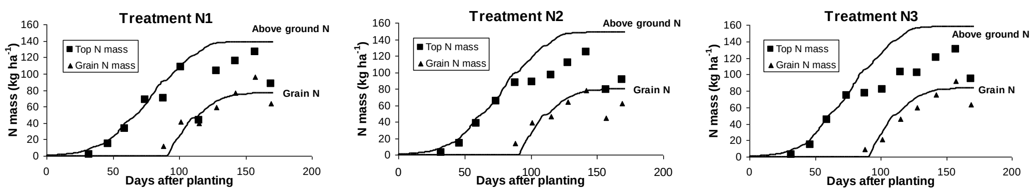

Figure 4.9 Aboveground and grain N mass for treatments N1, N2 and N3

Aboveground N mass was more accurately simulated than grain N mass for all the treatments (Table 4.9). Overall decreases in both aboveground N mass and grain N mass for the final measurement (Figure 4.9) should theoretically not be possible and contributed to the poor statistical values achieved for the simulations.

Table 4.9 Statistical evaluation of measured and simulated values for aboveground N mass and grain N

Treatment	Aboveground N mass			Grain N		
	r^2	D	MAE (%)	r^2	D	MAE (%)
N1	0.87	0.92	26	0.80	0.94	21
N2	0.88	0.88	35	0.73	0.88	26
N3	0.92	0.92	37	0.89	0.96	20

4.3.2.4 Soil inorganic N

Soil NO_3^- levels were well simulated for the 0-60 cm layer of all treatments, but over-estimated for the 60-180 cm layer for all treatments (Figure 4.10). Possible reasons for this over-prediction of NO_3^- in the lower soil layers could be an over-estimation of mineralization, or an under-estimation of crop N uptake and/or N leaching.

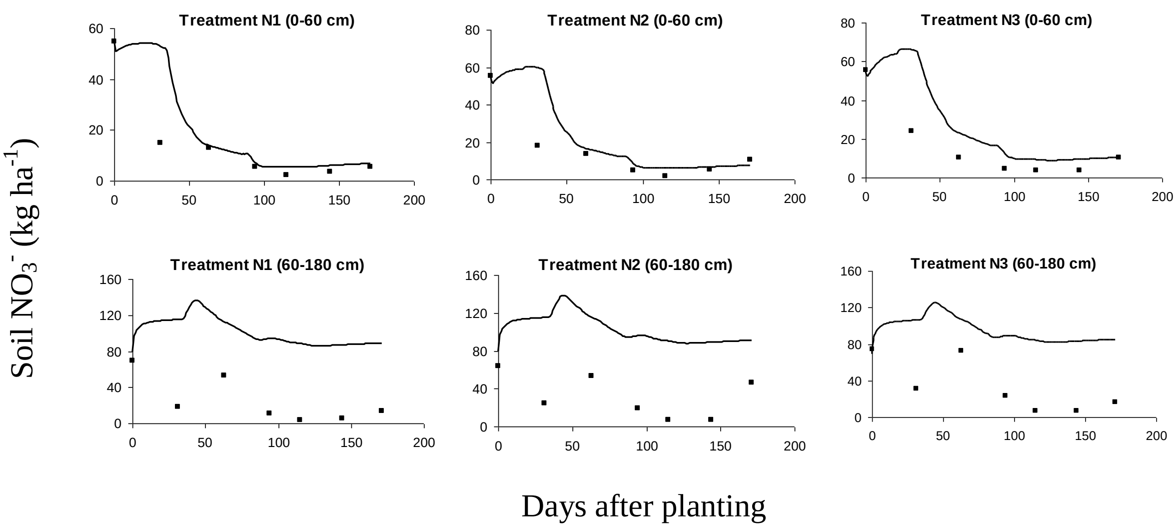

Figure 4.10 Soil NO_3^- content for treatments N1, N2 and N3 at depths of 0-60 and 60-180 cm

NH_4^+ was also generally well simulated except at the end of the season when a large NH_4^+ spike was observed in both layers (0-60, 60-180 cm) and for all three treatments (Figure 4.11). A similar phenomenon was observed for the previous season.

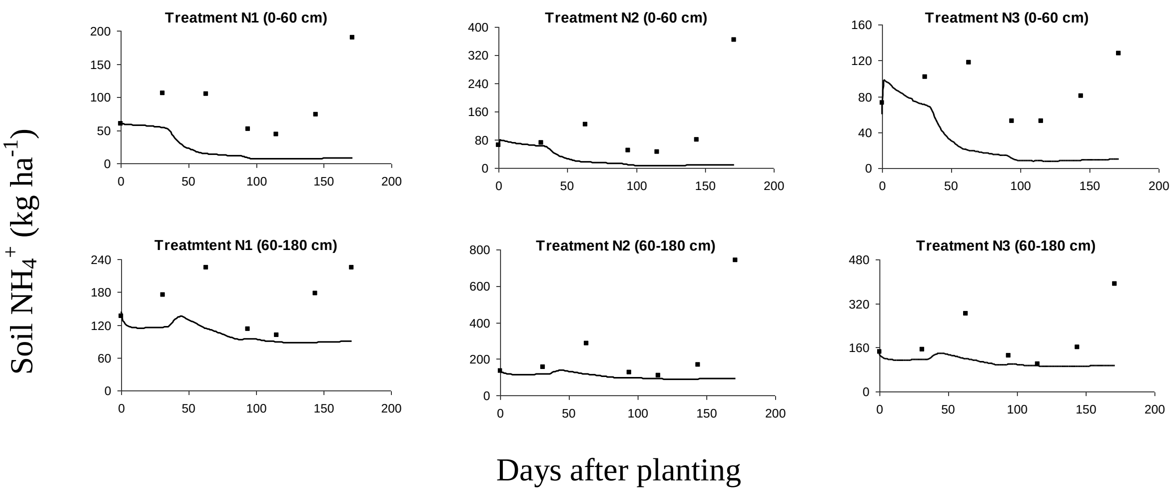

Figure 4.11 Soil NH_4^+ content for treatments N1, N2 and N3 at depths of 0-60 and 60-180 cm

The over-estimation of NO_3^- and under-estimation of NH_4^+ may also be an indication that the model is over-estimating the rate of nitrification.

4.4 GENERAL DISCUSSION

TDM was generally well simulated for the *Bouwing* trial, and complied with statistical criteria in almost all cases. The model was therefore able to model the relative effect of different N application rates on TDM well between treatments. Yield was also accurately simulated for the 1982/83 season but less accurately for the 1983/84 season. Addiscott et al. (1991) suggested that a possible reason for a better simulation of the first season as opposed to the second may be due to inappropriate assumptions of the potato crop grown in between. Although measured maize TDM and yield was similar for the three treatments in the *Glen* trial despite different rates of N application, the model was again judged to simulate these two variables well. Such similar dry matter production across treatments indicates that residual soil inorganic N or newly mineralized N was important and was also well accounted for in the model. Although the season was observed to be wetter than the long-term average, further rainfall may have caused significant differences between the treatments. Alternatively, another nutrient such as phosphorus or potassium may have been the limiting factor causing little difference between the three treatments.

Total aboveground and grain N mass was generally well simulated by the model when TDM and yield were also well simulated. Poor statistical results can be a result of inconsistencies in the measured data rather than poor model simulations in some cases (see Chapter 5). For example, in the *Glen* trial, a decline in yield (and the related grain N mass) relative to the previous measurement was observed at some stage for all three treatments, most noticeably for the N2 treatment. Reductions in total aboveground N mass were also observed for all three treatments. Although aboveground N losses from a crop are possible through physical means such as the loss of leaf matter from the crop, or chemical means associated with respiration, such losses are not expected for grain N. Whether the decline in aboveground N mass and the unexplained increase in soil inorganic N are related is speculative. That such increases were observed in the 60-180 cm soil layer makes this unlikely.

N stress was estimated by the model for all three treatments in both trials at some stage during the growth season. From this testing exercise it is apparent that the modified approach in SWB-Sci for simulating N available for translocation to the grain on a daily basis as opposed to using an end of season harvest index approach such as that used in CropSyst was adequate to predict grain N over the season.

In reviewing 14 N models that were run against the *Bouwing* data or similar datasets, De Willigen (1991) concluded that the main difficulties were in modelling soil processes (as opposed to crop growth and N uptake), especially soil biological processes. Soil inorganic levels were not subjected to statistical evaluation and in most cases would not have met the statistical criteria set out in this paper. The statistical criteria proposed by De Jager (1994) therefore do not seem appropriate to compare measured and simulated values of soil inorganic N when there is such high variability in the measured data. The 'disappearance' of N fertilizer or inability to detect increases in soil N following N fertilizer applications was observed in both trials. N immobilization can occur almost instantaneously after fertilizer application, and could therefore account for at least part of this 'disappearance' (Groot and De Willigen, 1991). This may also be due to spatial soil sampling that does not detect the effect of the added N on soil N levels. Finally it should be remembered that the simulation of inorganic N in soil represents only a small fraction, with 95-99% of N being in organic form (Brady and Weil, 1999). While total N was not measured for the *Bouwing* trial, total N was observed to fluctuate widely due to high spatial variability. This could be expected to contribute greatly to differences between measured and simulated results. Although error bars could have been included into the soil inorganic N graphs to represent this high spatial variability, it was decided not to include error bars due to a resultant reduction of clarity in the graphs.

During both seasons for the *Bouwing* and *Glen* trials the model did well in simulating profile water content. The assumption therefore is that soil available water for crop growth was also correctly simulated by the model. Because drainage and leached N was not measured the ability of the model to estimate these variables could not be tested. As these two measurements are very difficult to make, it is envisaged that a model such as SWB-Sci can play an important role in predicting N leaching losses from these types of cropping systems.

4.5 CONCLUSIONS

Mechanistic crop models such as SWB-Sci can be useful tools to investigate the interactions of water and N, crop growth responses to fertilizer applications and the risks of N leaching. Model testing and validation exercises are essential in providing confidence in a model's ability to adequately simulate in-field processes, and based on the results of this study SWB-Sci was judged to adequately simulate TDM, yield, aboveground N mass, grain N mass, soil water content, and to a lesser extent soil mineral N levels when compared to measured values. Due to high spatial variability, it is not always suitable to apply statistical analysis to measured and simulated values of soil mineral N levels. When spatial variability is clearly high for a given dataset, modelling may provide more useful insights and a more representative and consistent estimate of typical changes in soil N levels. Simple water and N balances for specific cropping systems can be useful to determine the fate of added fertilizer and to drive management decisions. Mechanistic models also allow for the careful study of N availability to the crop over the growth season and critical periods of runoff and leaching losses from the system. Freshly mineralized N is an important source of N to the crop, but management practices should aim to maintain adequate levels of soil organic matter levels rather than letting them decrease with time.

4.6 ACKNOWLEDGEMENTS

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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:

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

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.

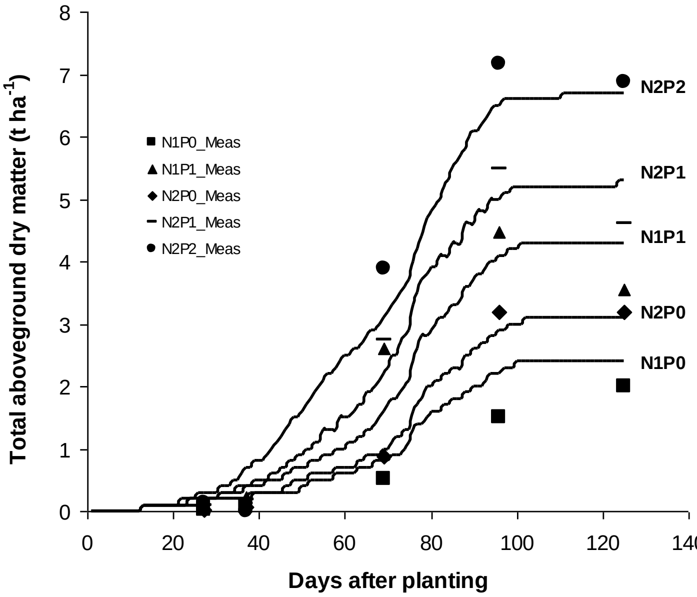

Figure 5.1 Measured and simulated values for total aboveground dry matter (TDM) production for the five treatments for the SR89 growth season

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.

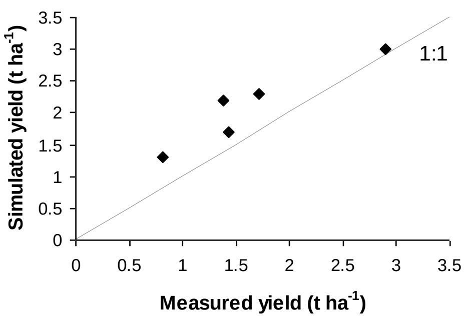

Figure 5.2 Measured versus simulated values for yield for the five treatments for the SR89 growth season

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.

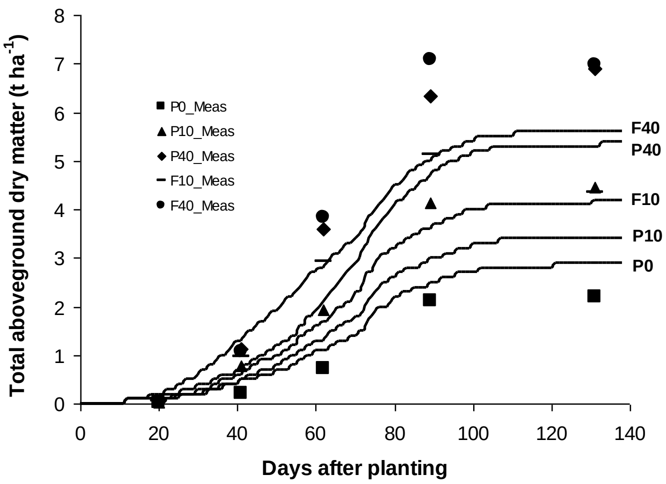

Figure 5.3 Measured and simulated values for total dry matter production for the five treatments for the LR90 growth season

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).

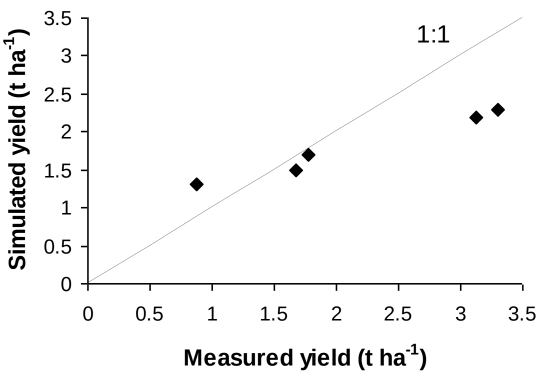

Figure 5.4 Simulated versus measured values for yield for the five treatments for the LR90 growth season

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.

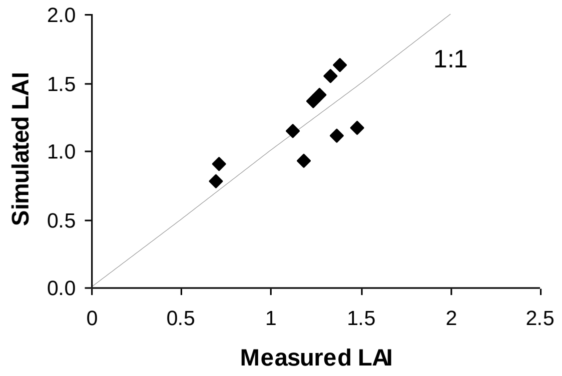

Figure 5.5 Simulated versus measured values for leaf area index (LAI) for the LR 90 growth season

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).

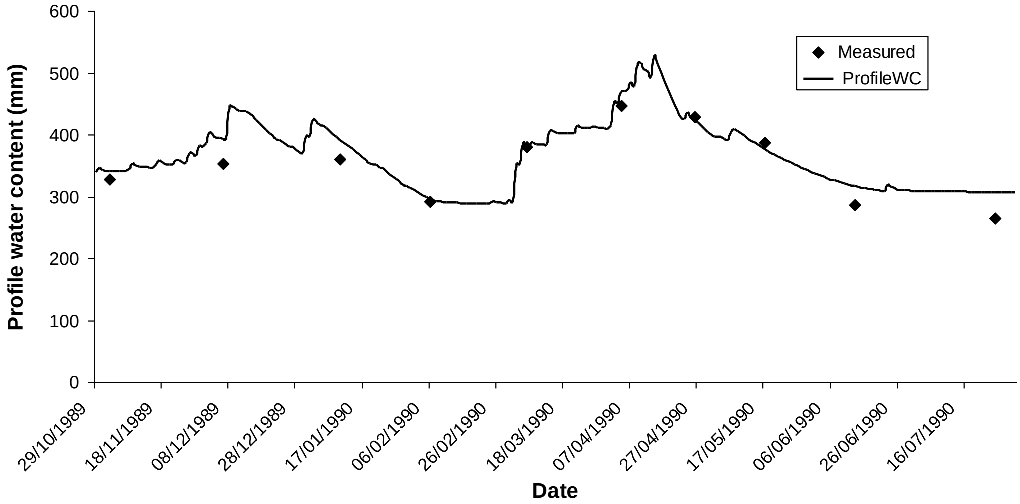

Figure 5.6 Profile water content (PWC) for the SR89 N2P1 treatment and the LR90 F40 treatment

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.

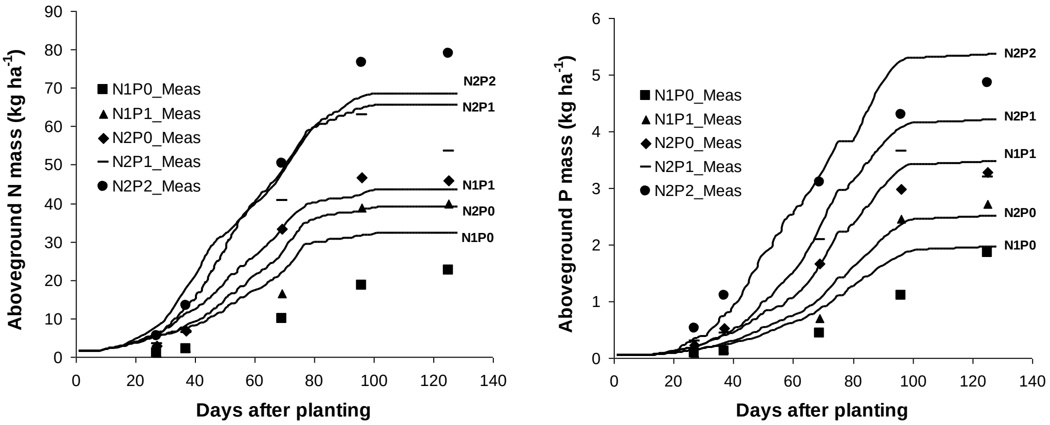

Figure 5.7 Measured and simulated values for aboveground N mass (left) and aboveground P mass (right) for the SR89 growth season

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.

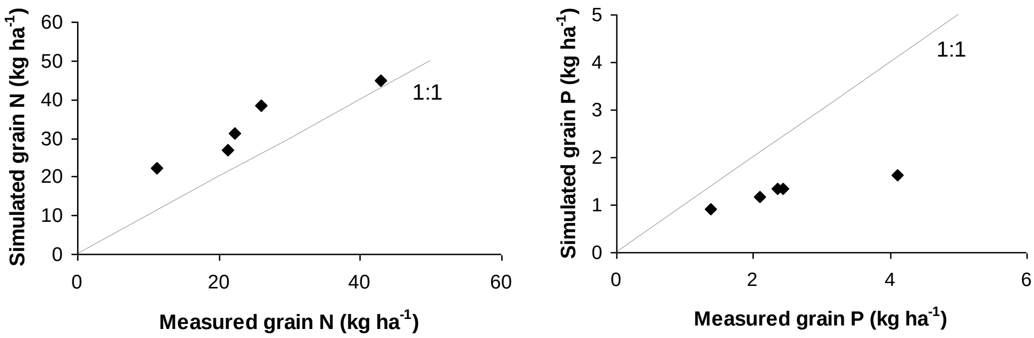

Figure 5.8 Simulated versus measured values for grain N mass (left) and grain P mass (right) for the SR 89 growth season

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.

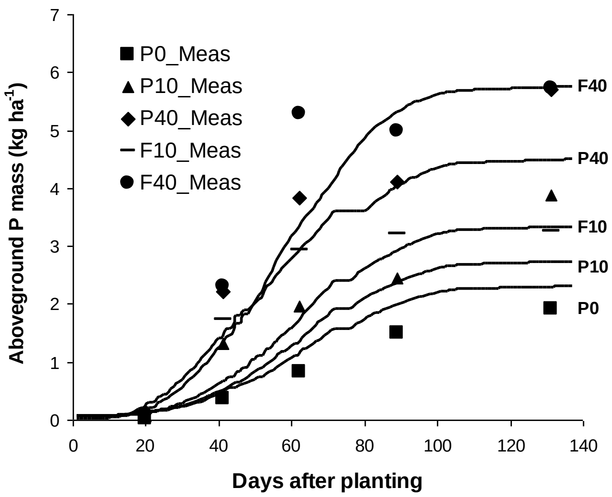

Figure 5.9 Measured and simulated values for aboveground P mass for the LR90 growth season

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.

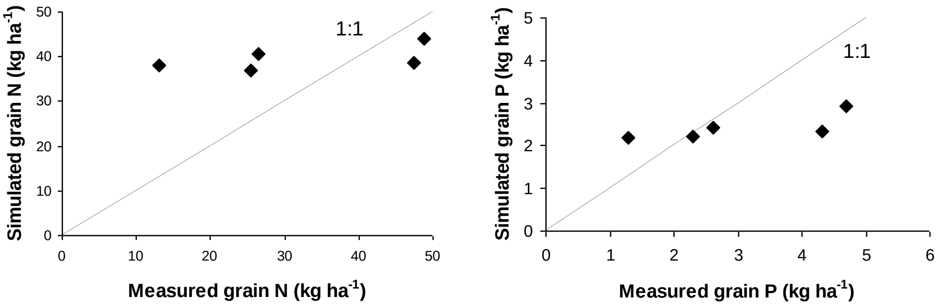

Figure 5.10 Simulated versus measured values for grain N (left) and grain P (right) for the LR90 growth season

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.

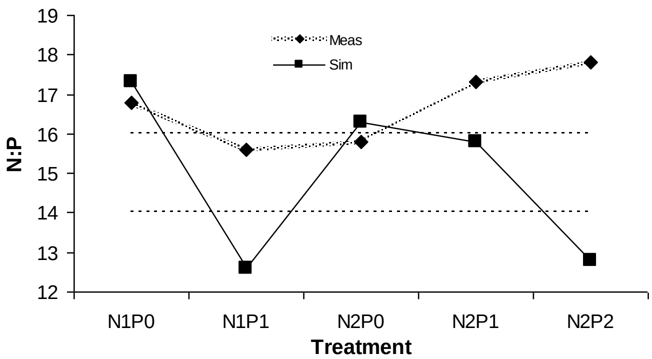

Figure 5.11 Measured and simulated shoot nitrogen:phosphorus ratios for the five treatments in the SR89 growth season. Measured data are based on analyses carried out on 5 February 1990 (before grain filling)

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.

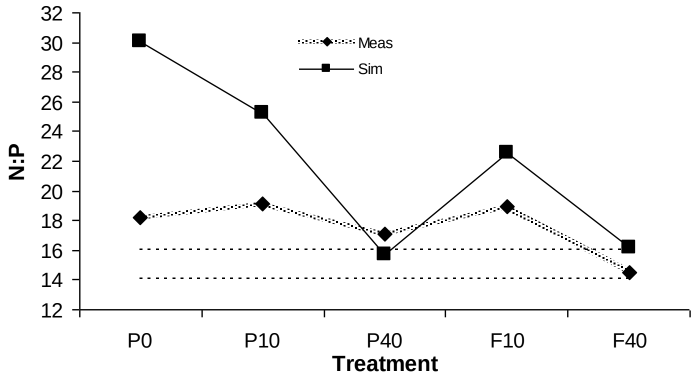

Figure 5.12 Measured and simulated shoot nitrogen:phosphorus ratios for the five treatments in the LR90 growth season for the analyses done on 12 June 1990 (before grain filling)

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$_2$O-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

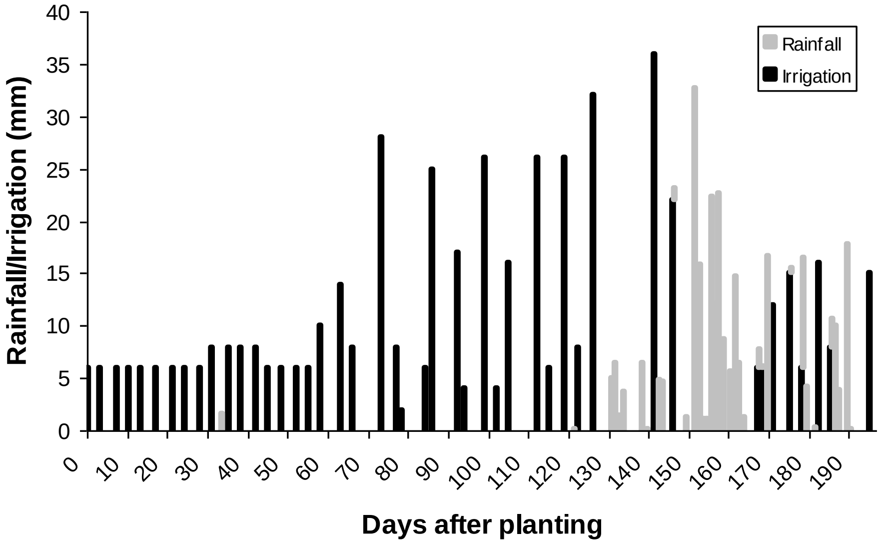

Figure 6.1 Rainfall and irrigation for the growth season

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.

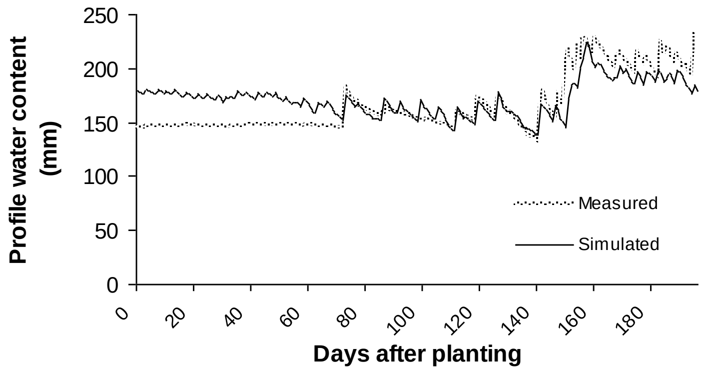

Figure 6.2 Measured and simulated profile water content over the growing season to a depth of 90 cm (measurements are based on data from the capacitance sensors)

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.

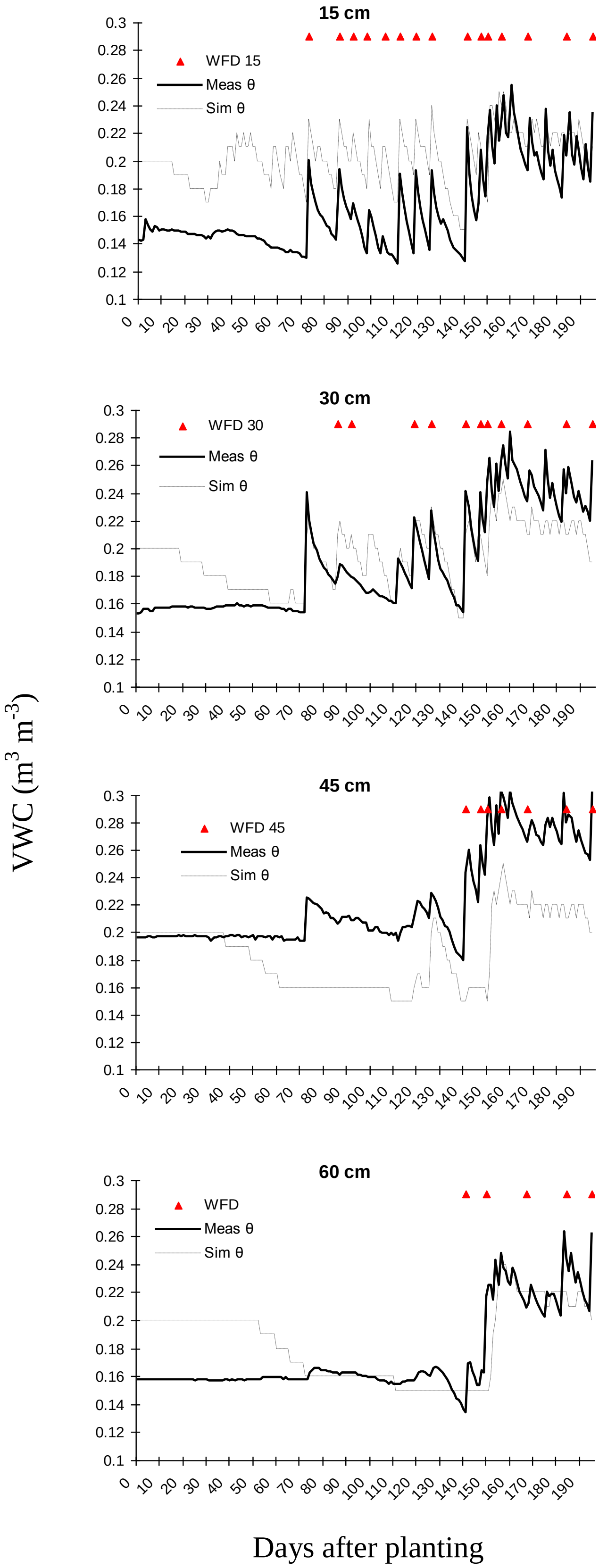

Figure 6.3 Measured and simulated volumetric water content (VWC), and WFD response at depths of 15, 30, 45 and 60 cm

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.

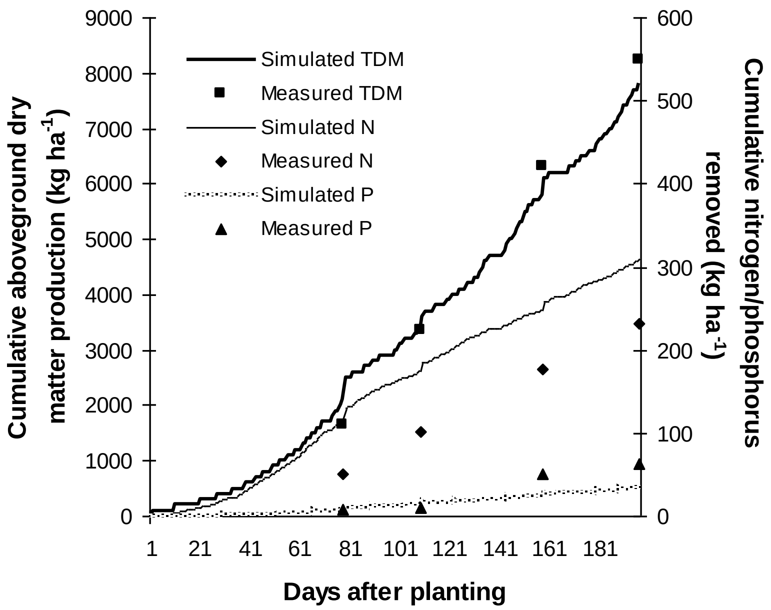

Figure 6.4 Cumulative aboveground dry matter (TDM) production (primary y-axis), and N and P removal (secondary y-axis) over the growth season

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.

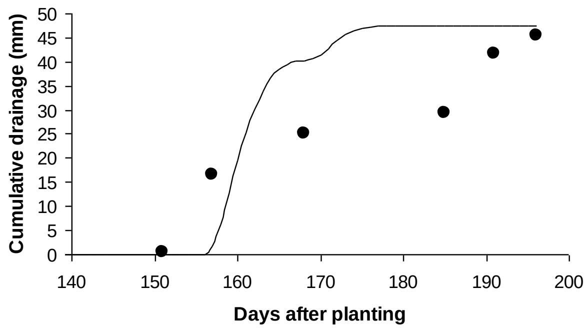

Figure 6.5 Measured and simulated cumulative drainage (mm) over the growth season

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.

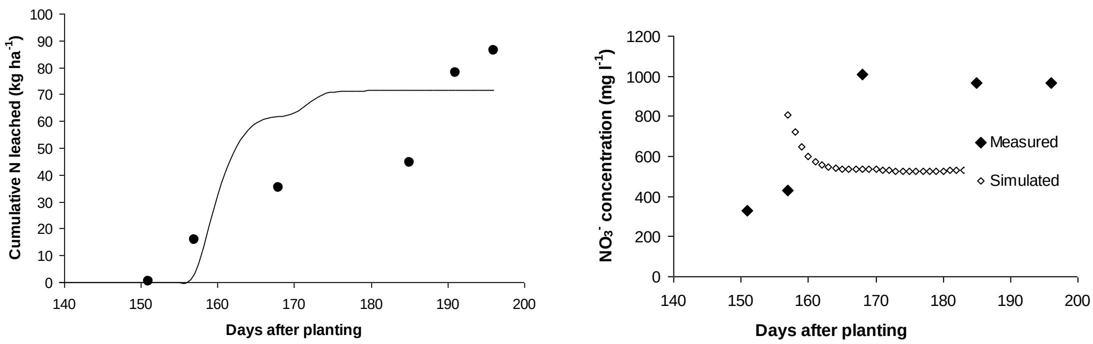

Figure 6.6 Measured and simulated cumulative N leached (left) and drainage water NO_3^- concentrations (right)

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.

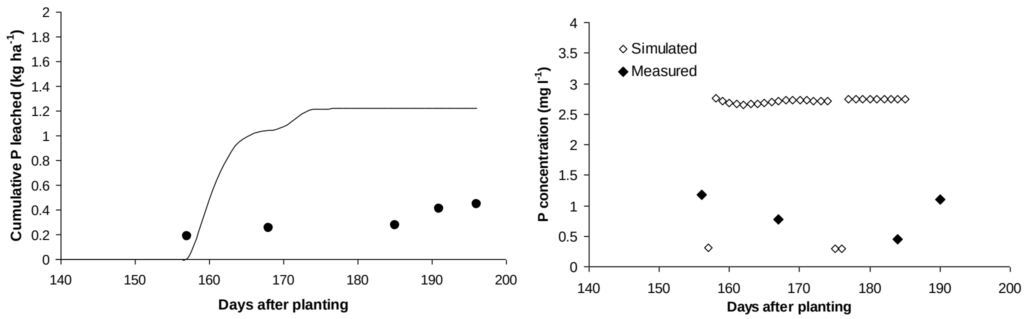

Figure 6.7 Measured and simulated cumulative P leached (left) and drainage water P concentrations (right)

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.

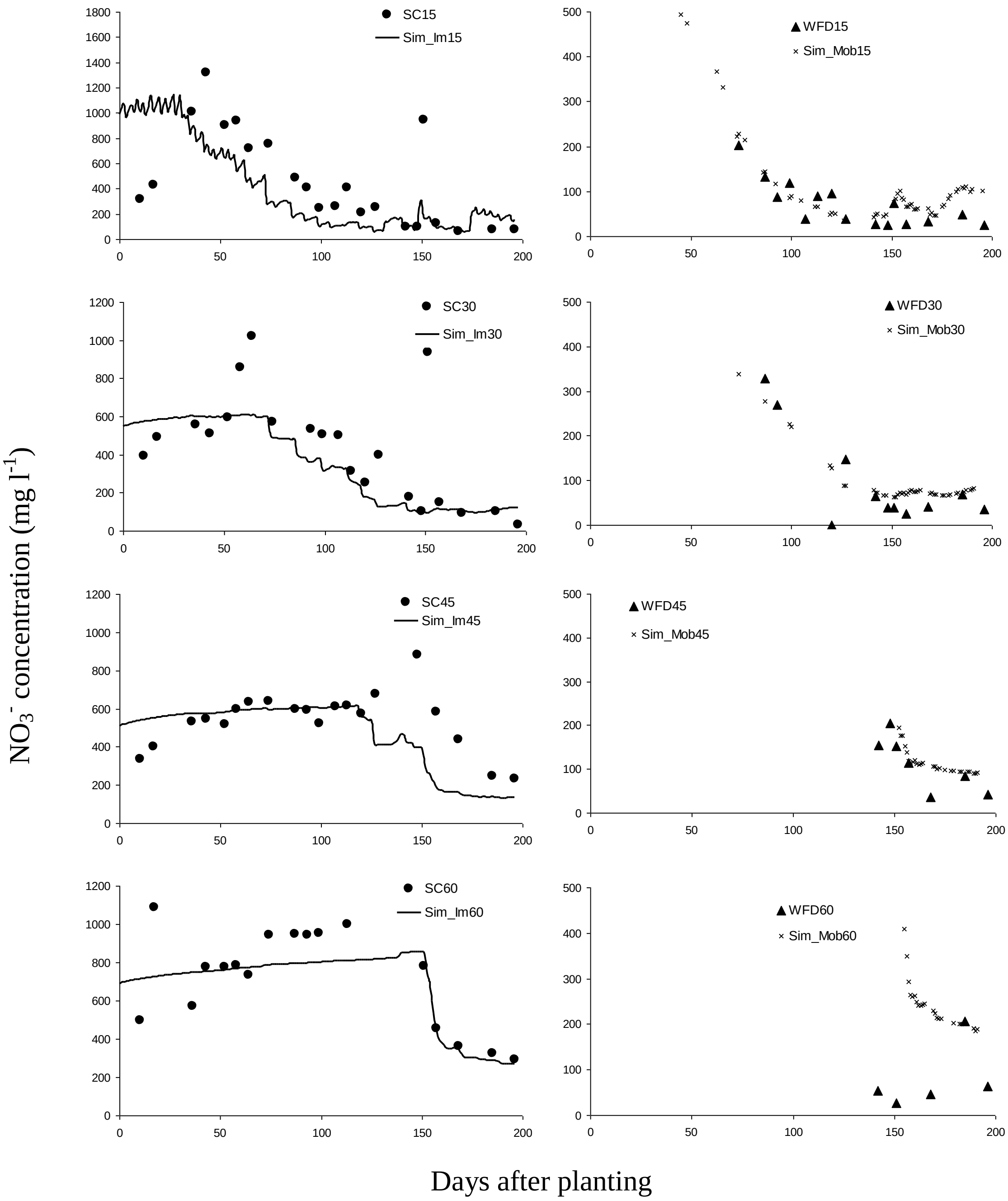

Figure 6.8 Measured NO_3^- concentrations from suction cups compared to simulated immobile soil water phase concentrations (Sim_Im; left) and measured NO_3^- concentrations from wetting front detectors compared to simulated mobile soil water phase concentrations (Sim_Mob; right) at depths of 15, 30,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

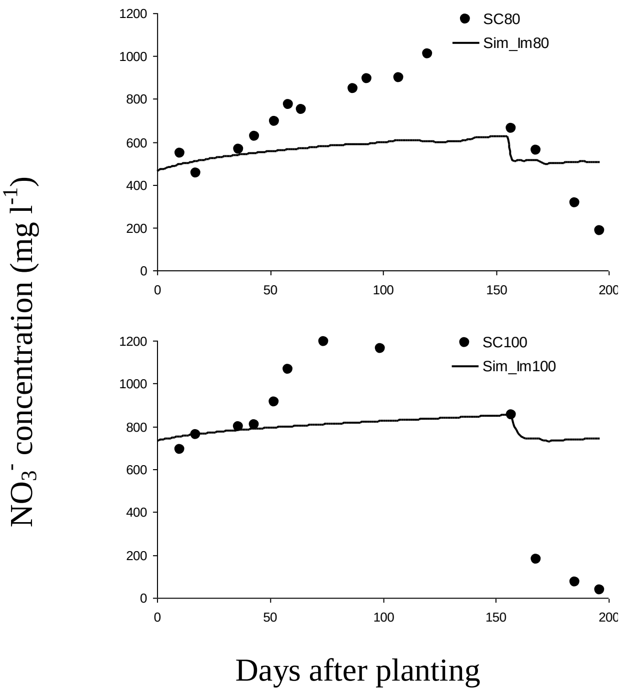

Figure 6.9 Measured NO_3^- concentrations from suction cups compared to simulated immobile soil water phase concentrations at depths of 80 and 100 cm

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.

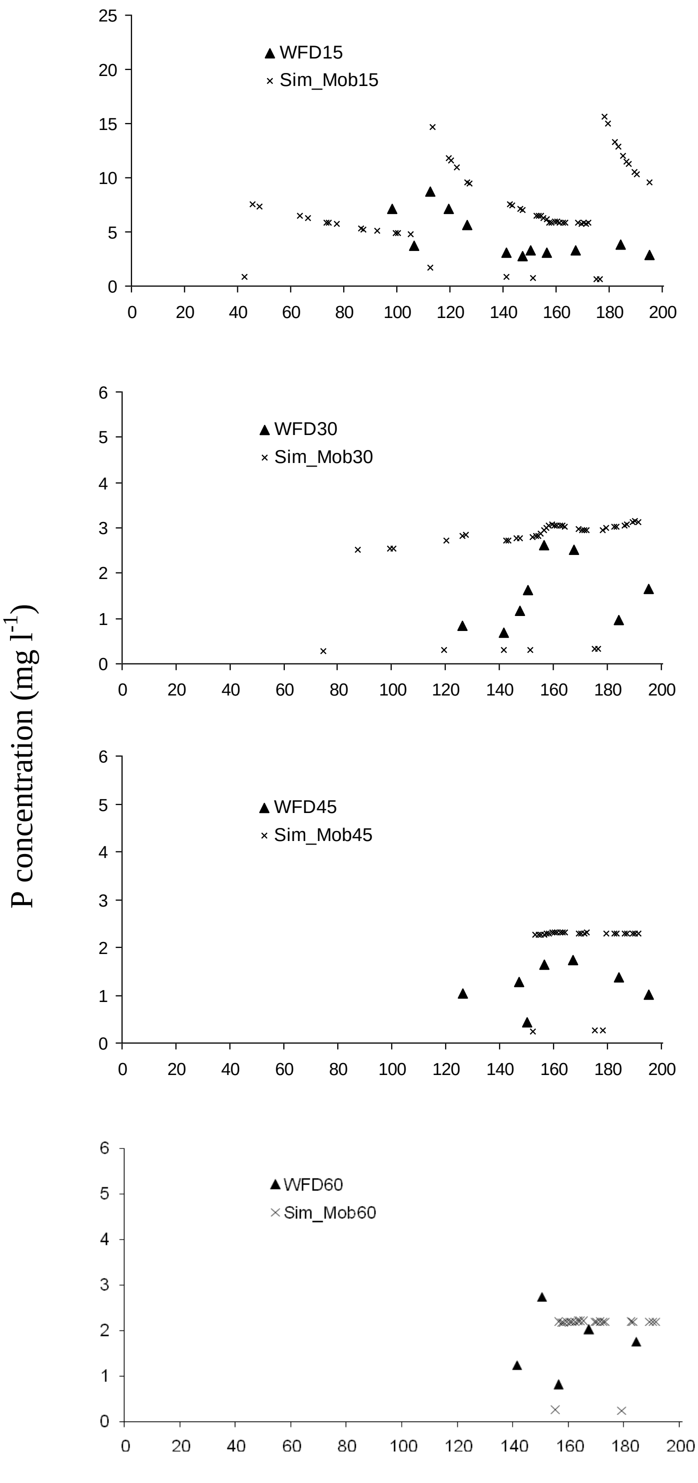

Figure 6.10 Measured P concentrations from wetting front detectors and simulated mobile soil water phase P concentrations at depths of 15, 30, 45 and 60 cm

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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CHAPTER 7

ANALYSIS OF NITROGEN AND PHOSPHORUS LEACHING FROM DRYLAND AND IRRIGATED CROPPING SYSTEMS USING LONG-TERM MODELLING

ABSTRACT

Cropping systems can potentially contribute high loads of non-point source (NPS) nitrogen (N) and phosphorus (P) pollution to ground and surface waters. Quantifying these contributions is however highly challenging. Long-term modelling at the local scale for a hypothetical field located on the South African Highveld was used to assess the potential contribution of irrigated and dryland crop production to N and P leaching losses in a monoculture maize cropping system. As irrigated systems present more management options, the effect of a 'room for rain' irrigation strategy and a maize-wheat crop rotation system on reducing N and P leaching losses were also investigated. Over a 30 year simulation period, irrigated crop production was observed to leach 480% more N and 420% more P than dryland production. A 'room for rain' irrigation strategy was able to reduce N leaching by 12% and P leaching by 14% compared to irrigating to field capacity. Despite increased irrigation and fertilization input requirements for a crop rotation system, significant reductions in N (23%) and P (24%) leaching losses were observed for this system compared to the monoculture system. From this trial it is clear that long-term modelling can be used effectively to investigate N and P leaching losses from different cropping systems and identify appropriate mitigation measures.

7.1 INTRODUCTION

Loss of nutrients from agricultural systems to waterways is a world-wide problem that can lead to eutrophication and jeopardize aquatic ecosystems and fresh water quality (Matson et al., 1997). Nitrogen (N) and phosphorus (P) are most frequently the limiting nutrients for algal growth and are therefore implicated as the primary nutrients leading to eutrophication (Walmsley, 2000). Negative spin-offs from eutrophication and toxic algae growth include: taste and odour problems in drinking water, oxygen depletion, increased fish and invertebrate mortality, waterway clogging interference in irrigated agriculture and recreational activities, increased treatment costs and a decline in aesthetic conditions (Toerien, 1974; Dunst et al., 1974). High nitrate (NO_3^-) levels in drinking water can also be hazardous to infants and livestock (Tredoux, 1993). Furthermore, N and P loss from agricultural soils can result in unwanted environmental impacts and substantial economic loss for farmers. N and P can be exported to waterways in inorganic or organic forms via runoff or leaching, making this type of pollution very difficult to measure.

The replacement of natural vegetation with cropping systems can drive major changes in water balances and cause the redistribution of water and solutes in the landscape (Keating et al., 2001). It can be commonly expected that irrigated and dryland cropping systems will have different water and nutrient balances. According to Bristow (2004), most current irrigation systems can be characterized by uniformity, discontinuity in nutrient dynamics (large fertilizer inputs at planting and large removal at harvest), excess deep drainage, and rising water tables and salinisation. The close spatial proximity of irrigated cropping systems to water sources results in these systems often having higher risk with regard to polluting potential due to the likelihood of increased delivery of nutrients to ground and surface waters. The focus of concern will lie with downstream water and ecological systems, as most water supply dams are usually upstream of irrigated areas. For these reasons, an increase in irrigation area can be expected to intensify the NPS nutrient pollution problem.

In developing countries, irrigated land consists of 20% of total arable land but produces 40% of all crops and close to 50% of cereal production (FAO, 2003). Further agricultural production intensification will be required to feed the increasing world population. According to the FAO, between the years 1960 and 2000, nitrogenous fertilizer consumption increased 7-fold and phosphate fertilizer consumption increased 3-fold, while total irrigated area doubled between 1960 and 1999 (http://faostat.fao.org). Tilman et al. (2001) used past global trends and their dependence on population size and GDP to obtain trajectories for global irrigated area and N and P fertilizer consumption in 2020 and 2050. The authors estimated that global N and P fertilization would increase 1.6- and 2.7-fold by 2020, and 1.9- and 2.4-fold for 2050, respectively, from 2000 values. They also estimated that irrigated area will increase 1.3-fold by 2020 and 1.9-fold by 2050, with most increases occurring in Latin America and sub-Saharan Africa. While statistics on the breakdown of nutrients used on dryland versus irrigated agriculture are not readily available one can assume that irrigated cropping systems will generally receive higher fertilizer inputs due to higher target yields. These large projected increases could have significant environmental impacts (Tilman et al., 2001), and necessitate improved mitigation measures.

High N leaching potential is often expected in relatively arid areas where intensively managed fruit and vegetable crops are common, as mild winters permit crop residue decomposition, and heavy rainfall can occur within a few winter months, promoting leaching (Coppock and Meyer, 1980). Similarly, leaching is also more predominant in coarse than fine textured soils. An array of studies investigating NO_3^- leaching have produced a wide range of results depending on experimental conditions, with amount of NO_3^- leached usually related to amount of fertilizer N applied and the volume of deep percolation. Nitrate losses greater than 100 kg N ha^{-1} have been observed in semi-arid surface irrigated areas in Spain and the USA (Causapé et al., 2004). Sexton et al. (1996) observed that the majority of NO_3^- leaching in a season occurred during only two major rainfall periods, highlighting the importance of specific leaching events in a season. In the US, higher groundwater NO_3^- concentrations are more often observed in areas under irrigation than in areas with no irrigation (Follet and Hatfield, 2004).

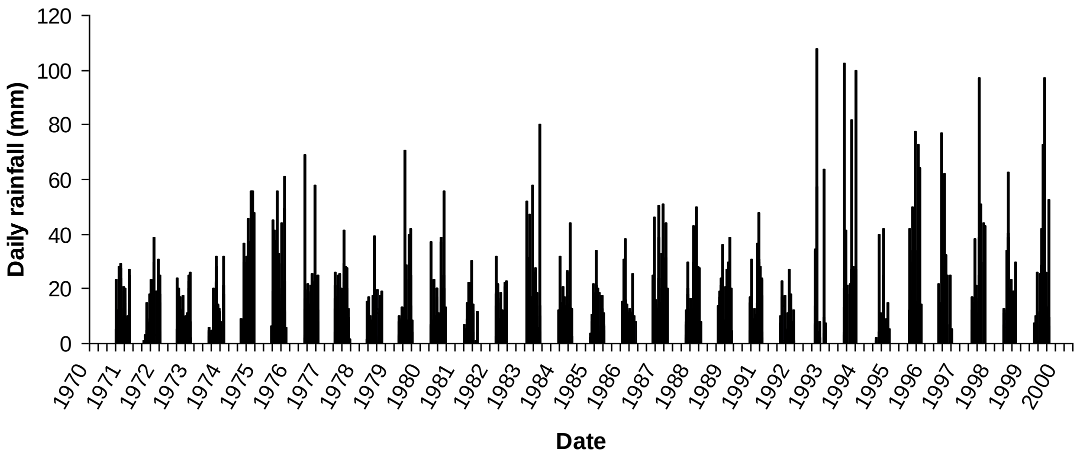
The movement of P through the soil profile is less well documented than P movement in surface runoff (Bush and Austin, 2001), but recently more attention is being given to P leaching. Toor et al. (2005) report that significant amounts of P can be lost shortly after P fertilizer applications when preferential transport takes place through cracks, root holes and worm borings in the soil. However, P leaching is usually minimal in soils through which water moves very slowly and there is prolonged contact with the soil matrix (Djodjic et al., 2004).

From field scale nutrient balances, Annandale and du Preez (2005) concluded that dryland crop production in South Africa has a limited impact on groundwater nitrate levels, especially on deeper soils. As irrigated systems are often characterized by intensive crops, higher nutrient application rates and wetter systems, it may be expected that these systems are ‘leakier’ relative to dryland production.

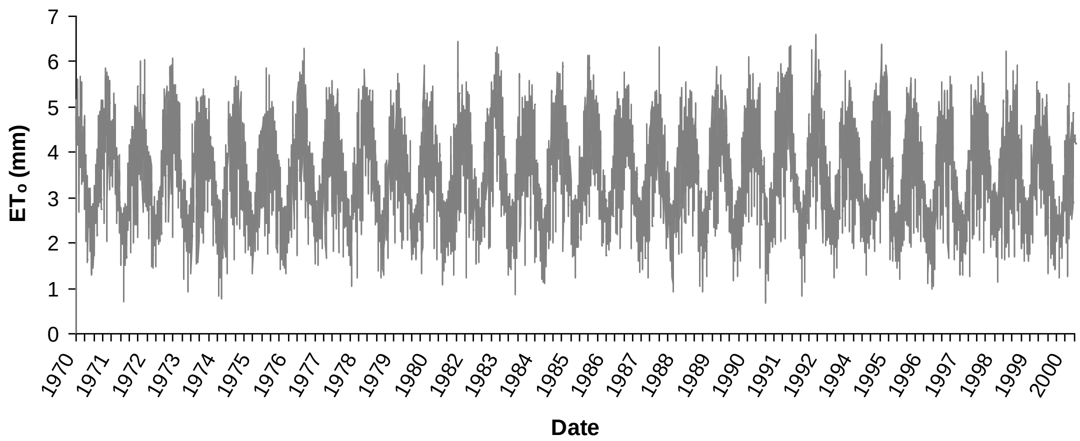
The objective of this study was firstly to compare the impact of dryland versus irrigated agriculture on expected N and P leaching losses from cropping systems. As irrigated systems often offer the highest flexibility in terms of mitigation management practices, N and P leaching was further investigated for two additional scenarios, the first employing a ‘room for rain’ irrigation strategy, and the second using a crop rotation strategy. Ultimately, the potential for using a local scale, mechanistic model such as SWB-Sci to estimate N and P leaching and find potential management practices to reduce these types of losses was assessed.

7.2 MATERIALS AND METHODS

SWB-Sci is a local scale crop model that can mechanistically model N and P dynamics in cropping systems (see Chapters 4, 5 and 6). The soil water balance is modelled using a simple cascading approach (Campbell and Diaz, 1977), and a daily crop dry matter increment is estimated as being either water supply (Tanner and Sinclair, 1983) or solar radiation limited (Monteith, 1977). This daily dry matter increment is then used to calculate daily crop N and P demand after which the lesser of any N or P stress on crop growth is accounted for through stress factors (see Chapter 5). The model was used to run 30 year simulations for a single dryland and three irrigation scenarios on a hypothetical field in the Bethal area, Mpumalanga, South Africa. The soil profile used in the simulations was based on the soil used in an N and P leaching trial conducted in a drainage lysimeter in Pretoria, South Africa (see Chapter 6). Briefly, the 1.5 m deep soil has a sandy clay loam texture with a clay content of 20% and a sand content of 70%. Soil organic matter ranges from 1.0 to 1.3%, pH(H_2O) ranges from 5.9 to 6.2, and Bray I P ranges from 20 to 6.6 mg kg^{-1} with depth. Rainfall and ET_o data used in the simulation for the 30 year period are presented in Figure 7.1. No N and P additions via rainfall or irrigation were simulated.



(a)



(b)

Figure 7.1 Daily rainfall (a) and daily ET_o (b) for the Bethal area for the simulation period (1970 -2000)

The first scenario simulated a dryland maize system (DM = dryland maize) totally dependent on rainfall. Following 15 September, daily rainfall was summed and maize was planted immediately after 20 mm of rainfall had occurred. At planting, the crop was fertilized with 40 kg N ha^{-1} in the form of limestone ammonium nitrate (LAN) and 15 kg P ha^{-1} in the form of superphosphate which was banded at a depth of 10 cm.

For the second scenario maize was grown under irrigation (IM = irrigated maize). The crop was planted on 25 October each year and fertilized on this day with 40 kg P ha^{-1} in the form superphosphate banded at 10cm. Nitrogen fertilizer was applied in split applications of 100 kg N ha^{-1} each at plating and 6 weeks after planting. Soil in the root zone was irrigated to field capacity when root zone plant available water (PAW) reached a deficit of 40%.

The third scenario was exactly as for IM, except that instead of irrigating the root zone to field capacity, irrigation was applied to allow for 30 mm of 'room for rain' (IMrr). This strategy was not applied for the initial, establishment phase of the crop when the root zone was irrigated to field capacity.

The fourth scenario (IMwr) was also exactly as for IM, except that a crop rotation system involving wheat was used. Wheat was planted on 1 May of every year and fertilized with 80 kg N ha^{-1} (LAN) and 10 kg P ha^{-1} (superphosphate, banded at 10 cm). A further 60 kg N ha^{-1} was applied 6 weeks after planting. Irrigation scheduling used the same approach as for IM.

Maize and wheat crop parameters were obtained from model calibration and testing work done for a dryland maize and wheat trial receiving different N applications conducted in Glen, near Bloemfontein, South Africa (Schmidt, 1993) and a maize trial receiving different N and P application rates conducted in Kenya (Probert and Okalebo, 1992). For both crops, the radiation use efficiency (kg MJ^{-1}) was increased and the day degrees to maturity were decreased to represent cultivars with higher yield potentials and shorter growth durations.

Direct comparisons were made between DM and IM, IM and IMrr and IM and IMwr, and thereafter all four scenarios were considered together.

7.3 RESULTS

7.3.1 Dryland versus irrigated cropping systems

As expected, final yield data for the 30 year simulation period was observed to be higher and more consistent for the irrigated (IM) than for the dryland (DM) scenario (Figure 7.2). Yields of between 8.9 and 11.6 tons were achieved for the irrigated system, while yield fluctuated from below 0.1 to 8.5 t ha^{-1} for the dryland scenario depending on seasonal rainfall.

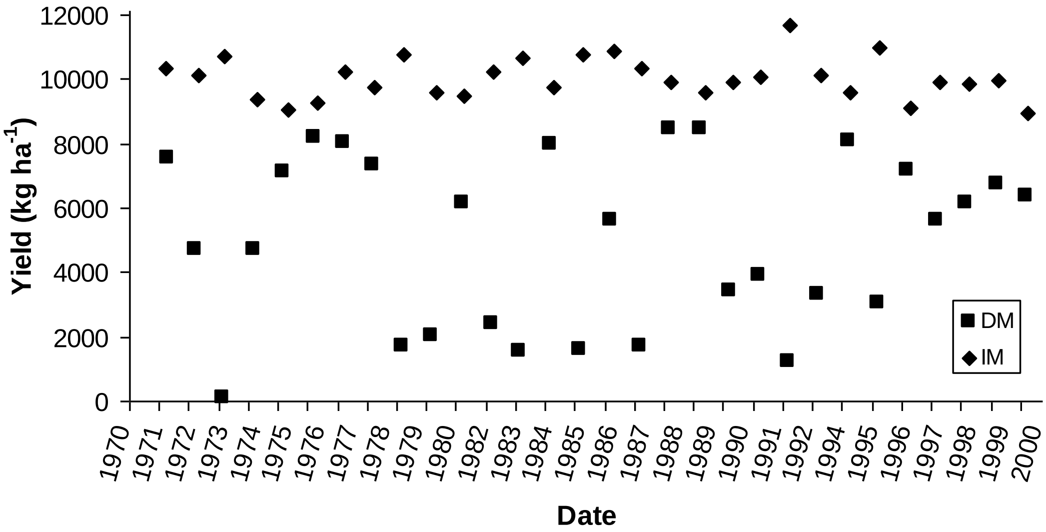


Figure 7.2 Seasonal yields over the 30 year simulation period for the Dryland Maize (DM) and Irrigated Maize (IM) scenarios

As a result of irrigation leading to a ‘wetter’ soil profile with little additional space for rainfall, higher cumulative profile drainage was simulated for the irrigated scenario than for the dryland scenario (Figure 7.3). Over the 30 year simulation period, in addition to 22029 mm of rainfall, 6328 mm of irrigation was applied resulting in 3495 mm of deep drainage leaving the root zone and 48 mm of runoff for IM. For the dryland scenario, we simulated 787 mm of deep drainage and 17 mm of runoff. No deep drainage occurred over entire growth seasons for long periods, most notably between 1970 and 1983. Irrigation therefore led to a 4.4-fold increase in cumulative deep drainage over the 30 year period.

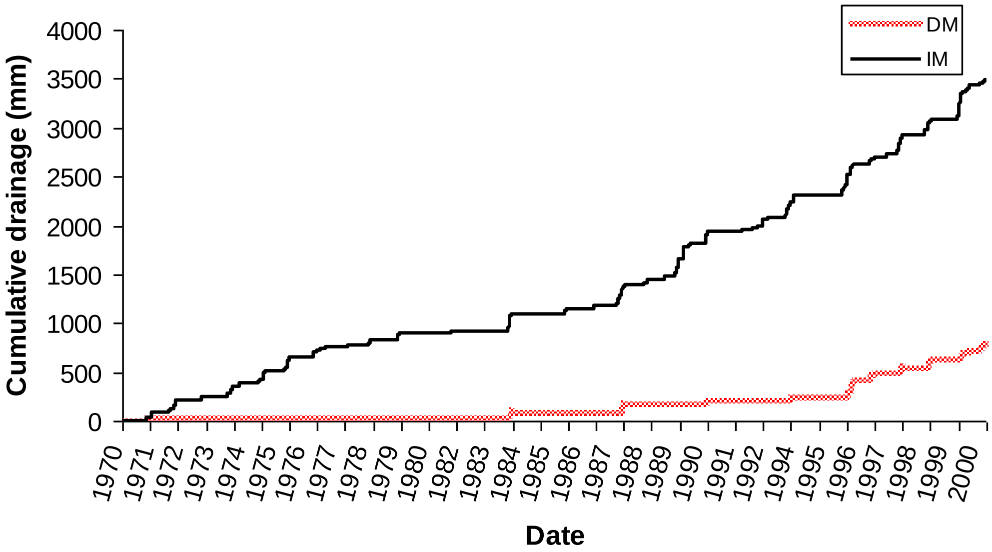
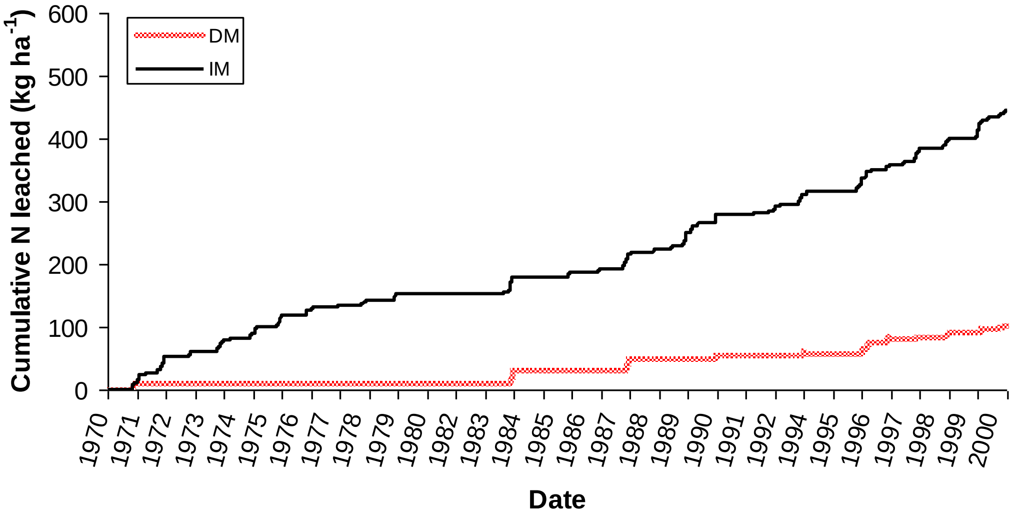
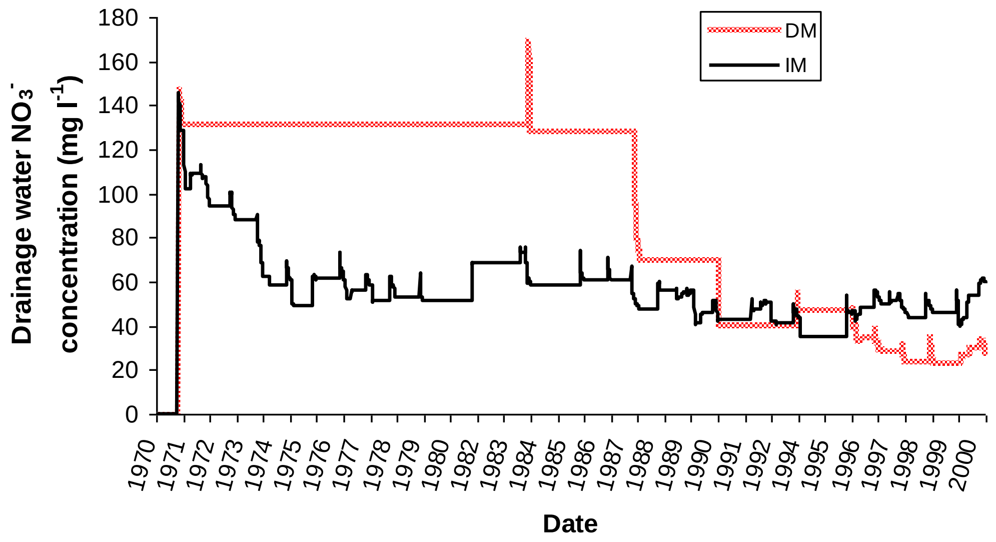


Figure 7.3 Cumulative deep drainage (mm) over the 30 year simulation period for the Dryland Maize (DM) and Irrigated Maize (IM) scenarios

For the IM scenario, 497 kg N ha^{-1} of the 6000 kg N ha^{-1} applied was estimated to have leached, and for the DM scenario 103 kg N ha^{-1} of the 1200 kg N ha^{-1} applied was simulated to have leached (Figure 7.4). Cumulative N leaching for the irrigation scenario was therefore 4.8-fold higher than for the dryland scenario. For the first 20 years, despite less N fertilizer being applied to the DM than to the IM scenario, higher drainage NO_3^- concentrations were observed for the DM scenario. The highest NO_3^- concentration of 168 mg l^{-1} was observed for the DM scenario in the first deep drainage event following a long period during which no deep drainage occurred. Following the first season, NO_3^- concentrations fluctuated between 40 and 100 mg l^{-1}, for the IM scenario. For the DM scenario especially, sudden sharp increases in cumulative N leached highlighted that leaching is clearly event driven.



(a)



(b)

Figure 7.4 Cumulative N leached (a) and drainage water NO_3^- concentrations (b) over the 30 year simulation period for the Dryland Maize (DM) and Irrigated Maize (IM) scenarios

Cumulative P leaching over the simulation period is presented in Figure 7.5. For the IM scenario, 88 kg P ha^{-1} of the 1200 kg P ha^{-1} applied was estimated to have leached, while for the dryland scenario, 21 kg P ha^{-1} of the 450 kg P ha^{-1} applied was estimated to have leached over the 30 year period. This represents a 4.2-fold difference between the two scenarios and is reflects the differences in cumulative deep drainage. P concentrations in the drainage water were similar for both scenarios, remaining constant at around 2.6 mg l^{-1}. Averaged over the simulation period, 0.7 kg P ha^{-1} a^{-1} was estimated to leach from the dryland scenario and 2.9 kg P ha^{-1} a^{-1} was estimated to leach from the irrigated scenario. For the IM scenario, P leaching was therefore simulated to be slightly above 7.3% of applied fertilizer P.

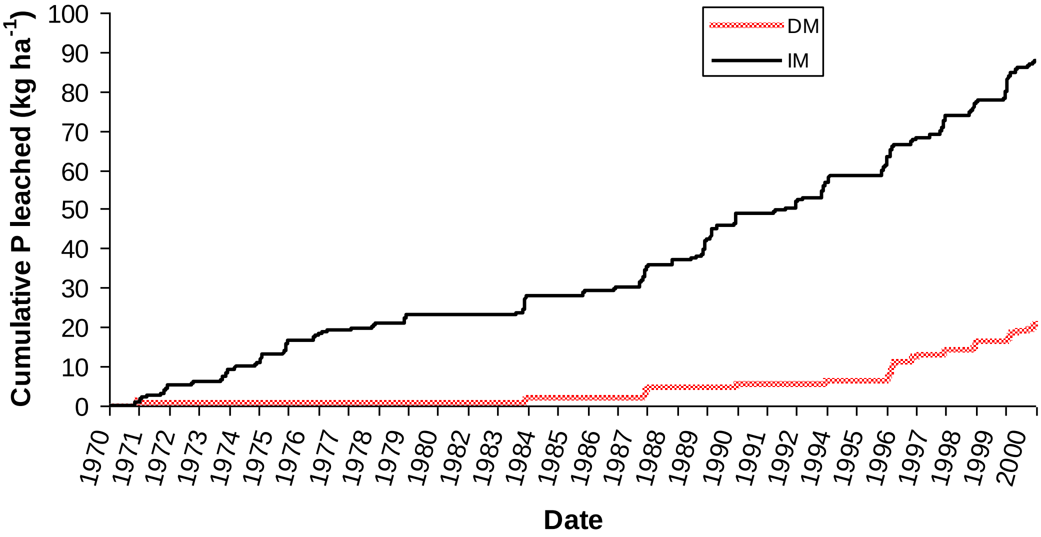


Figure 7.5 Cumulative P leached over the 30 year simulation period for the Dryland Maize (DM) and Irrigated Maize (IM) scenarios

7.3.2 Irrigation scheduling

Applying an irrigation refill strategy that allowed 30 mm 'room for rain' (IMrr) had little effect on final yield relative to a strategy that refilled the root zone to field capacity (IM) (Figure 7.6). In several cases yield for IMrr was marginally higher than for IM and this may have been due to slightly less nutrient leaching occurring for the IMrr scenario.

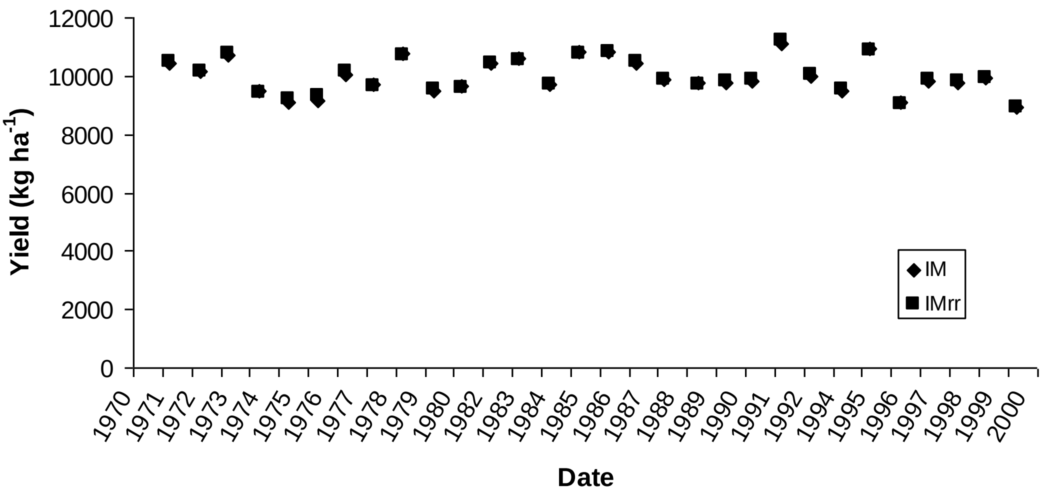


Figure 7.6 Seasonal yields over the 30 year simulation period for Irrigated Maize (IM) scenarios and Irrigated Maize 'room for rain' (IMrr) scenarios

As expected, deep drainage for the IMrr scenario was less than for the IM scenario. Cumulative drainage at the end of the 30 year simulation period was 2986 mm for the IMrr scenario and 3495 mm for the IM treatment (Figure 7.7). This equates to a yearly average of 17 mm less deep drainage occurring for the IMrr scenario, or a 15% reduction in drainage compared to the IM scenario.

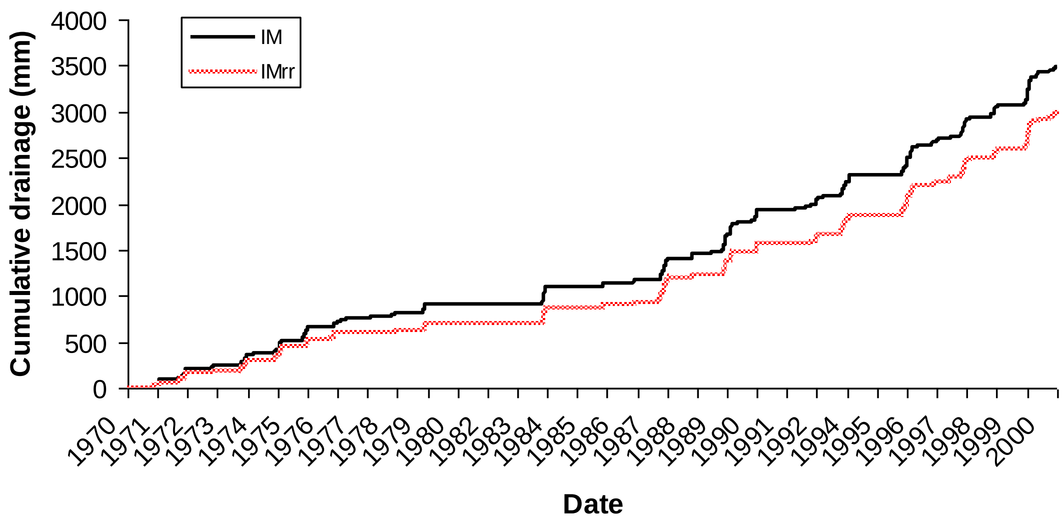


Figure 7.7 Cumulative deep drainage (mm) over the 30 year simulation period for the Irrigated Maize (IM) and Irrigated Maize 'room for rain' (IMrr) scenarios

While the 'room for rain' strategy was not judged to be highly effective in reducing profile drainage over the long-term, it is important when designing and implementing management strategies to understand the implications of seasonal variations. To explore this two contrasting seasons were analyzed more closely. Cumulative drainage data for a selected period during the 1975/76 maize growth season is presented in Figure 7.8. During this season, the 'room for rain' strategy clearly contributed to reducing total drainage as the drainage that did take place occured later in the season for the IMrr than for the IM scenario, and at the end of the season there was 50 mm less drainage for the IMrr scenario than for the IM scenario. Considering that over the 30 year simulation period, drainage was observed to be 509 mm less for the IMrr than for the IM scenario, the 1975/76 growth season represents 10% of the total over the 30 year simulation period. This again highlights the significance of particular events, and the danger of relying solely on averages.

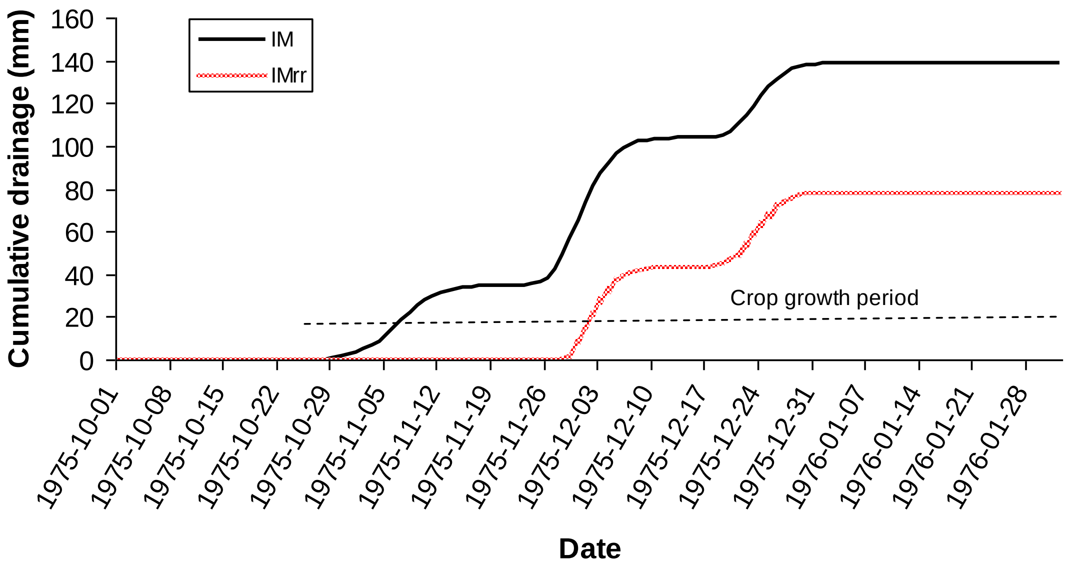
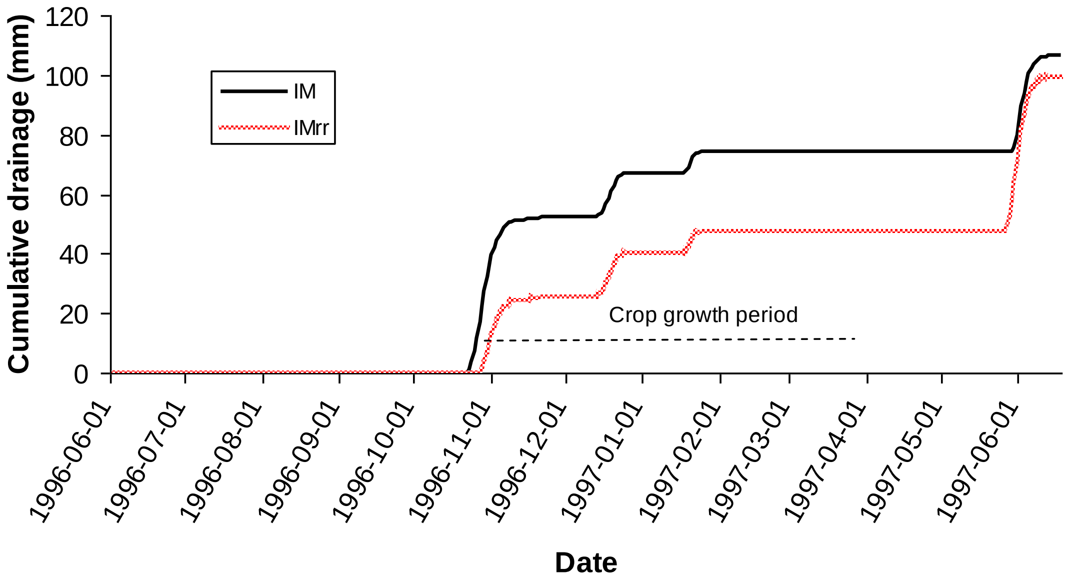
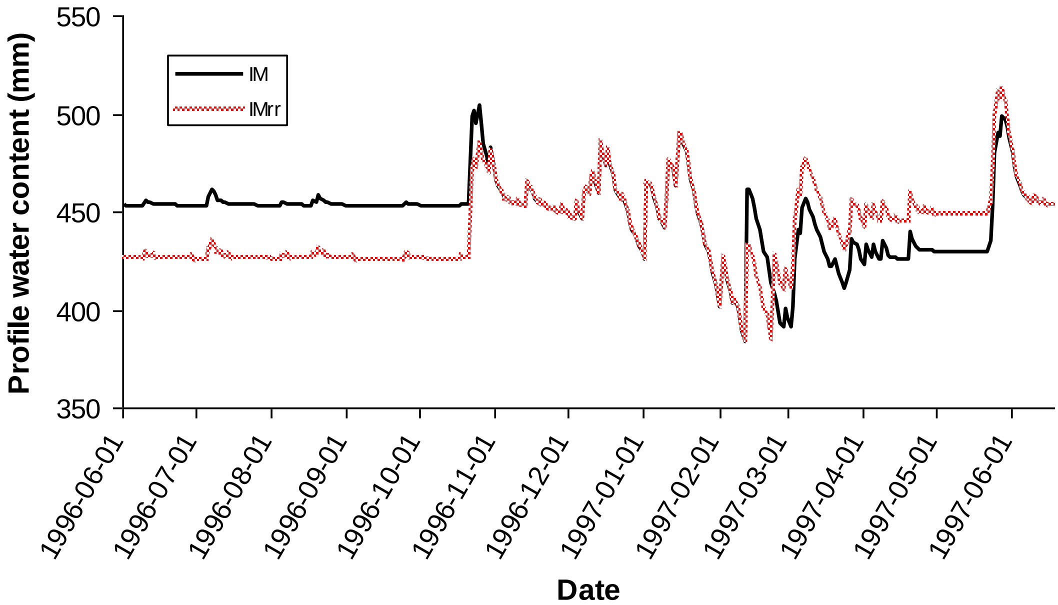


Figure 7.8 Cumulative deep drainage (mm) over a selected period within the 1975/76 maize growth season

For the 1996/97 growth season, the 'room for rain' strategy was observed to be much less effective in reducing drainage. On closer inspection of the deep drainage for the time period, it was observed that during the actual maize growth season, the 'room for rain' strategy led to a 27 mm reduction in deep drainage. The IMrr strategy which requires more frequent irrigation applications, in this case led to a wetter soil profile at the end of the growth season (Figure 7.9), and as a result rainfall that occurred after the crop was harvested resulted in more drainage from the IMrr scenario than from the IM scenario. Considered over a longer period, the 'room for rain' strategy only led to an 8 mm decrease in cumulative drainage, therefore.



(a)



(b)

Figure 7.9 Cumulative deep drainage (mm) (a) and profile water content (b) over a selected period within the 1996/97 maize growth season

As with drainage volumes from the two scenarios, cumulative N leaching was very similar. After the 30 year simulation period, the 'room for rain' strategy led to a 60 kg ha^{-1} decrease in N leaching, from 497 to 437 kg N ha^{-1} (Figure 7.10). The 'room for rain' strategy was therefore only effective in reducing N leaching by 2 kg ha^{-1} a^{-1}, which represents a 13% reduction per year. Similar to N leaching, the 'room for rain' strategy led to a very small decrease in P leaching of 12 kg ha^{-1} over the 30 year simulation period.

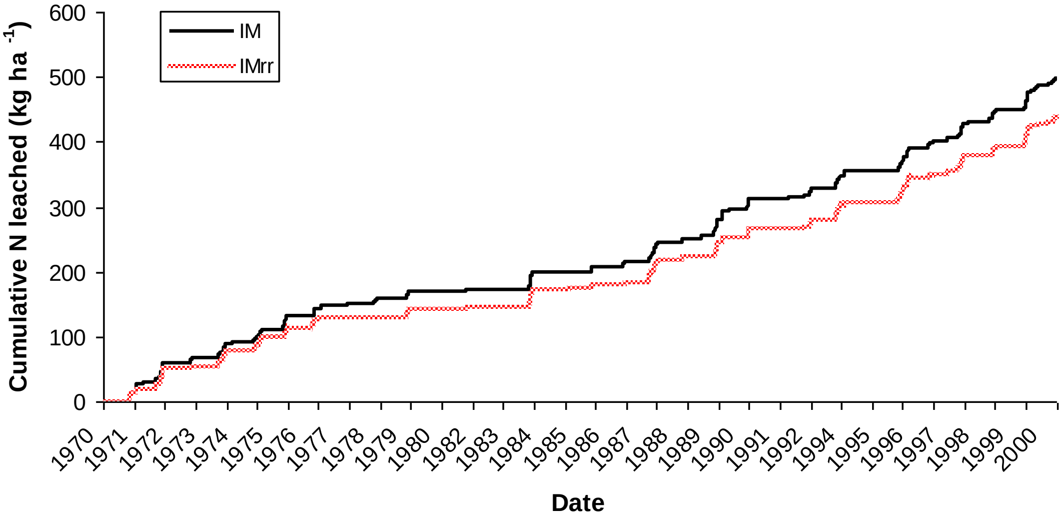


Figure 7.10 Cumulative N leached over the 30 year simulation period for the Irrigated Maize (IM) and Irrigated Maize 'room for rain' scenarios

7.3.3 Crop rotation

Maize yields were observed to be very similar for the monoculture (IM) and crop rotation (IMwr) scenarios (Figure 7.11). In some years, yields for the IMwr scenario were observed to be slightly higher than for the IM scenario, and this may be due to the excess N and/or P fertilizer that was applied to the wheat crop for the IMwr scenario. For the irrigated wheat crop, yields were observed to range between 5.5 and 8.0 t ha^{-1}.

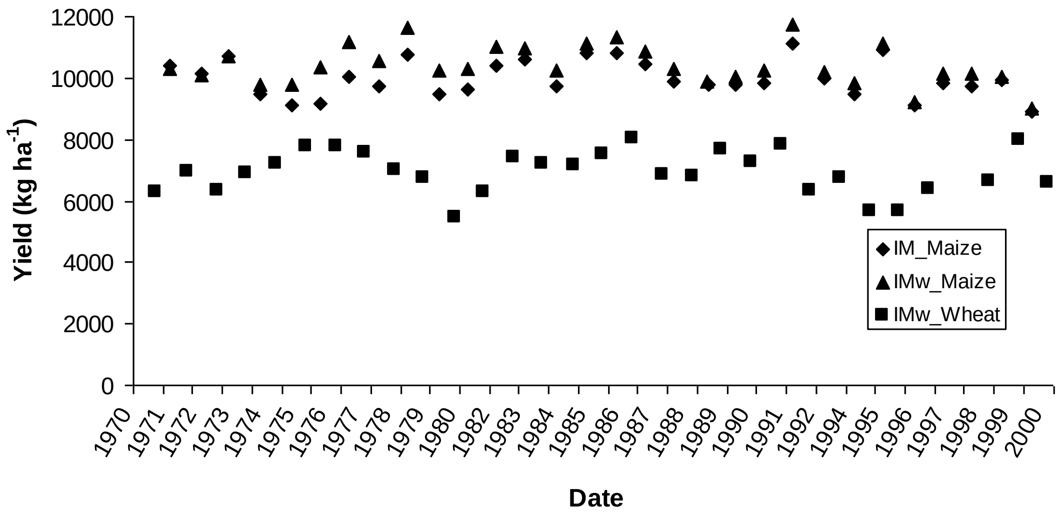


Figure 7.11 Seasonal yields over the 30 year simulation period for the Dryland Irrigated Maize (IM) and Irrigated Maize-wheat rotation (IMwr) scenarios

Using a crop rotation system with wheat grown over the winter season clearly reduced seasonal profile drainage in comparison to maize monoculture (Figure 7.12). In comparison to the 3495 mm of cumulative drainage that occurred for the IM scenario, 2584 mm cumulative drainage was simulated for the IMwr scenario, representing a 911 mm reduction. This is despite an additional 10108 mm of irrigation water being applied for the IMwr scenario. Using a crop rotation system therefore resulted in an average of 30 mm a^{-1} less deep drainage than for a monoculture system, indicating that a significant amount of drainage was likely occurring before or after the actively growing maize crop season.

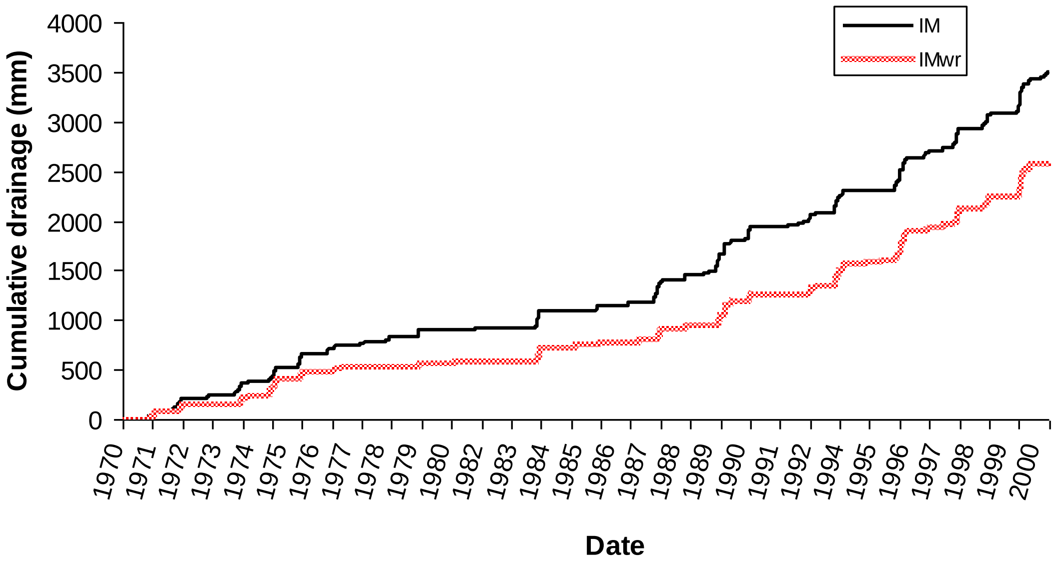


Figure 7.12 Cumulative deep drainage (mm) over the 30 year simulation period for the Irrigated Maize (IM) and Irrigated Maize-wheat rotation (IMwr) scenarios

As a result of decreased drainage volumes for the IMwr scenario, cumulative N leached was also reduced for this scenario; 497 to 383 kg ha^{-1}, a 114 kg ha^{-1} reduction over the 30 year period (Figure 7.13). This represents a greater reduction in N leaching than was achieved for the IMrr scenario.

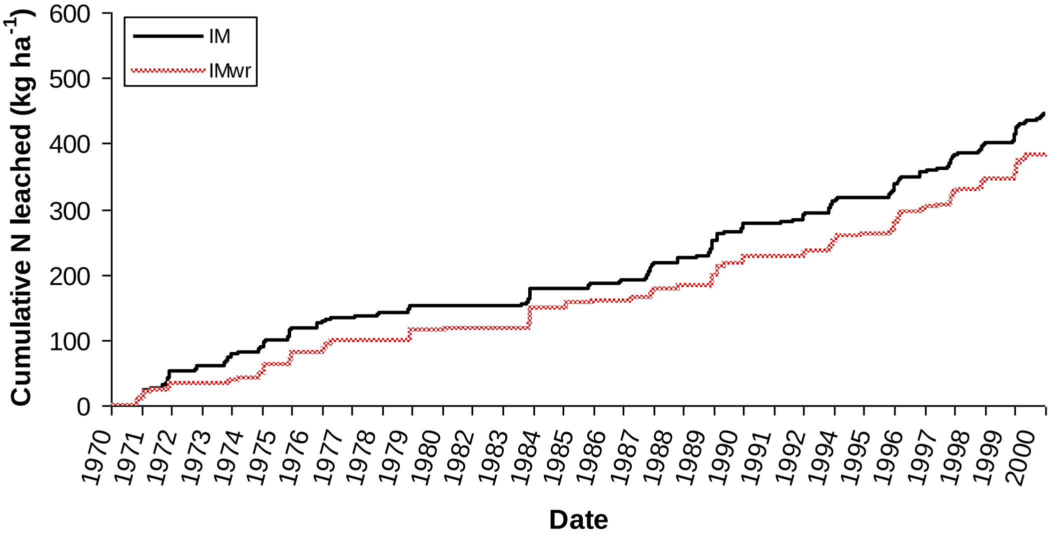


Figure 7.13 Cumulative N leached over the 30 year simulation period for the Irrigated Maize (IM) and Irrigated Maize-wheat rotation (IMwr) scenarios

Cumulative P leached was also reduced, from 88 kg ha^{-1} for scenario IM to 67 kg ha^{-1} for scenario IMwr (Figure 7.14). Reductions of N and P leaching of 23 and 24%, respectively, were therefore similar and closely correlated to the 26% reduction in cumulative deep drainage.

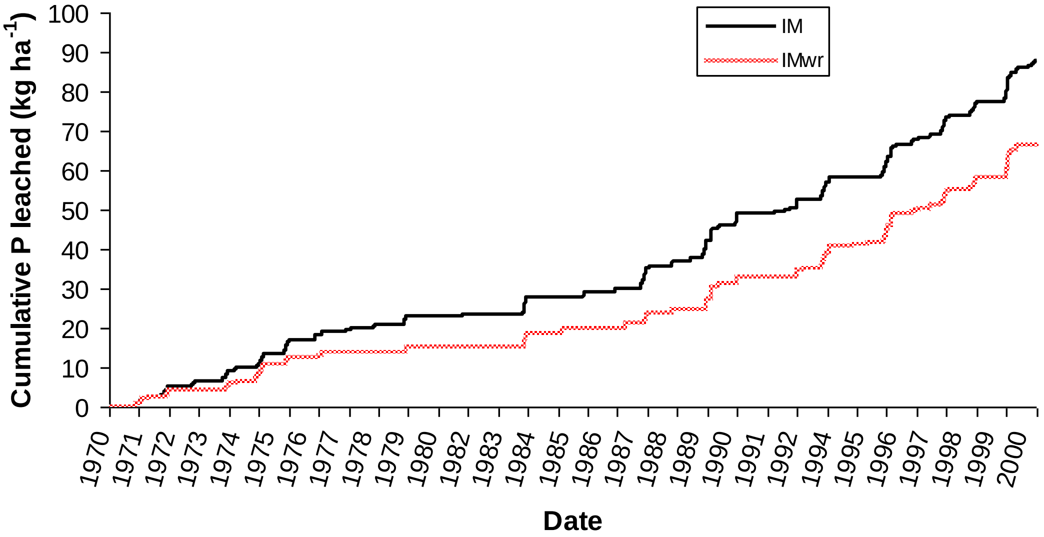


Figure 7.14 Cumulative P leached over the 30 year simulation period for the Irrigated Maize (IM) and Irrigated Maize-wheat rotation (IMwr) scenarios

7.4 OVERVIEW AND DISCUSSION

The highest N and P leaching losses occurred for the IM scenario, while the lowest occurred for the DM scenario (Table 7.1). Compared to the IM scenario, using a ‘room for rain’ irrigation strategy reduced N leaching by 12%, while using a crop rotation system reduced N leaching by 23%, despite much higher overall irrigation and N and P applications. Correspondingly, P leaching loads were reduced by 14 % for IMrr and by 24% for IMwr.

Table 7.1 Cumulative water, N and P additions and losses for the IM, DS, IMrr and IMwr scenarios after the 30 year simulation period

	DM	**IM**	**IMrr**	**IMwr**
Rainfall (mm)	22 029	22 029	22 029	22 029
Irrigation (mm)	0	6328	5916	16 436
Drainage (mm)	787	3495	2986	2584
Runoff (mm)	17	48	17	79
Transpiration (mm)	9206	12 729	17	23573
Evaporation (mm)	11 199	11 107	11 190	10867
Yield (kg ha^{-1})	6273	9995	10 017	10 414/6939*
N fertilization (kg ha^{-1})	1200	6000	6000	10200
P fertilization (kg ha^{-1})	450	1200	1200	1500
N removed (kg ha^{-1})	3119	4848	4864	8836
P removed (kg ha^{-1})	230	337	336	595
N leached (kg ha^{-1})	103	497	437	383
P leached (kg ha^{-1})	21	88	76	67

*Values for maize/wheat

Although average yield for the IM scenario was observed to be 160% higher than for the DM scenario, N leaching was observed to be 482% higher and P leaching 420% higher for the IM scenario. From an environmental standpoint, farming larger surface areas under dryland production will therefore potentially pollute less than irrigated production on smaller surface areas. High yield fluctuations due to unreliable rainfall and limited land availability disfavour such an approach, however. Overall therefore, the IMwr crop rotation system can be expected be more efficient with regards to producing high yields while maintaining relatively low N and P leaching rates. But although crop rotation was observed to play an important role in retaining N in the system, when the crop senesces the N is returned to the soil and can contribute to N leaching (Goulding, 2000). An additional risky period when a second crop’s residues are present on the soil will potentially be included therefore. The same will apply for P. The use of a simple cover crop will be expected to have the same beneficial effects as a crop rotation system on reducing N and P leaching.

For scenarios IM, IMrr and IMwr, more N was applied as fertilizer than was removed in the grain of the crop, but this was not the case for the DM scenario in which a net 'mining' of soil N was observed. Therefore although the lowest leaching losses were simulated for this scenario, a depletion of soil organic matter over time can be expected and the long-term sustainability of such a system requires further investigation. In practice, P fertilization is often adjusted according to soil P tests which give an indication of crop available P in the soil. It is therefore plausible that P fertilization could have been reduced for the scenarios investigated in this study if there was a build up of P, and this may have reduced the amount of P leaching from the profile. Ultimately, the aim is to supply nutrients as and when needed to match crop demand in order to minimize leaching losses.

The South African Department of Water Affairs and Forestry set effluent discharge standards for NO_3^- at 44.3 mg l^{-1} and for P at 1 mg l^{-1} (DWAF, 1996). Whether such a discharge standard should apply to leaching from cropping systems is debatable. NO_3^- concentrations in the leachate from IM, IMrr and IMwr were observed to fluctuate between 40 and 100 mg l^{-1}. The highest drainage water NO_3^- concentration of 168 mg l^{-1} was observed for the DM scenario following a long period in which no drainage took place. Consequently, although dryland exports a smaller long-term N load, a build-up of N deeper in the soil profile during the periods when no drainage occurs can lead to high NO_3^- fluxes entering water systems when drainage finally does occur. For P, leaching concentration for all scenarios remained relatively stable, ranging from 2.3 mg l^{-1} to 2.7 mg l^{-1}.

Other forms of N loss from cropping systems such as denitrification and volatilization were not considered in this paper. It is plausible that higher gaseous losses could have been expected from the more intensively fertilized scenarios, including higher denitrification from the irrigated scenarios. Such losses should also be considered in designing improved nutrient management practices to minimize unwanted environmental impacts of different cropping systems.

In modelling studies of this nature, it is important that all important processes are represented accurately (Keating et al., 2001). Two major uncertainties in this study were N and P mineralization rates in the soil and soil sorption of P, both of which could have influenced leaching losses. Unfortunately 1-D modelling does not account for the added effects of irrigation systems with low uniformity on N and P leaching from cropping systems. Furthermore, any potential preferential flow that may have occurred in the wetter irrigated profile was not simulated. Nonetheless, this study shows that long-term modelling can be used to provide insights into N and P dynamics in cropping systems, and the suitability of different mitigation measures in reducing N and P leaching losses. Modelling work of this nature can also be done in conjunction with field measurements and to plan field trials more effectively.

7.5 CONCLUSIONS

Deterioration of water quality as a result of N and P export from cropping systems requires innovative management practices at the local scale to reduce this type of non-point source (NPS) pollution. As N and P leaching losses from cropping systems are difficult to measure and monitor, the use of long-term modelling can effectively improve understanding on N and P export, as demonstrated in this study.

SWB-Sci was successfully used to compare N and P leaching losses for four different management scenarios. Maize under irrigation was shown to leach far greater loads of N and P compared to dryland maize production. Using a ‘room for rain’ strategy reduced N and P leaching relative to a standard irrigation scheduling system, but the effectiveness of the strategy varied between seasons. Including a wheat crop over the winter season also reduced N and P leaching, despite increased rates of irrigation and fertilization.

The continued use of models such as SWB-Sci to conduct long-term simulations to analyse critical N and P leaching periods for different cropping systems is recommended. This will lead to the identification of effective management practices to reduce these losses. In addition, modelling can also assist in the planning of field trials and monitoring programmes to further enhance our understanding of these issues. Finally, further research is needed on the optimal management of deep drainage to remove unwanted salts while minimizing the losses of valuable plant nutrients, and here too modelling has an important role to play.

7.6 ACKNOWLEDGEMENTS

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CHAPTER 8
CONCLUSIONS AND RECOMMENDATIONS

8.1 OVERVIEW OF STUDY

Nitrogen (N) and phosphorus (P) leaching losses from the rootzone of cropping systems can lead to deterioration of fresh water quality and represents an economic loss to farmers. Quantification of these leaching losses requires accurate estimation of deep drainage and the N and P concentrations in this deep drainage, but these two variables are difficult to measure. For this reason modelling is often used to estimate N and P fluxes from the rootzone. This study was done improve understanding of the leaching losses of these two nutrients and encompassed the development, testing and application of a modelling tool that could effectively be used to analyse leaching losses at the local scale. Following the inclusion of N and P subroutines into the locally developed SWB-Sci model, initial testing was done using three historical datasets and data collected from a drainage lysimeter trial as part of this study. Long-term simulations were then used to compare N and P leaching losses for dryland versus irrigated agriculture and to explore the effect of best management practices on reducing N and P leaching losses.

8.2 GENERAL CONCLUSIONS AND RECOMMENDATIONS FOR MODELLING N AND P AT THE LOCAL SCALE

Nitrogen and P simulating capabilities have now been successfully incorporated into the SWB-Sci model (see Chapter 2). Although algorithms were primarily obtained from existing models, this exercise provided an excellent learning opportunity on N and P dynamics in cropping systems and the different approaches used to model these dynamics. The existence of a range of similar models worldwide is acknowledged, but having the ability to edit and modify source code allows greater flexibility when simulating a diverse range of cropping systems and for long-term modelling exercises. Considerable de-bugging and testing was required following the inclusion of N and P algorithms. During the development phase and the design of interface screens, achieving high user-friendliness in the model was a priority. It is expected that the SWB-Sci model will continue to undergo refinement and be widely used by researchers in the future, building on the large amount of work that has already been done on the simulation of the soil water balance, crop growth, and salt dynamics. The highly mechanistic approach, the generic way in which crop growth is simulated, and the ability to simulate a wide range of morphologically different crops favours the wide applicability of this model.

Early on during this study it was realised that obtaining the soil parameters required to model P for South African soils is not a straightforward exercise. It is anticipated that soil parameterization work and the guidelines developed as part of this research will increase the effort directed to P measurement and modelling in South Africa to further reduce loss of P from cropping systems and minimise unwanted impacts of NPS pollution (see Chapter 3). Further work is needed to test the general applicability of the equations used to estimate the quantity of *Labile P* and the P availability index (PAI) of local soils. A follow-on study is currently underway to improve understanding of the soil characteristics important in determining P sorption in soils (Du Preez – personal communication), and it is envisaged that this work will assist in further improving the algorithms used to model P interactions with the soil matrix. The appropriateness of the guidelines provided in this thesis to categorize South African soil forms as calcareous, slightly weathered or highly weathered also requires further development. A lack of suitable P data collected locally and across scales is still a limitation in testing these algorithms and guidelines. New monitoring to collect this type of data and the continuation of existing monitoring is therefore recommended to improve our ability to better manage P.

During model testing exercises with the N datasets from the Netherlands and South Africa, the model performed well in simulating N dynamics in cropping systems (see Chapter 4). The new approach to simulate the effect of N stress on yield on a daily basis following flowering, as opposed to simulating the effect of N stress on the harvest index as used in CropSyst, proved to be effective. As also observed by De Willigen (1991), aboveground N variables were more accurately simulated than belowground N variables. For both the South African and Netherlands datasets, correlation between measured and simulated soil inorganic N levels were not evaluated according to statistical criteria as was the case for other variables. This was because low overall correlations, most likely due to high soil variability, make these prescribed statistical criteria too stringent. In some cases, added fertilizer N was observed to 'disappear' in the measured data, adding to the difficulty in trying to compare measured and simulated values. Nonetheless, simulated changes in soil inorganic N levels and trends over the growth season were often similar to measured values. In simulating soil organic matter in soils, the model requires that users input the size of the different fractions making up the soil organic matter (SOM), including the 'microbial biomass', 'active labile SOM', 'active meta-stable SOM' and 'passive SOM', at different soil depths. These fractions influence mineralization and immobilization rates significantly, so it is important that they are accurately represented for the particular soils being simulated. Freshly mineralized inorganic N is clearly an important contribution to crop available N (see Chapter 4), and development of a simple laboratory procedure to assist users to obtain these values could be highly beneficial. It is also suggested that the model be modified to simulate the influences of the stony fraction in soils on organic matter mineralization, soil water movement and other relevant processes in order to improve overall accuracy.

New algorithms to simulate crop P demand and uptake, P stress effects on crop growth, and banded P fertilizer applications were included into SWB-Sci (see Chapter 5). During testing exercises using a dryland maize dataset collected in Kenya, the model was observed to simulate aboveground dry matter production (TDM), yield, leaf area index (LAI), profile water content, aboveground N and P mass and grain N and P mass with varying levels of accuracy. Unfortunately soil N and P levels were not measured in this trial so this made testing and comparison of measured and simulated values more difficult. Except for aboveground P mass, agreement between measured and simulated values was almost always better for the first growth season (SR89) than for the second growth season (LR90). Exact reasons for poorer performance by the model during the second season are not immediately clear. There could have been something that happened in the field when transitioning from the one season to the next that is not adequately captured in the simulations, or some of the newly developed algorithms still need further improvement, so further testing and refinement of these newly included algorithms is recommended.

Similar research on the critical assessment of a model to mechanistically estimate the effects of both N and P stress on crop growth, and to statistically evaluate model performance using a wide range of variables including TDM, yield, LAI, profile water content, aboveground N and P mass and grain N and P mass, could not be identified in the literature. Work done in this thesis therefore contributes significantly to the future inclusion of the simulation of P stress effects on crop growth to the great amount of mechanistic, local scale N modelling that is carried out. Good datasets for testing mechanistic P models are still lacking. Field trials involving the extensive measurement of crop P uptake, soil P and runoff and P leaching losses are required to improve our ability to study P dynamics and further progress our ability to simulate P at the local scale.

During the testing exercises discussed above, several areas where further research and the inclusion of additional processes could help improve the model were identified. Work on the effects of N and/or P stress on leaf development and crop LAI for different crops is recommended. The incorporation of a special stress factor that accounts for P stress on LAI, as exists for N, should be considered. These improvements would potentially lead to better estimation of crop water use. In addition to the crops maize, wheat and swiss chard modelled as part of this research, testing the model with other crops, especially with regards to P uptake, is recommended to more fully explore the generic applicability of the SWB-Sci model. It is also proposed that the model be further adapted to simulate N and P dynamics under drip and micro-irrigation as these two forms of irrigation are gaining in popularity as methods to irrigate more efficiently world wide.

Although runoff losses of soluble N and P are simulated in the model, the leaching focus of this research meant that the runoff algorithms were not tested. Further testing of these algorithms, and the incorporation of routines to simulate erosion, which will enable N and P sediment loss estimations, is recommended for SWB-Sci. In the application of the model, it is always essential for users to fully understand what they want to accomplish with a model (Sharpley, 2007), and further knowledge of the strengths and weaknesses of the model will assist with this. A comprehensive, up-to-date user's manual incorporating the crop, soil, weather, salt and nutrient units is recommended to assist future users in the practical application of the model.

8.3 MONITORING AND MODELLING MOBILE AND IMMOBILE SOIL WATER PHASE SOLUTE CONCENTRATIONS

The accurate estimation of solute leaching from agro-ecosystems is highly important in maintaining fresh water quality, but suitable and universally applied techniques to estimate drainage fluxes and solute concentrations in these drainage fluxes are lacking. A drainage lysimeter trial was used to more closely evaluate our ability to simulate vertical solute movement in soils, focusing on the role of mobile and immobile soil water phase NO_3^- and P concentrations (see Chapter 6). As hypothesized, WFD NO_3^- and P concentrations were observed to align closely with simulated mobile phase concentrations, and SC NO_3^- concentrations were observed to align closely with simulated immobile phase concentrations. These results highlight the potential for the use of measuring and modelling together to estimate leaching. Two approaches are possible. The first involves using measurements to calibrate the model and test long-term model accuracy. The second involves measuring solute concentrations with active and/or passive samplers, and modelling to estimate drainage fluxes only, and using these values together to estimate leaching. In both these approaches, WFD and SC data can be valuable in assisting users to estimate the drainage factor, drainage rate (mm d^{-1}) and solute mixing factor for the soil. Additional research, encompassing studies done on a wide range of soils and for cropping systems with varying fertilization and irrigation management practices is needed to test and develop this approach further. Nonetheless, the suggestion provided here is meant as a pragmatic approach to enable the immediate estimation of N and P leaching in critical areas where no similar, simple to implement approaches have been adopted.

Although a wide range of approaches have been developed to model solute movement in soils, instances when these algorithms were tested by someone other than the developer are rare (Addiscott and Wagenet, 1985). It is hoped that the ability of SWB-Sci to simulate N and P dynamics, especially in the mobile and immobile soil water phases, will be further investigated by other researchers for a wide range of soils. The approach used to model incomplete solute mixing is relatively simple, and should be considered for inclusion into larger scale models such as ACRU-NPS.

Finally, SCs, WFDs and modelling can also be used effectively to address and manage salinity issues in the rootzone and NPS salt pollution from cropping systems, and further work is needed to assess nutrient and salinity management together to reduce the overall negative impact of cropping systems on the environment.

8.4 LONG-TERM SIMULATIONS TO INVESTIGATE N AND P LEACHING LOSSES FROM CROPPING SYSTEMS

Long-term modelling with SWB-Sci was successfully used to study N and P leaching from different cropping systems (see Chapter 7). In such an approach, validity depends on the assumption that historical climate data is a guide to future climate data, and that the model provides a realistic representation of the biophysical processes (Keating et al., 2001). Although a model such as SWB-Sci cannot be ‘validated’ in the sense that it can provide unequivocally accurate simulations (Keating et al., 2001), confidence in a model is generated through extensive testing.

Using 30 year simulations, monoculture maize production under irrigation was observed to leach higher loads of N and P from the profile compared to a similar dryland production system. On numerous occasions, zero leaching losses were observed over multiple consecutive years for the dryland scenario. Application of a ‘room for rain’ irrigation strategy was observed to reduce N leaching by 12% and P leaching by 14%. A crop rotation system was even more effective, reducing N leaching losses by 23% and P leaching losses by 24%, despite the application of much higher amounts of irrigation water and fertilizer.

Nitrogen and P leaching losses were clearly event-driven, and amounts leached often varied widely between seasons. For this reason, long-term modelling is crucial in assessing and comparing the long-term effectives of different BMPs. Long-term modelling can also be used to guide planning and monitoring approaches when designing field trials.

8.5 BEST MANAGEMENT PRACTICES (BMPs)

With increasing environmental pressures on farmers, and rising fertilizer and production costs, current farming practices will need to shift towards more environmentally and economically sustainable management strategies. An ability to accurately estimate N and P leaching losses in different cropping systems is essential for the identification of suitable BMPs. Existing agronomic guidelines often do not adequately consider environmental implications; for example, soil P test recommendations are based on crop responses and not environmental risks such as runoff P enrichment potential (Sims and Sharpley, 1998). Several BMPs were investigated in this study. In the drainage lysimeter trial, using WFDs to guide irrigation was judged to be successful as drainage from the bottom of the profile was only caused by rainfall later in the season (see Chapter 6). Having WFDs buried at 45 and 60 cm served to ensure that over-irrigation was not occurring. Applying N fertilizer to the swiss chard crop only when NO_3^- concentrations measured from the WFDs located in the root zone was below 100 mg l^{-1} was not assessed to be completely successful in reducing N leaching from the profile. Accounting for N that is available to the crop deeper in the soil is also clearly important, and high N leaching from the profile could potentially have been reduced by not applying subsequent N fertilizer, forcing the crop to remove N from deeper in the soil profile. This may have made negative effects on yield and could represent a trade-off between economics and the environment.

In the long-term modelling study, a 'room for rain' irrigation scheduling strategy and a crop rotation strategy were found to reduce N and P leaching losses, with the crop rotation strategy proving more effective (see Chapter 7). Future work exploring BMPs at the local scale could include analysing the effect of fertilizer application timing, applying smaller amounts of fertilizer at a time in the irrigation water (fertigation), application of fertilizer with different rates of availability, more efficient irrigation systems and scheduling practices. It is also recommended that similar scenarios be investigated for cropping systems in different climatic zones in South Africa, especially for intensive horticultural crop production. In addition to this, the role of soil depth in N and P leaching is also recommended for further investigation. In such work identifying 'leaky' cropping systems and exploring appropriate BMPs, economists clearly have a major role to play in assessing feasibility.

In its current form, SWB-Sci can be used as a research tool to address many of the abovementioned issues and thereby play an important role in reducing N and P leaching from agricultural systems to fresh water systems.

8.6 REFERENCES

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SUMMARY

Nitrogen (N) and phosphorus (P) leaching from croplands to fresh water systems can lead to eutrophication and deterioration in water quality. Intensification of agricultural practices and extending cultivated areas to feed a growing population makes this type of non-point source pollution a growing concern. As leaching losses are highly challenging to monitor and quantify, modelling is becoming increasingly important as a tool to improve our ability to estimate N and P leaching losses. Such modelling is carried out at different scales, ranging from the local scale to represent a single field, to the larger catchment scales which account for the both the sources of these pollutants as well as the hydrological pathways to the receiving water bodies. Modelling at the local scale is often most effective in addressing the impacts of different water and crop management practices on N and P leaching, and is the scale focused on in this study.

In order to improve our ability to understand and manage N and P leaching, subroutines to simulate these two nutrients were included into the locally developed, local scale SWB-Sci crop model. In some cases existing algorithms were modified or new approaches developed as required. Most notably, new approaches to simulate N stress effects on yield; crop P demand, uptake and stress effects on crop growth; banded P fertilization applications; and incomplete solute mixing in soil water were included into the model. The decision to build N and P simulating capabilities into SWB-Sci was taken despite the existence of similar models primarily because of the flexibility and increased capacity that having an in-house model provides in simulating a diverse range of cropping systems and testing fine scale processes.

Following development and debugging, the ability of the model to simulate N and P dynamics in cropping systems was tested using several historical datasets from the Netherlands, Kenya and South Africa, as well as a dataset collected as part of this research. Variables tested included total aboveground dry matter production, yield, leaf area index, profile water content, aboveground N and P mass, grain N and P mass, and soil inorganic N content. Measured and simulated values were subjected to statistical analyses in order to assess model performance in all cases except for soil inorganic N. The model was observed to simulate the various variables tested with a

range of accuracy, and in almost all cases, the model simulated the effect of nutrient stress on crop growth well. Although the new model was judged to be robust, continued testing of the various processes and refinement of approaches and algorithms is recommended to improve the model further.

A drainage lysimeter installed with wetting front detectors and suction cups was used to study vertical solute movement more closely. Previous research has shown that estimating solute concentrations in the mobile soil water phase is important when modelling leaching losses. As wetting front detectors are able to collect a water sample from a wetting front (0 to -3 kPa) and suction cups are able to collect a sample from the immobile or resident soil water (-60 to -70 kPa), it was hypothesized that nitrate (NO_3^-) concentrations measured in wetting front detectors and suction cups would align with simulated NO_3^- concentrations in the mobile and immobile soil water phases, respectively, and this was observed through experimentation. Phosphorus concentrations measured in the wetting front detectors and those simulated in the mobile soil water phase were also observed to align, but not as closely as for NO_3^-. These results demonstrate the value of measuring and modelling together to provide more accurate estimates of solute leaching from the rootzone. Additional research, including studies using a wide range of soils and irrigation and fertilization techniques is recommended to develop this approach further. From this trial, high potential was also observed in the use of wetting front detectors and suctions cups in guiding irrigation and fertilization management practices.

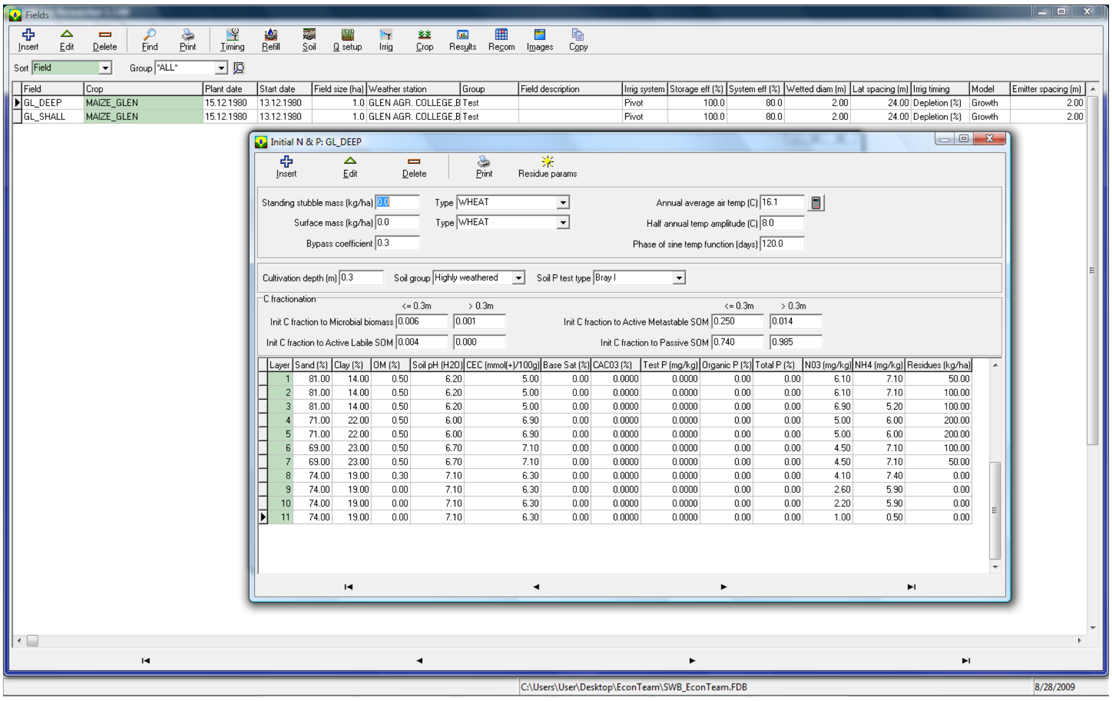
Long-term (30 year) modelling with SWB-Sci was used effectively to analyse and compare N and P leaching losses from dryland and irrigated cropping systems. An irrigated maize monoculture system was simulated to export higher N and P leaching loads compared to dryland production, with N leaching being 480% higher and P leaching being 420% higher. For the irrigated monoculture maize system, irrigating to maintain 30 mm ‘room for rain’ in the soil profile reduced N leaching by 12% and P leaching by 14% over the 30 year simulation period. A crop rotation system, which incorporated irrigated wheat in the winter months, resulted in an even greater reduction in leaching losses despite higher overall applications of N and P fertilizer and irrigation water. Compared to the irrigated monoculture maize scenario, the crop rotation systems led to a 23% decrease in N leaching and a 24% decrease in P

leaching. Nitrogen and P leaching losses were usually associated with large rainfall events and often varied widely between seasons. Long-term modelling was therefore confirmed as an important tool in analysing N and P leaching losses, designing field trials and monitoring experiments, and exploring appropriate best management practices.

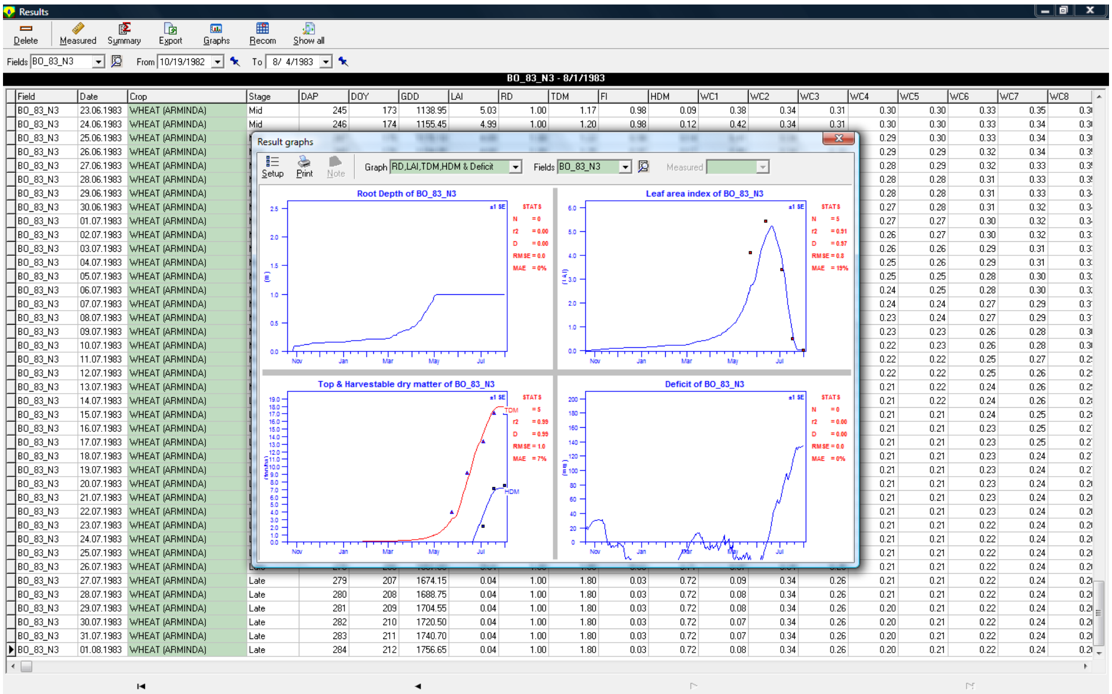
As a result of this study, it is strongly envisaged that enhanced understanding of N and P dynamics in cropping systems, and the use of SWB-Sci as a tool to increase our understanding further, will lead to the reduction of N and P leaching losses through improved management practices.

APPENDIX

Appendix 2.1 SWB-Sci N and P simulation soil initialization (a) and results (b) interface screens



(a)



(b)

Appendix 2.2 Incorporation and Mixing efficiencies of various tillage implements

Tillage implement	Incorporation efficiency	Mixing efficiency
Anhydrous ammonia applicator	0.05	0.05
Bedder--lister	0.95	0.05
Burn	0	0
Chisel	0.1	0.05
Cultivator--field	0.1	0.1
Cultivator--row	0.1	0.1
Digger--peanut	0.05	0.05
Digger--potato	0.15	0.05
Disk harrow--offset	0.85	0.6
Disk harrow--tandem	0.75	0.5
Disk tiller	0.3	0.05
Disk plough	0.8	0.4
Disk plough--one way	0.5	0.5
Do-all	0.1	0.25
Drill--deep furrow (dempster)	0.3	0.05
Drill--small grain	0.05	0.05
Harrow--spike tooth	0.05	0.05
Harrow--spring tooth	0.05	0.05
Moldboard plough	1	0.25
Paraplough	0.05	0.05
Planter--in-row chisel	0.05	0.05
Planter--knife, disk, sweep	0.05	0.05

Appendix 2.3 Soil organic matter (SOM) constants and fractions

Residue C to CO_2 fractions

C_Fraction_From_Fast_Cycling_Residue_To_CO2 = 0.6

C_Fraction_From_Slow_Cycling_Residue_To_CO2 = 0.7

C_Fraction_From_Lignified_Residue_To_CO2 = 0.3

SOM decomposition constants

Microbial biomass = 0.005 (d^{-1})

Labile = 0.01 + 0.00001 (d^{-1})

Metastable = 0.0003 + 0.00001 (d^{-1})

Passive = 0.00001 (d^{-1})

Appendix 2.4 Hard-coded C3 and C4 crop N concentration constants

Plant N concentration constants	C3	C4
N Maximum Conc. At Emergence	0.07	0.055
Biomass To Start Dilution Maximum N Conc.	1.5	1
Biomass To Start Dilution Critical N Conc.	1.5	1
Biomass To Start Dilution Minimum N Conc.	0.5	0.5
Scaling Factor Critical N Conc.	0.65	0.65
Scaling Factor Minimum N Conc.	0.45	0.45
Slope*	-0.45	-0.38
N Maximum Conc. At Maturity	0.0235	0.018
N Critical Conc. At Maturity	0.0152	0.0117
N Minimum Conc. At Maturity	0.0065	0.005

* Can be changed by the user in the interface

Appendix 2.5 Nitrogen:Phosphorus ratios of various crops used to determine P uptake

Crop type	N:P ratio		Crop type	N:P ratio
Alfalfa-seed	5.6		Spring oats-grain	3.5
Alfalfa-hay	5.6		Spring oats-grain+straw	3.5
Winter Barley-grain	5.6		Onions	5.8
Winter Barley-grain+straw	6.2		Orchardgrass	7.0
Spring Barley-grain	5.6		Peas	7.7
Spring Barley-grain+straw	6.2		Pepper, bell	11.7
Beans-dry	3.3		Peanuts	17.6
Beans-snap	10.6		Potatoes-Irish	8.2
Beets	6.0		Rape seed	8.5
Bermuda grass	6.7		Rice	4.8
Bluegrass	7.4		Winter rye-grain	5.7
Broccoli	16.5		Winter rye-grain+straw	5.7
Bromegrass	7.5		Spring rye-grain	5.7
Brussel sprouts	8.1		Spring rye-grain+straw	5.7
Cabbage	9.3		Safflower	4.5
Cantaloupes	6.2		Sorghum-grain	5.1
Carrots	5.8		Sorghum-forage	4.5
Cauliflower	9.3		Soybeans, row	5.3
Clover	5.0		Soybeans, broadcast	5.3
Maize-grain	5.9		Spinach	8.3
Maize-pop	5.9		Squash	6.0
Maize-silage	5.9		Sugar beets	6.0
Maize-sweet	7.8		Sugarcane	5.1
Cotton	5.8		Sunflower	4.5
Cowpeas-hay	4.3		Sweet potatoes	7.0
Cucumbers	6.0		Timothy grass	6.0
Eggplant	6.0		Tobacco	11.7
Lettuce-leaf	7.9		Tomatoes	8.6
Lettuce-head	7.9		Trees-conifer	4.5
Lespedeza	5.0		Trees-hardwood	4.5
Millet, row-grain	5.0		Turnips	8.3
Millet, row-grain+forage	5.0		Watermelon	6.0
Millet, broadcast-grain	5.0		Winter wheat-grain	5.3
Millet, broadcast-grain+forage	5.0		Winter wheat-grain+straw	5.3
Mustard greens	8.3		Spring wheat-grain	5.3
Winter oats-grain	3.5		Spring wheat-grain+straw	5.3
Winter oats-grain+straw	3.5		Weeds	7.0