

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 $7 \text{ kg ha}^{-1} \text{ a}^{-1}$, and for a Mgeni sub catchment the agricultural NPS P load was observed to be $0.12 \text{ kg ha}^{-1} \text{ a}^{-1}$. 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).

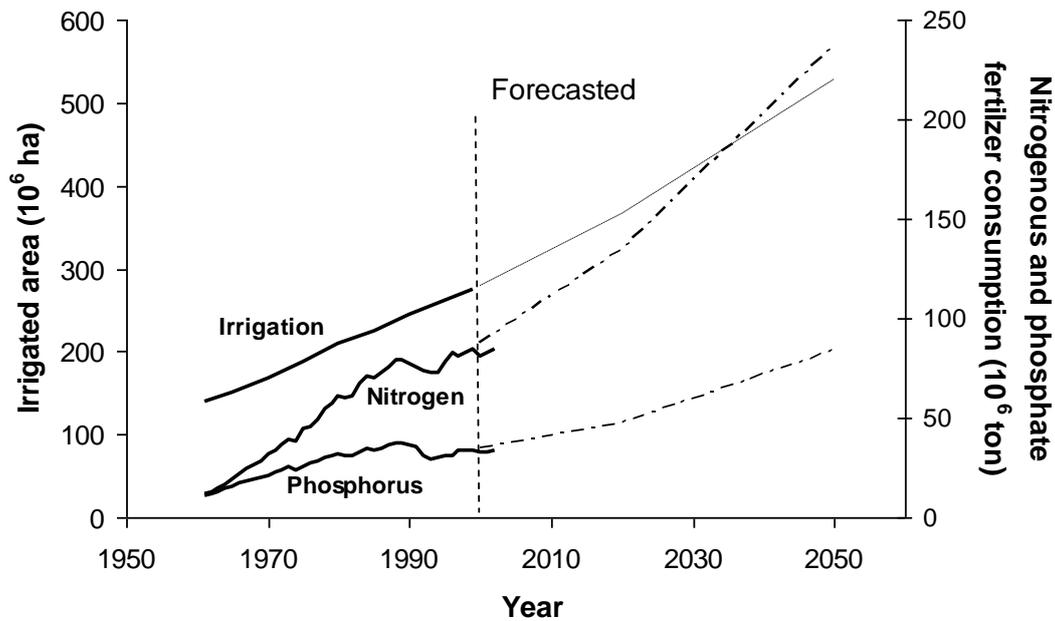


Figure 1.1 Total global increase in irrigated area and nitrogenous and phosphate fertilizer since the 1960's (www.worldwater.org; <http://faostat.fao.org>) and forecasted increase in irrigated area and nitrogenous and phosphate fertilizer consumption until 2050 (from Tilman et al., 2001)

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 $[(\text{NH}_2)_2\text{CO}]$. 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 NO₃⁻

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 $20 \text{ ML ha}^{-1} \text{ yr}^{-1}$ of water with a nitrate concentration of $10 \text{ mg NO}_3\text{-N}$ will add $200 \text{ kg N ha}^{-1} \text{ yr}^{-1}$, 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):

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

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-ECOSYSTEMS

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 assess 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 ($\sim 1 \text{ m}^2$), plot ($\sim 25 \text{ m}^2$), hillslope ($\sim 1 \text{ ha}$), field (broadly defined), small catchment ($\sim 1 \text{ km}^2$), and large catchment ($\sim 1000 \text{ km}^2$) 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 ₂ O)	-	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	°C	No	
Annual temperature amplitude	°C	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 CaCO₃ 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:

$$\text{Slightly weathered: } PAI = 0.0054 \times \text{BaseSat\%} + 0.116 \times \text{pH}(\text{H}_2\text{O}) - 0.73 \quad (2.1)$$

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

$$\text{Calcareous soils: } PAI = 0.58 - 0.061 \times [\text{CaCO}_3] \quad (2.3)$$



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 NO₃-N concentrations are not inserted, the model uses the following equation to estimate NO₃-N concentration (mg kg⁻¹):

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

where d = layer lower boundary depth (m)

If NH₄-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:

$$T_Minimum = -5^{\circ}C$$

$$T_Optimum = 35^{\circ}C$$

$$T_Maximum = 50^{\circ}C$$

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

$$Temperature_Function = \frac{(T[i] - T_Minimum)^Q \times (T_Maximum - T[i])}{(T_Optimum - T_Minimum)^Q \times (T_Maximum - T_Optimum)} \quad (2.6)$$

where T = layer soil temperature

$$Q = \frac{T_Minimum - T_Optimum}{T_Optimum - T_Maximum} \quad (2.7)$$

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 (WFP_{low} = 0.5) and a WFP high threshold value for maximum response (WFP_{high} = 0.7) are hard-coded into the model. If WFP is between WFPmin and WFP_{low}, the *Soil Water Function* is calculated using Equation 2.8:

$$Soil_Water_Function = \frac{WFP - WFP\ min}{WFP\ low - WFP\ min} \quad (2.8)$$

$$\text{where } WFP = \frac{\theta}{\theta_s} \quad (2.9)$$



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

$$Soil_Water_Function = WC_{sat} + (1 - WC_{sat}) \times \sqrt{\frac{1 - WFP}{1 - WFP_{high}}} \quad (2.10)$$

2.2.4.3 Soil pH Function

Minimum (pH_{min}) and maximum pH (pH_{max}) 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:

$$pH_Function = \frac{pH - pH_{min}}{pH_{max} - pH_{min}} \quad (2.11)$$

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 CO₂ fraction which is hard-coded (Appendix 2.3). Potential C decomposition is calculated as follows:

$$Potential_C_Decomposed = C_Mass_Org_Residue \times Contact_Fraction \times (1 - e^{(-Decomp_Constant \times Temperature_Function)}) \times Moisture_Function \quad (2.12)$$

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:

$$Decomp_Reduc_Fact = \frac{N_Immobilization_Demand - Deficit_For_Immobilization}{N_Immobilization_Demand} \quad (2.13)$$

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:

$$\text{Layer}_N\text{Nitrified} = \left(\text{NH}_4[i] - \frac{\text{NO}_3[i]}{\text{NO}_3\text{NH}_4\text{Ratio}} \right) \times \left(1 - e^{(-\text{Nitrification_Constant} \times \text{pH_Function} \times \text{Soil_Temperature_Function})} \right) \times \text{Nitrification_Moisture_Function} \quad (2.14)$$

where $\text{Nitrification_Constant} = 0.2$

$\text{Nitrification_Moisture_Function}$ is the same as the $\text{Soil_Water_Function}$ (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, denitrification is not assumed to occur on the following day. The Potential_Denitrification constant is hard-coded as $0.000032 \text{ kg N kg soil}^{-1} \text{ d}^{-1}$, and the *Denitrification Half Rate* is hard-coded as $0.00006 \text{ kg N kg soil}^{-1} \text{ d}^{-1}$. When a denitrification event does occur, Equation 2.15 is used to estimate the amount of NO_3^- lost through denitrification:

$$\text{Layer}_N\text{Denitrified} = \frac{\text{Potential}_\text{Denitrification}}{\text{Soil}_\text{Mass} \times \text{Denitrification}_\text{Factor}} \quad (2.15)$$

where the Denitrification_Factor is the minimum of:

$$\text{Re}_\text{piration}_\text{Re}_\text{ponse}_\text{Function} = \frac{\text{CO}_2\text{Loss}_\text{Per}_\text{Unit}_\text{Soil}_\text{Mass}}{\text{CO}_2\text{Re}_\text{piration}_\text{Threshold}} \quad (2.16)$$

$$\text{Nitrate}_\text{Re}_\text{ponse}_\text{Function} = \frac{\text{NO}_3\text{Conc}_\text{Dry}_\text{Soil}}{\text{NO}_3\text{Conc}_\text{Dry}_\text{Soil} + \text{Denitrification}_\text{Half}_\text{Rate}} \quad (2.17)$$

$$\text{Denitrification}_\text{Moisture}_\text{Function} = 1 \text{ (1st day)}, 0.5 \text{ (2nd day)} \quad (2.18)$$

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:

$$\text{Nitrogen_Fixation} = \text{Minimum}[\text{Crop_N_Demand} \times \text{N_Fixation_Factor}, \text{Min_Daily_N_Fixation_Mass}] \quad (2.19)$$

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

N_Fixation_Factor is the minimum of the following factors:

N_Fix_Temp Factor: 1 for temperatures $> 36^\circ\text{C}$

0.7 for temperatures between $0\text{-}36^\circ\text{C}$

0 for temperatures $< 0^\circ\text{C}$

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

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

$1 - \frac{\text{Root_Zone_N_Mass} - 100}{300}$ for root zone N masses

between $100\text{-}300 \text{ kg ha}^{-1}$ (2.20)

$$\text{N_Fix_Moisture_Function} = \frac{\text{PAW_Top_30} - 0.5}{0.5} \quad (2.21)$$

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:



$$\begin{aligned}
 \text{Labile_Active_P_Flux} &= 0.1 \times \text{Moisture_Function} \times e^{(0.115 \times \text{Soil_Temp} - 2.88)} \\
 &\times (\text{Labile_P} - \text{Active_P} \times \frac{\text{PAI}}{1 - \text{PAI}})
 \end{aligned}
 \tag{2.22}$$

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:

$$\text{Active_Stable_P_Flux} = \text{P_Flux_Coeff} \times (4 \times \text{Active_P} - \text{Stable_P})
 \tag{2.23}$$

where PFluxCoeff = 0.00076 for calcareous soils

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

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 NO₃⁻ and 5.6 for NH₄⁺. 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:

$$Root_Activity_Factor = 1 + 2 \times \left(1 - \left(\frac{Cumulative_Biomass}{Biomass_For_Increased_Root_Activity}\right)^3\right) \quad (2.25)$$

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:

$$Grain_N_Stress_Factor = \frac{N_Available_For_Distribution}{Grain_N_Demand} \quad (2.30)$$

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:

$$Crop_P_Uptake_Factor = (Labile_P+Banded_P) \times Active_Uptake_Factor \times Moist_Function \quad (2.31)$$

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:

$$Potenital_P_Uptake = Avail_P_Conc \times Layer_Transpiration \times Crop_P_Uptake_Factor \quad (2.32)$$

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

$$InitialAbstraction = 0.2 \times (SL_SaturatedWC - SurfaceLayerWC) \quad (2.36)$$

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

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

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

Finally actual soluble P runoff loss is calculated as follows:

$$RunoffLabileP = RunoffLabilePConc \times RunOff \quad (2.39)$$

2.2.5.5.2 Nitrogen

NH₄⁺ runoff losses are calculated as for P, except the partitioning coefficient is calculated using Equation 2.40:

$$NH4PartitionCoeff = 1.34 + 0.083 \times Clay\% \quad (2.40)$$

In the case of NO₃⁻, 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:

$$\text{Mobile_Solute_Concentration} = \frac{\text{Layer_Solute_Mass} \times \text{Solute_Mixing_Fraction}}{\text{Layer_VWC} \times \text{Layer_Depth} \times \text{WaterDensity}} \quad (2.41)$$

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 $1 - \gamma$ 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.

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