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.

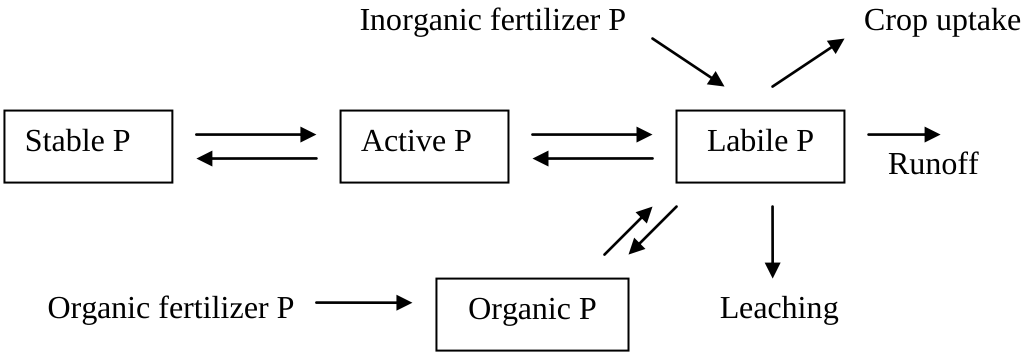

Figure 3.1 Structural diagram of the various P pools simulated using the EPIC approach

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:

$$\mathrm{BP1} = 1.23 \times \mathrm{AP} + 3.82 \tag{3.1}$$

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):

$$\mathrm{BP1} = 0.42 \times \mathrm{BP2} + 1.44 \tag{3.2}$$

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:

$$\mathrm{IP} = 1.49 \times \mathrm{BP1} + 1.07 \tag{3.3}$$

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[ɿ]	n/a		= 0.43CP + 4.21[†]		0.84
= 0.24BP2 + 5.9[ɿ]	n/a		= 0.64MP3 + 5.72[†]		0.71
= 0.38IP[*]+ 4.69[ɿ]	n/a		= 0.50AP + 7.12[ɿ]	n/a	
			= 0.17BP2 + 6.14[ɿ]	n/a	
Highly weathered	20		= 0.28IP + 5.25[ɿ]	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[ɿ]	n/a		P_{lab} = 0.69BP1 – 1.76[†]		0.35
= 0.059BP2 + 4.4[ɿ]	n/a		= 0.96OP – 0.19[†]		0.90
= 0.09IP + 4.1[ɿ]	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[ɿ]	n/a				
= 0.23BP2 + 6.89[ɿ]	n/a				
= 0.37IP + 5.70[ɿ]	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)

[ɿ] 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: $$\text{PAI} = 0.58 - 0.0061 \times \text{CaCO}_3 \quad (3.4)$$

Slightly weathered: $$\text{PAI} = 0.0054 \times \text{BaseSat\%} + 0.116 \times \text{pH}(\text{H}_2\text{O}) - 0.73 \quad (3.5)$$

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

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):

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

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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3.9 REFERENCES

ARNOLD JG, SRINIVASA R, MUTTIAH RS and WILLIAMS JR (1998) Large area hydrological modeling and assessment Part 1: Model development. *J. Am. Water Resour. Assoc*. **34** 73-89.

BUEHLER S, OBERSON A, RAO IM, FRIESEN DK and FROSSARD E (2002) Sequential phosphorus extraction of a 33P-labeled Oxisol under contrasting agricultural systems. *Soil Sci. Soc. Am. J.* **66** 868-877.

BURESH RJ, SMITHSON PC and HELIUMS DT (1997) Building soil phosphorus capital in Africa. In: Buresh RJ, Sanchez PA and Calhoum F (eds.). Replenishing soil fertility in Africa. *SSSA Special Publication Number 51*.111 pp.

BRAY RH and KURTZ LT (1945) Determination of total, organic, and available forms of phosphorus in soils. *Soil Sci.* **59** 39-45.

BUYS AJ and VENTER GCH (1980) Correlations between Bray 1, Bray 2 and ISFEI (Volume) soil-P extractants. *Fert. Soc. S. Afr.* **1** 13-18.

CAMPBELL KL, KIKER GA and CLARK DJ (2001) Development and testing of a nitrogen and phosphorus process model for Southern African water quality issues. ASAE Annual International meeting. *Paper No. 012085*, St. Joseph, MI.: ASAE.

CHANG SC and JACKSON ML (1957) Fractionation of soil phosphorus. *Soil Sci.* **84** 133-144.

COPE JT, EVANS CE and WILLIAMS HC (1981) Soil test fertility recommendations for Alabama crops. Alabama Agric. *Station Circular No. 251*.

GROENENDIJK P and KROES JG (1999) Modelling the nitrogen and phosphorus leaching to groundwater and surface water; ANIMO 3.5. *Report 144*. DLO Winand Staring Centre, Wageningen.

HENRY PC and SMITH MF (2003) The relationship between phosphorus requirement and some phosphorus characteristics of selected soils of the South African tobacco industry. *S. Afr. J. Plant Soil* **20** 18-24.

HENRY PC and SMITH MF (2004) An improved phosphorus desoprtion index for the routine determination of the Ambic 2 phosphorus requirement factor for South African soils. *S. Afr. J. Plant Soil* **21** 13-20.

JACKSON ML and SHERMAN GD (1953) Chemical weathering of minerals in soils. *Advances in Agron.* **5** 219-318.

JOHNSTON MA, MILES N and THIBAUD GR (1991) Quantities of phosphorus fertilizer required to raise the soil test value. *S. Afr. J. Plant Soil* **8** 17-21.

JONES CA, COLE CV, SHARPLEY AN and WILLIAMS JR (1984) A simplified soil and plant phosphorus model: I. Documentation. *Soil Sci. Soc. Am. J.* **48** 800-805.

KARPINETS TV, GREENWOOD DJ and AMMONS JT (2004) Predictive mechanistic model of soil phosphorus dynamics with readily available inputs. *Soil Sci. Soc. Am. J.* **68** 644-653.

KEATING BA, CARBERRY PS, HAMMER GL, PROBERT ME, ROBERTSON MJ, HOLZWORTH D, HUTH NI, HARGREAVES JNG, MEINKE H, HOCHMAN Z, MCLEAN G, VERBURG K, SNOW V, DIMES JP, SILBURN M, WANG E, BROWN S, BRISTOW KL, ASSENG S, CHAPMAN S, MCCOWN RL, FREEBAIRN DM and SMITH CJ (2003) An overview of APSIM, a model designed for farming systems simulation. *Eur. J. Agron.* **18** 267-288.

LAND TYPE SURVEY STAFF (1985) Land types of South Africa. ARC-Institute for Soil, Climate and Water, Pretoria.

MACVICAR CN, DE VILLIERS JM, LOXTON RF, VESTER E, LAMBRECHTS JJN, MERRYWEATHER FR, LE ROUX J, VAN ROOYEN TH and HARMSE HJ (1977) Soil Classification. A binomial system for South Africa. *Sci. Bull.* 390. Dept. Agric. Tech. Serv., RSA, Pretoria.

MCGECHAN MB and LEWIS DR (2002) Sorption of phosphorus by soil, Part 1: Principles, Equations and Models. *Bios. Eng.* **82** 1-24.

MEHLICH A (1984) Mehlich 3 soil test extractant: A modification of Mehlich 2 extractant. *Commun. Soil Sci. Plant Anal.* **15** 1409-1416.

MENGEL K (1997) Agronomic measures for better utilization of soil and fertilizer phosphates. *Eur. J. Agron.* **7** 221-233.

MYERS RG, SHARPLEY AN, THIEN SJ and PIERZYNSKI GM (2005) Ion-sink phosphorus extraction methods applied on 24 soils from the continental USA. *Soil Sci. Soc. Am. J.* **69** 511-521.

NEITSCH SL, ARNOLD JG, KINIRY JR, WILLIAMS JR and KING KW (2002) Soil Water Assessment Tool Theoretical Documentation. Grassland, Soil and Water Research Laboratory, Temple, Texas. *GSWRL Report* 02-01.

PROBERT ME (2004) A capability in APSIM to model phosphorus responses in crops. In: Delve RJ and Probert ME (eds.) Modelling Nutrient Management in Tropical Cropping Systems. Australian Centre for International Agricultural Research (ACIAR) Proceedings no. 114. 92-100 pp.

RADCLIFFE DE and CABRERA ML (2007) Suggestions to improve modeling of phosphorus. In: Radcliffe DE and Cabrera ML (eds.) *Modeling phosphorus in the environment.* CRC Press, New York, USA. 405-415 pp.

SCHMIDT CJJ, ADRIAANSE FG and DU PREEZ CC (2004) Relationships between Ambic 1 and Bray 1 extractable phosphorus in some South African soil. *S. Afr. J. Plant Soil* **21** 71-79.

SHARPLEY AN (2007) Modeling phosphorus movement from agriculture to surface waters. In: Radcliffe DE and Cabrera ML (eds.) *Modeling phosphorus in the environment.* CRC Press, New York, USA. 3-19 pp.

SHARPLEY AN, JONES CA, GRAY C and COLE CV (1984) A simplified soil and plant phosphorus model. II Prediction of labile, organic and sorbed phosphorus. *Soil Sci. Soc. Am. J.* **48** 805-809.

SHARPLEY AN, KLEINMAN PJA, MCDOWELL RW, GITAU M and BRYANT RB (2002) Modeling phosphorus transport in agricultural watersheds: Processes and Possibilities. *J. Soil Water Conserv.* **57** 425-439.

SHARPLEY AN, SINGH U, UEHARA G and KIMBLE J (1989) Modeling soil and plant phosphorus dynamics in calcareous and highly weathered soils. *Soil Sci. Soc. Am. J.* **53** 153-158.

SHARPLEY AN, TIESSEN H and COLE CV (1987) Soil phosphorus forms extracted by soil tests as a function of pedogenesis. *Soil Sci. Soc. Am. J.* **51** 362-365.

SHARPLEY AN and WILLIAMS JR (eds.) (1990) EPIC-Erosion/Productivity Impact Calculator: 1. Model Documentation. U.S. Department of Agriculture, Agricultural Research Service, Technical Bulletin No.1 768.

SINGELS A, ANNANDALE JA, DE JAGER JM, SCHULZE RE, INMAN-BAMBER NG, DURAND W, VAN RENSBURG LD, VAN HEERDEN PS, CROSBY CT, GREEN GC and STEYN M. Modelling crop growth and crop water relations in South Africa: Past achievements and lessons for the future. *S. Afr. J. Plant Soil, in press.*

SOIL CLASSIFICATION WORKING GROUP (1991) Soil Classification – a Taxonomic System for South Africa. *Memoirs on the Agricultural Natural Resources of South Africa No. 15*. Department of Agricultural Development, Pretoria.

THOMAS GW (1996) Soil pH and soil Acidity. In: Sparks DL, Page AL, Helmke PA, Loeppert RH, Soltanpour PN, Tabatabai MA, Johnston CT and Summer ME (eds.) Method of soil analysis. Part 3. Chemical methods. *SSSA Book Ser. 5*. SSSA, Madison, WI. 475-490 pp.

VADAS PA, KROGSTAD T and SHARPLEY AN (2006) Modeling phosphorus transfer between labile and nonlabile soil pools: Updating the EPIC model. *Soil Sci. Soc. Am. J.* **70** 736-743.

WATANABE FS and OLSEN SR (1965) Test of an ascorbic acid method for determining phosphorus in water and NaHCO3 extracts from soil. *Soil Sci. Soc. Am. J.* **29** 677-678.

WILLIAMS JR, RENARD KG and DYKE PT (1983) EPIC Erosion Productivity Impact Calculator: A new method for assessing erosion's effect on soil productivity. *J. Soil Water Conserv.* **38** 381-383.

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).

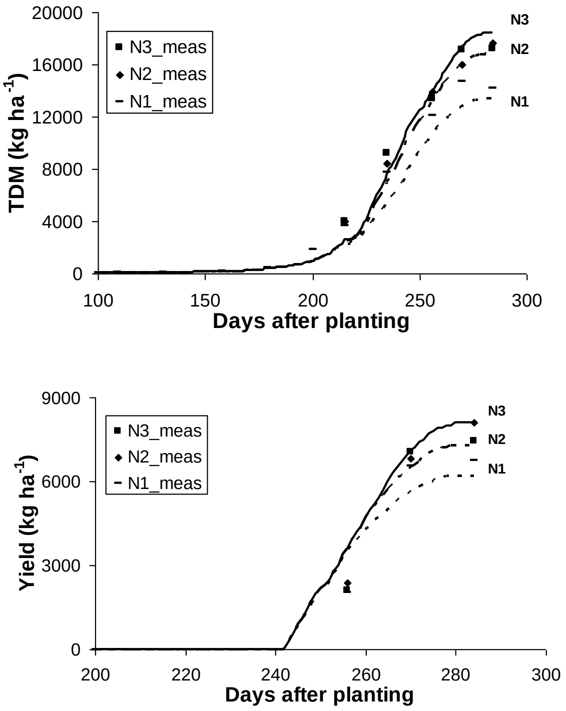

Figure 4.1 Total aboveground dry matter (TDM) and wheat grain yield for treatments N1, N2 and N3 for the 1983/83 growth season

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.

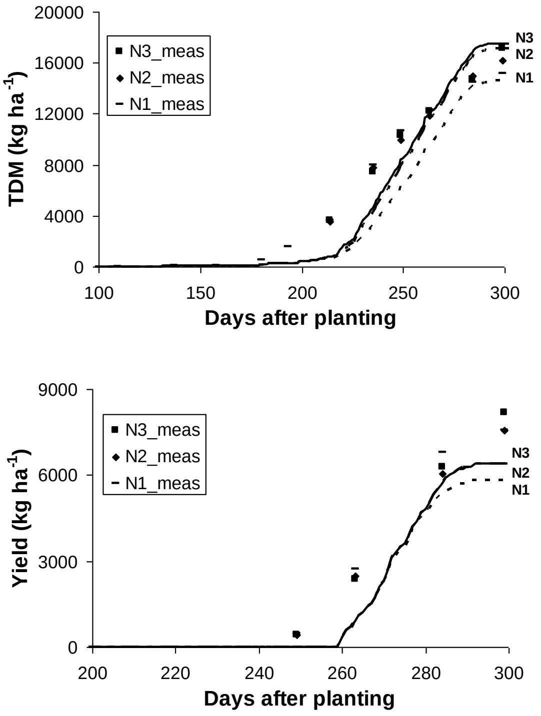

Figure 4.2 Total aboveground dry matter (TDM) and yield for treatments N1, N2 and N3 for the 1983/84 growth season

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.

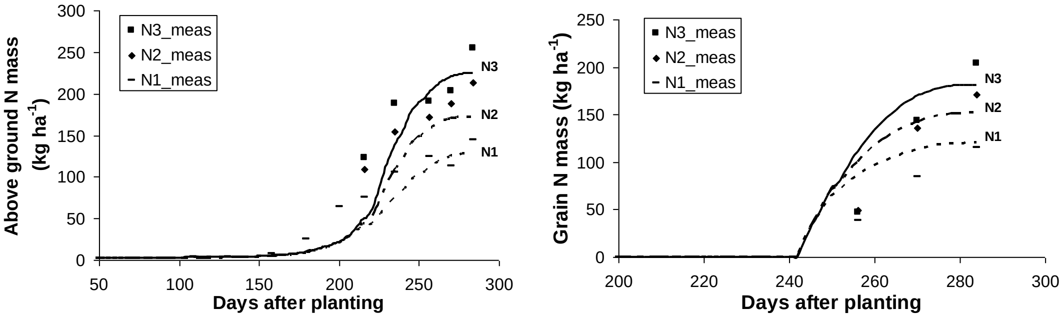

Figure 4.3 Aboveground N mass (left) and grain N mass (right) for the 1982/83 growth season

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.

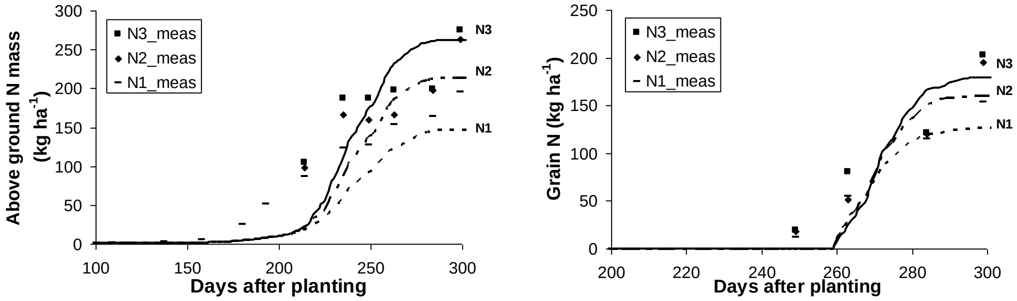

Figure 4.4 Aboveground N mass (left) and grain N mass (right) for the 1983/84 growth season

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.

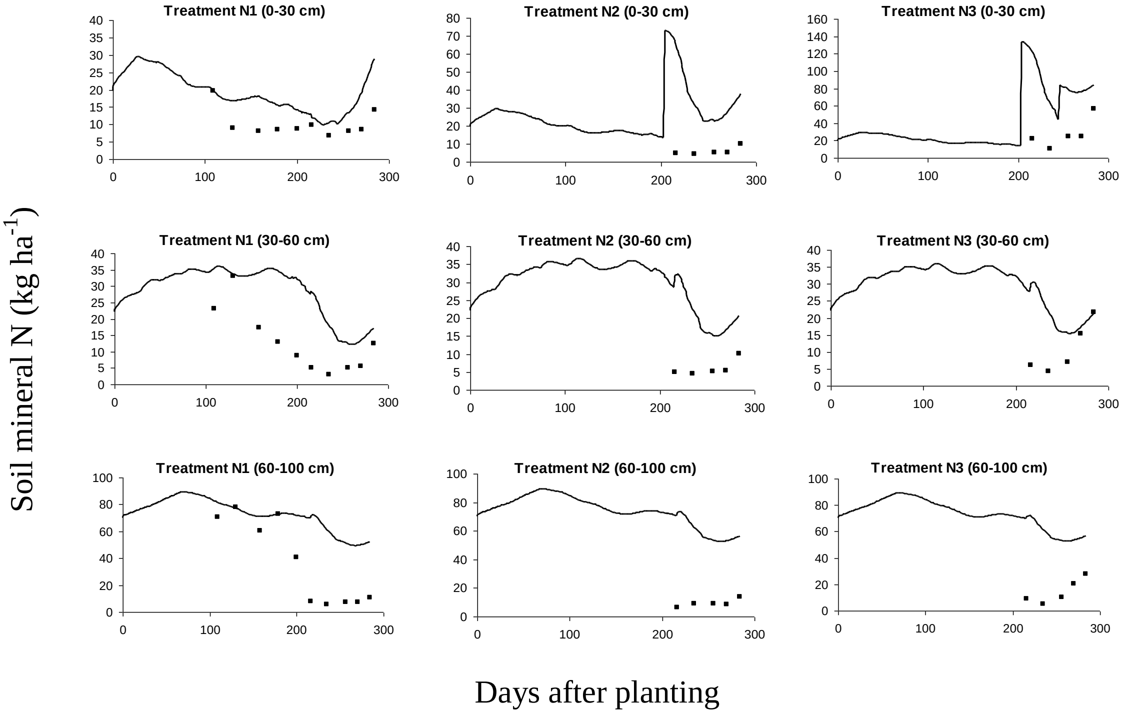

Figure 4.5 Soil mineral N content for the 1982/1983 growth season for treatments N1, N2 and N3 at depths of 0-30, 60-30 and 60-100cm

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.

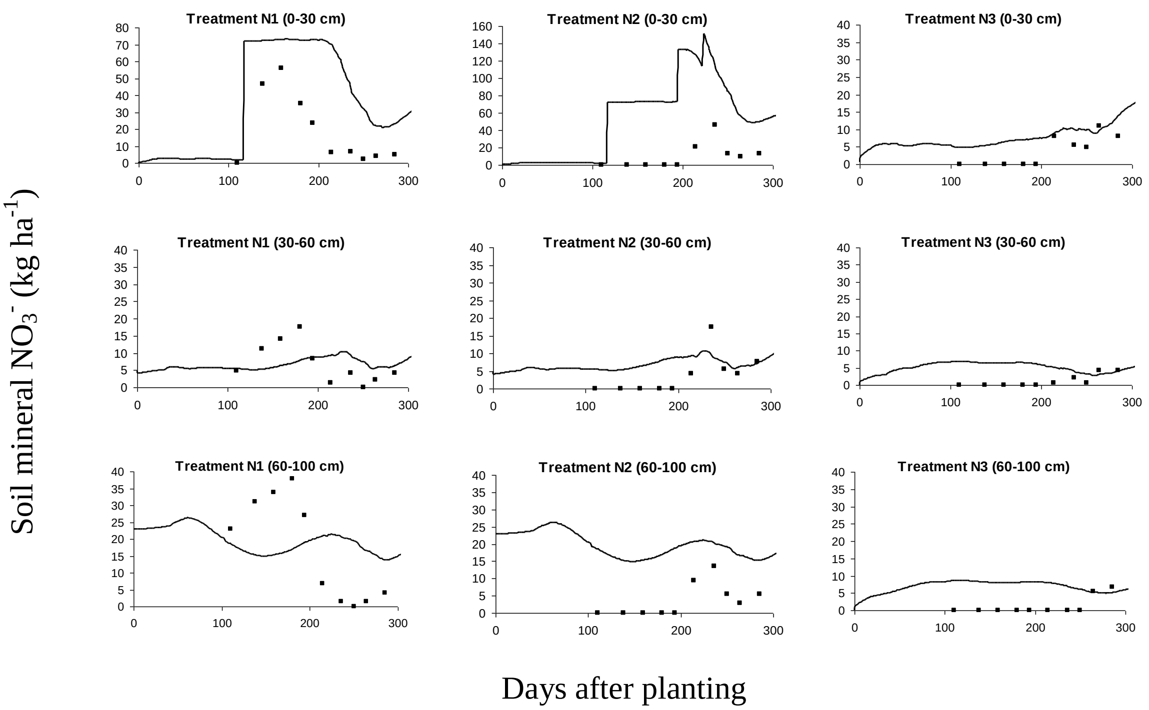

Figure 4.6 Soil NO_3^- content for the 1983/84 growth season for treatments N1, N2 and N3 at depths of 0-30 cm, 60-30 cm and 60-100cm

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).

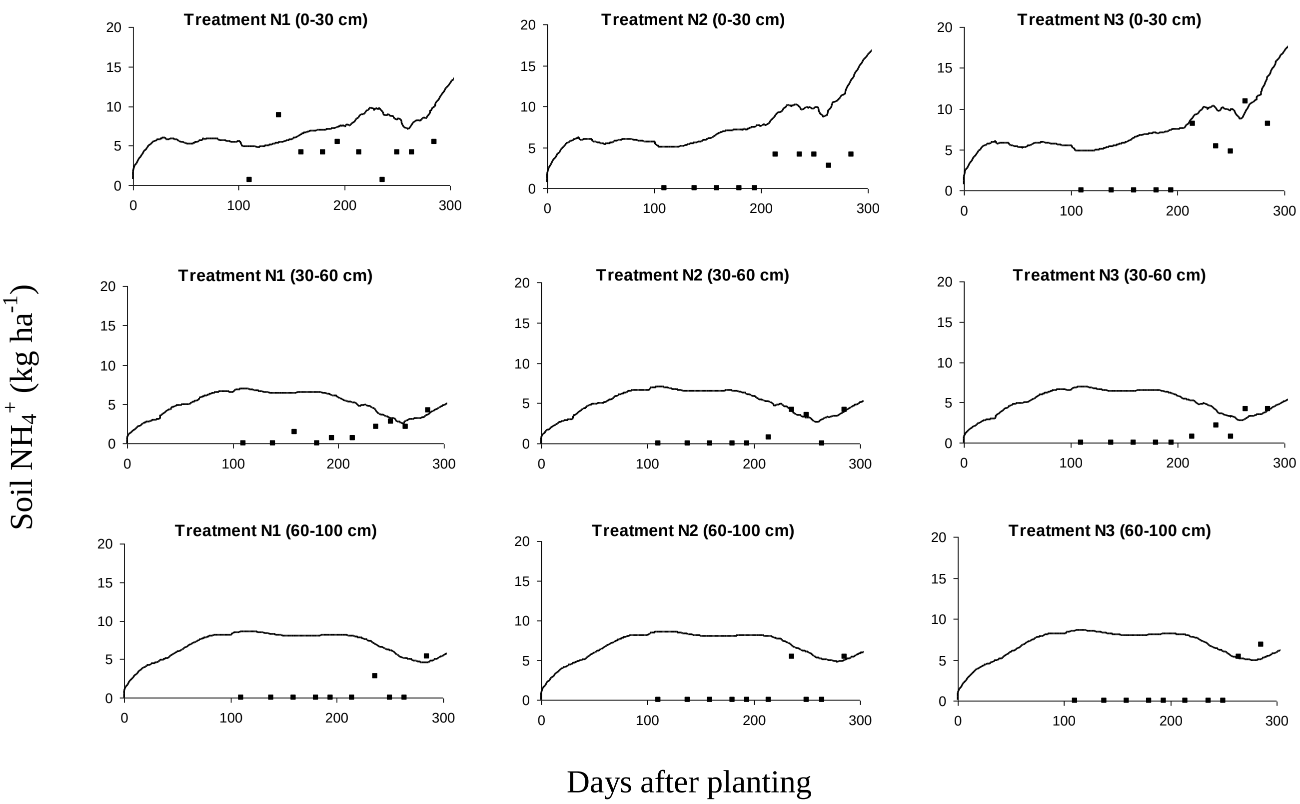

Figure 4.7 Soil NH_4^+ levels for the 1983/1984 growth season for treatments N1, N2 and N3 at depths of 0-30, 60-30 and 60-100 cm

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).

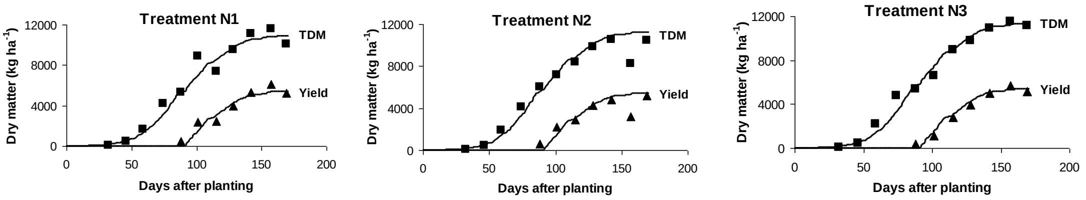

Figure 4.8 Total aboveground dry matter (TDM) and yield for treatments N1, N2 and N3

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.

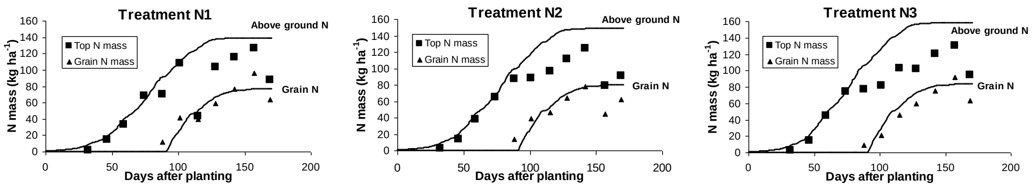

Figure 4.9 Aboveground and grain N mass for treatments N1, N2 and N3

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.

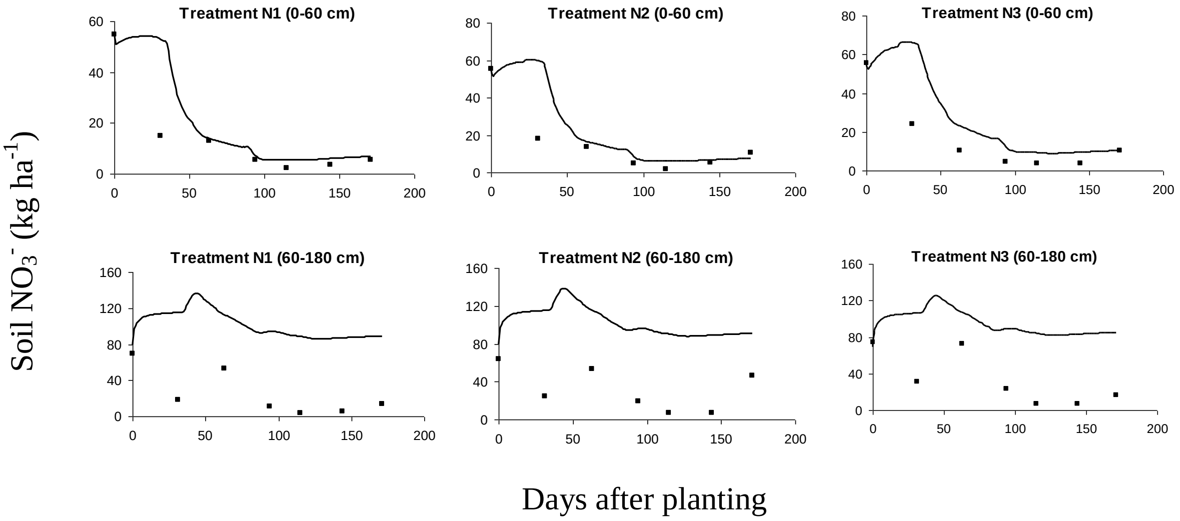

Figure 4.10 Soil NO_3^- content for treatments N1, N2 and N3 at depths of 0-60 and 60-180 cm

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.

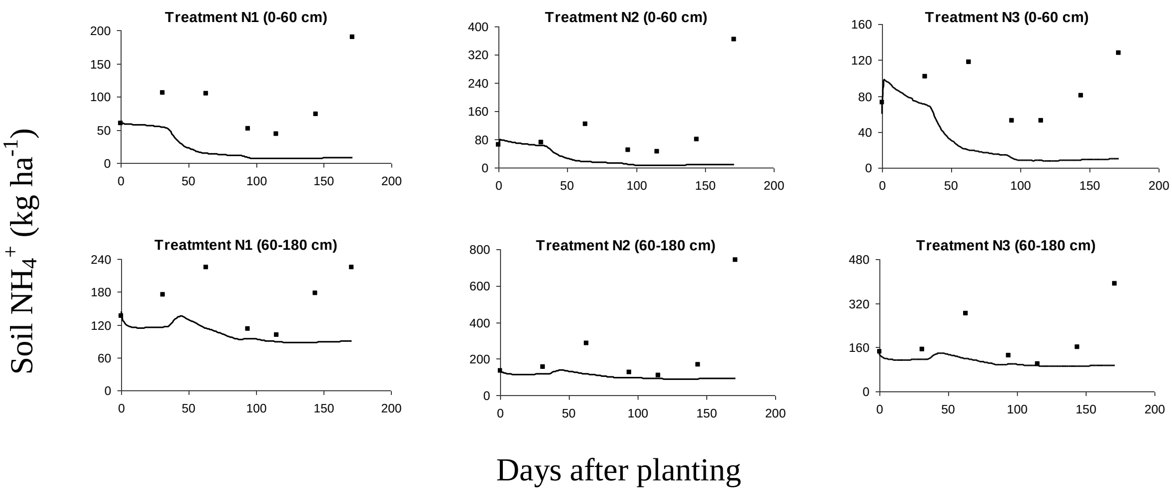

Figure 4.11 Soil NH_4^+ content for treatments N1, N2 and N3 at depths of 0-60 and 60-180 cm

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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4.7 REFERENCES

ADDISCOTT TM, BAILEY NJ, BLAND GJ and WHITMORE AP (1991) Simulation of nitrogen in soil and winter wheat crops: a management model that makes the best use of limited information. *Fert. Res.* **27** 305-312.

ANNANDALE JG, BENADE N, JOVANOVIC NZ, STEYN JM and DU SAUTOY N (1999a) Facilitating irrigation scheduling by means of the Soil Water Balance model. *WRC report No. 753/1/99*. Pretoria, South Africa.

ANNANDALE JG, JOVANOVIC, NZ, BENADE N and TANNER PD (1999b) Modelling the long term effect of irrigation with gypsiferous water on soil and water resources. *Agric. Ecosyst. Environ.* **76** 109-119.

ANNANDALE JG, JOVANOVIC NZ, CLAASSENS AS, BENADE N, LORENTZ SA, JOHNSTON MA, TANNER PD, AKEN ME and HODGSON FDI (2002) Modelling and monitoring crop production, soil properties and drainage water under centre pivot irrigation with gypsiferous mine water. *WRC Report No. K5/858.* Pretoria, South Africa.

ANNANDALE JG and DU PREEZ CC (2005) Nutrients – Agricultural contribution, management and modeling. In: Rossouw JN and Görgens AHM (eds.). Knowledge review of modelling non-point source pollution in agriculture from field to catchment scale. *WRC Report No. 1467/1/05,* Pretoria.

BELETSE YG (2004) Modelling the soil water and salt balance of irrigated pastures with sodium sulphate rich mine effluent. M.Sc. (Agric.) diss. University of Pretoria, Pretoria, South Africa.

BRADY NC and WEIL RR (1999) The Nature and Properties of Soils. 12th ed. Prentice Hall, New Jersey.

DE JAGER JM (1994) Accuracy of vegetation evaporation ratio formulae for estimating final wheat yield. *Water SA* **20** 307-314.

DE WILLGEN P (1991) Nitrogen turnover in the soil-crop system; comparison of fourteen simulation models. *Fert. Res.* **27** 141-150.

GROOT JJR and DE WILLIGEN P (1991) Simulation of the nitrogen balance in the soil and a winter wheat crop. *Fert. Res.* **27** 261-272.

GROOT JJR and VERBENE ELJ (1991) Response of wheat to nitrogen fertilization, a data set to validate simulation models for nitrogen dynamics in crop and soil. *Fert. Res.* **27** 349-383.

JOVANOVIC NZ, ANNANDALE JG and MHLAULI NC (1999) Field water balance and SWB parameter determination of six winter vegetable species. *Water SA* **25** 191-196.

KEATING BA, CARBERRY PS, HAMMER GL, PROBERT ME, ROBERTSON MJ, HOLZWORTH D, HUTH NI, HARGREAVES JNG, MEINKE H, HOCHMAN Z, MCLEAN G, VERBURG K, SNOW V, DIMES JP, SILBURN M, WANG E, BROWN S, BRISTOW KL, ASSENG S, CHAPMAN S, MCCOWN RL, FREEBAIRN DM and SMITH CJ 2003 An overview of APSIM, a model designed for farming systems simulation. *Eur. J. Agron.* **18** 267-288.

MULLER S and GREGORY J (2003) Ground Water Loading Effects of Agricultural Management Systems. University of Florida, Department of Agricultural and Biological Engineering.

NEITSCH SL, ARNOLD JG, KINIRY JR, WILLIAMS JR and KING, KW (2002) Soil Water Assessment Tool Theoretical Documentation. Grassland, Soil and Water Research Laboratory, Temple, Texas. *GSWRL Report 02-01*.

SCHMIDT CJJ (1993) Kwantifisering van die stikstofbalans op die Glen-Shorrocks gewasekotoop. Finale Projekverslag GB5111/32/8/10, Instituut vir Grond, Klimaat and Water, Pretoria.

SINCLAIR TR and SELIGMAN N (2000) Criteria for publishing papers on crop modeling. *Field Crop. Res.* **68** 165-172.

STOCKLE CO, DONATELLI M and NELSON R (2003) CropSyst, a cropping systems simulation model. *Eur. J. Agron.* **18** 289-307.

VAN KEULEN H, PENNING DE VRIES FWT and DREES EM (1982) A summary model for crop growth. In: Penning de Fries FWT and van Laar HH (eds.) Simulation of crop growth and production, pp 87-97. Pudoc, Wageningen.

VREECKEN H, VANCLOOSTER M and SWERTS M (1990) A model for the estimation of nitrogen leaching with regional applicability. In: R Merckx, H Vereecken and K Vlassak (eds.). Fertilization and the environment, pp 250-263. Leuven University Press, Leuven, Belgium.

VREECKEN H, VANCLOOSTER M, SWERTS M and DEIS J (1991) Simulating water and nitrogen behaviour in soils cropped with winter wheat. *Fert. Res.* **27** 233-234.

WILMOT CJ (1982) Some comments on the evaluation of model performance. *Bull. Am. Meteorol. Soc.* **64** 1309–1313.

YANG J, GREENWOOD DJ, ROWELL DL, WADSWORTH GA and BURNS IG (2000) Statistical methods for evaluating a crop nitrogen simulation mode, N_ABLE. *Agric. Sys.* **64** 37-53.