QUANTIFYING NITROGEN LEACHING IN WHEAT (*TRITICUM AESTIVUM*) USING LYSIMETERS, STABLE ISOTOPES, CONSERVATIVE TRACER AND MODELLING TECHNIQUES

by

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DECLARATION

I, Tapera Elias Mangwende declare that the dissertation, which I hereby submit for the degree MSc (Agric) Agronomy at the University of Pretoria, is my own work and has not been submitted by me for a degree at this or any other tertiary institution.

Signed: ……………………………

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LIST OF ABBREVIATIONS

AEC	Anion exchange capacity
APSIM	Agricultural Production System siMulator
APSRU	Agricultural Production Systems Research Unit
BD	Bulk density
Br^-	Bromide
C	Carbon
CEC	cation exchange capacity
CERES	Crop Environment REsource Synthesis
Cl-	Chloride
CropSyst	Cropping Systems Simulator
CSIRO	Commonwealth Scientific and Industrial Research Organisation
D	Index of agreement
D_r	Drainage
DAP	Days after planting
DCT	Divergence control tube
DNDC	Denitrification-Decomposition
DSSAT	Decision Support System for Agrotechnology Transfer
DUL	Drained upper limit
ET	Evapotranspiration
FNUE	Fertiliser N use efficiency
GS-GOGAT	glutamine synthatase–glutamate synthatase
HCL	Hydrochloric acid
HPO	Haloperoxidases

I	Infiltration
K_s	Saturated hydraulic conductivity
LAI	Leaf area index
LAN	Lime ammonium nitrate
L_i	Lateral inflow
LL	Lower limit
L_o	Lateral outflow
MAE	Mean absolute error
MCPA	2-methyl-4-chlorophenoxyacetic acid
N	Nitrogen
N_2	Dinitrogen gas
N_2O	Nitrous oxide
Ndff	Nitrogen derived from fertiliser
NH_3	Ammonia
NH_4^+	Ammonium
NO_2^-	Nitrite
NO_3^-	Nitrate
NO_3-N	Nitrate nitrogen
NO_x	Nitrogen oxide
P	Precipitation
R	Runoff
r^2	Square of the correlation coefficient
RMSE	Root mean square error
RUE	Radiation use efficiency

RZWQM	Root Zone Water Quality Model
SAT	Saturation
SC	sandy clay
SCL	sandy clay loam
SCs	Suction cups
SOILN	Soil nitrogen
SoilWat	Soil and Water
SOM	Soil organic matter
SPAW	Soil-Plant-Air-Water
SWB	Soil Water Balance
SWIM3	Soil Water Infiltration and Movement version 3
T	Tensiometer
TDM	Total above ground dry matter
UOM	unit of measurement
VPD	Vapour pressure deficit
VWC	Volumetric water content
WFDs	Wetting front detector
$\delta^{15}N$	Nitrogen with atomic mass of 15
ΔS	Change in soil water
‰	per milli

ABSTRACT

Nitrogen (N) leaching is one of the important pathways that leads to water pollution, and previous studies have highlighted the difficulty in measuring it. The purpose of this study was to evaluate different techniques used to quantify nitrate-N (NO_3-N) leaching load and determine fertiliser N use efficiency (FNUE). Lysimeter and field trial sites were planted with wheat (*Triticum aestivum*) (PAN3400 cultivar) at the University of Pretoria Experimental Farm, Hatfield, Pretoria. Two weighing lysimeters and a drain gauge were installed at the lysimeter trial site. Water content sensors and suction cups (SCs) were installed at 0.15, 0.3, 0.5 and 0.7 m depths in the weighing lysimeters and close to the drain gauge, while SCs, wetting front detectors (WFDs) and water content sensors were installed at 0.25 and 0.5 m in the field trial site. The crop was fertilised with 200 kg N ha^{-1} at both sites, but no fertiliser was applied on unfertilised control plots at the field trial site. High density drip irrigation was used at both sites, and bromide (Br^-) was applied to all field plots at 0.020 kg m^{-2}. Water was sampled from the SCs, WFDs and the bottom of weighing lysimeters and drain gauge to determine soil water NO_3-N and Br^- concentrations. Soil samples collected before and after the trial, and plant samples taken at tillering, flowering and physiological maturity were analysed for plant N% and stable ^{15}N natural abundance using a mass spectrometer. Phenological and growth data from the lysimeter trial were used to calibrate Agricultural Production Systems sIMulator (APSIM) model for the first time (according to our knowledge) on wheat in South Africa. The model was then validated using data from the field trial. The drain gauge drained more frequently and in greater amounts than the weighing lysimeters, and NO_3^- was observed in drainage water from the drain gauge, but was undetectable from the weighing lysimeters drainage possibly because of saturated bottom layer that promoted denitrification. Based on stable ^{15}N natural abundance, the FNUE was 68%, so the fertilised crop did not use 32% of the applied fertiliser. Good correlation was noted between the flag leaf and total plant N% at physiological maturity, indicating that flag leaf can be used to determine the FNUE without requiring whole plant analysis. The potential NO_3-N leaching determined using a Br^- conservative tracer was 51.5 kg ha^{-1} $season^{-1}$. In fertilised plots, the calibrated model predicted NO_3-N leaching of 22.7 kg ha^{-1} $season^{-1}$, which was slightly lower than the drain gauge measured NO_3-N leaching 24.9 kg ha^{-1} season. Therefore, the drain gauge

shows excellent promise in quantifying N leaching but will require further testing under a range of cropping systems. Since the measured drain gauge and simulated NO_3-N leaching agreed, and variables such as grain yield, total above dry matter, leaf area index and soil water content were reasonably simulated, the APSIM model can be applied to wheat cropping systems to improve N management decisions. The model confirmed that proper timing of N applications can reduce leaching losses, but further tests are required in several wheat growing agro-ecological zones to explore N management options that minimise N leaching losses. Even without measurements and/or modelling of N losses and crop uptake, results of this study for wheat indicate that the ^{15}N stable isotopes can be used on its own to estimate FNUE, but more studies from different soil types and on wheat varieties are required to verify the trends observed in this study.

INTRODUCTION

Nitrogen (N) is a major element limiting crop growth in most cultivated soils, and it is supplemented by an application of inorganic N forms (Fageria and Baligar 2005). High rates of N are used during commercial production poses a high risk of N export into aquatic systems (Ladha et al. 2005). Besides the environmental pollution and high cost of inorganic N that demands for better N management, poor fertiliser N use efficiency (FNUE) of less than 50% were still reported worldwide in several studies with annual crops (Smil 1999, Fageria and Baligar 2005, Edmonds et al. 2009, Cameron et al. 2013). Poor FNUE can be attributed partially to leaching, but N may also be made unavailable for plant uptake through immobilisation, or lost via volatilization, surface runoff and denitrification which make N studies complex (Ladha et al. 2005, Van der Laan 2009). Strategies to minimise N loss need further development due to a growing need for sustainable crop production. Furthermore, techniques to accurately measure and quantify field N loss are still lacking (Van der Laan et al. 2014).

Monitoring of water and N dynamics is central in sustainable crop production, and with the aid of crop models, they can improve the understanding of solute movement. Since N dynamics in the soil are still not yet fully understood (Van der Laan et al. 2010, Van der Laan et al. 2011, Van der Laan et al. 2014), more information about N leaching needs to be generated. Challenges to quantify the drainage and the corresponding N concentrations being leached out of the soil profile still exist (Van der Laan 2009, Van der Laan et al. 2010). Previously, research to evaluate N losses due to leaching using wetting front detectors and suction cups was done (Van der Laan et al. 2010), and was not able to equate concentration to respective solute and water fluxes. Since N concentration can be measured over time, the measured data can be incorporated into crop models such as APSIM (Agricultural Production Systems sIMulator) (Asseng et al. 1998, Keating et al. 2003) to simulate soil solute movement and establish the solute flux. Models are accessible and able to provide scenario analysis for various management options, which are usually resource, labour and time consuming if exclusively done as field experiments. Once models are calibrated, they can be used to evaluate the impacts

of N leaching for various agronomic strategies, so that the best management options can be adopted.

Another technique used to quantify N and water dynamics is the use of lysimeters. A lysimeter is a device used to measure and study water or solute movement in the soil profile (Martin et al. 1994, Martin et al. 2001). Essentially, the two main types of lysimeters consist of passive tension (wetting front detector, weighing lysimeters) and active tension (suction cups and wick drain gauges) (Weihermuller et al. 2007). Mostly, weighing lysimeters are permanently installed, which makes them unsuitable for studying solute and water transport in soils for a number of different sites (Martin et al. 2001, O'Kane and Barbour 2003). A wick drain gauge, Decagon G3, is now available commercially, which is portable and capable of measuring drainage, but its accuracy in different soils is unknown (Gee et al. 2009, Fisher 2012). These drain gauges need to be further tested against weighing lysimeters and other techniques to ascertain their accuracy. Besides their portability and versatility, drain gauges provide a cheaper option, and it has the advantage of being deployed at several research sites to measure N and water dynamics. In this study, the wick drain gauge will be referred as a drain gauge.

Solute dynamics can also be investigated using tracer techniques, for example conservative, natural isotopic abundance and labelled fertiliser (enriched or depleted forms) tracers. Bromide (Br^-) and chloride (Cl^-) are frequently used conservative tracers (Dusek et al. 2015, Frey et al. 2012, Schwen et al. 2014), as they do not interfere with plant growth and development (Tilahun et al. 2006, Wishkerman 2006). Bromide movement is unrestricted in soils with less dominant anion exchange capacity (AEC), and move more preferably in soils with high clay and organic matter content. Stable ^{15}N isotopes can potentially be used in N studies, as a quick and direct method to quantify N use efficiency and trace its fate in the soil profile (Adams and Grierson 2001, Evans 2001, Dawson et al. 2002, Van Cleemput et al. 2008, Cameron et al. 2013). As labelled (enriched or depleted) can contaminate the mass spectrometers if not properly used (Handley and Raven 1992, Handley and Scrimgeour 1997), ^{15}N natural abundance is often preferred as an alternative tracer

(Handley and Raven 1992). Spatial and temporal variability exhibited by ^{15}N natural abundance limit its use as a tracer, however, valuable information on N processes such as mineralisation, denitrification and leaching can be derived (Handley and Raven 1992).

The aim of the study was to evaluate different techniques (drain gauge, conservative Br$^-$ tracer, natural stable ^{15}N isotopes and modelling) used to quantify and predict NO$_3$-N leaching load, and to determine fertiliser N use efficiency (FNUE).

Hypotheses

i.   A drain gauge can accurately quantify deep drainage and NO$_3$-N leaching.
ii. Stable N isotope analysis techniques can provide an integrated measurement of FNUE, without needing to measure or estimate various N in and outflows in cropping systems.
iii. Conservative tracers can be effectively used to estimate potential NO$_3$-N leaching in a soil.
iv. Measurements of volumetric water content and NO$_3$-N concentration over time from soil water content sensors, SCs and WFDs can accurately estimate leaching loads when combined with a mechanistic model.

Objectives

i.   To compare the performance of a drain gauge to a calibrated weighing lysimeter in measuring deep drainage and NO$_3$-N leaching.
ii. To determine the FNUE of a wheat crop using stable ^{15}N isotope analysis.
iii. To quantify potential NO$_3$-N leaching using a conservative tracer.
iv. To evaluate and validate the performance of APSIM after calibration with experimental data to simulate soil water and N dynamics.

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CHAPTER 1: LITERATURE REVIEW

1.1 Introduction

Knowledge on water and nitrogen (N) dynamics is essential to sustainably produce crops and reduce the export of this nutrient to aquatic environments. A key factor in the export of N to the environment is failing to fully utilise applied N (Ladha et al. 2005, Lamb et al. 2014). Poor fertiliser N use efficiency (FNUE), fertiliser recovered by plants from total applied, of less than 50% is often reported globally for annual field crops (Raun and Johnson 1999, Smil 1999, Brye et al. 2003, Fageria and Baligar 2005, Gu et al. 2016), and it is mostly attributed to leaching losses, although inorganic N is also lost via volatilization, denitrification, and surface runoff, or transformed into plant unavailable N through immobilisation. The various N loss pathways complicate N studies, yet detailed information on N balance is required to increase knowledge and formulate effective strategies to counter N nonpoint source pollution.

Nitrogen studies are required to address key production and pollution challenges, so that high quality crops are produced, while also aimed at reducing the detrimental nutrient loading that pollutes the environment. Most agricultural soils are deficient of N, and cultivated plants benefit from N application, as it is required for high biomass accumulation (Cambui et al. 2011). A lot of work has been done and shown that N is required in several plants' metabolic activities, as it forms a basic constituent of chlorophyll, enzymes, proteins and genetic material (Baligar et al. 2001, Delgado et al. 2006). However, there are also several pitfalls associated with mismanaging N use. These challenges include deteriorating water quality, eutrophication, greenhouse gas emission and loss of biodiversity (Nye 1986, Chen et al. 2014, Sainju et al. 2016). Therefore, a gap still remains to quantify N processes that determine N availability and distribution in cultivated soils (Bojović and Marković 2009), so that production and environmental costs can be reduced.

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Since several N transformation processes occur in agricultural soils, precise quantification of N loss is difficult, especially of nitrate (NO_3^-) leaching (Van der Laan 2009, Van der Laan et al. 2011, Van der Laan et al. 2014). The N cycle complexity in cultivated soil means that pragmatic approach is required to determine the contribution of individual N processes (Oelmann et al. 2007), so that N dynamics can be quantified. Therefore, in this chapter N dynamics will be reviewed with a specific interest on ways to evaluate N leaching using lysimeters, conservative tracers, stable isotopes and crop models.

1.2   Field lysimeters

Lysimeter are devices used to measure and study water or solute movement in a soil profile (Martin et al. 2001), and they are grouped into two main types which are passive and active suction lysimeters. The passive suction can be classified as pan, for example, wetting front detector and free draining weighing lysimeters, and the active suction are also classified into static tension e.g. suction cups and controlled tension, for example, use constant/varying vacuum. Although there are several types of lysimeters, the most used are weighing and static tension lysimeters (Abichou et al. 2006, Goss et al. 2010), which are shown on Figure 1.1.

1.2.1   Passive tension lysimeters

1.2.1.1   Weighing lysimeters

A weighing lysimeter is a tank used to measure the amount of water transpired by vegetation and can also determine the movement of water and chemicals (Martin et al. 2001). A weighing lysimeter consists of a cell filled with soil, preferably with an undisturbed soil core, which will be resting on a balance (Figure 1.1). The cell may have a load cell, which can be connected to a data logger, so that data collection and monitoring is automated. According to Howell et al. (1985), weighing lysimeters can be sub-classified into continuous or intermittent weighing. The main difference between the continuous and intermittent weighing lysimeter is the time when the measurement is taken, logging system capturing weight changes at very short intervals (even every second) are usually used for a continuous weighing system,

but an intermittent weighing ones will be weighed occasionally, mostly on a daily or weekly basis.
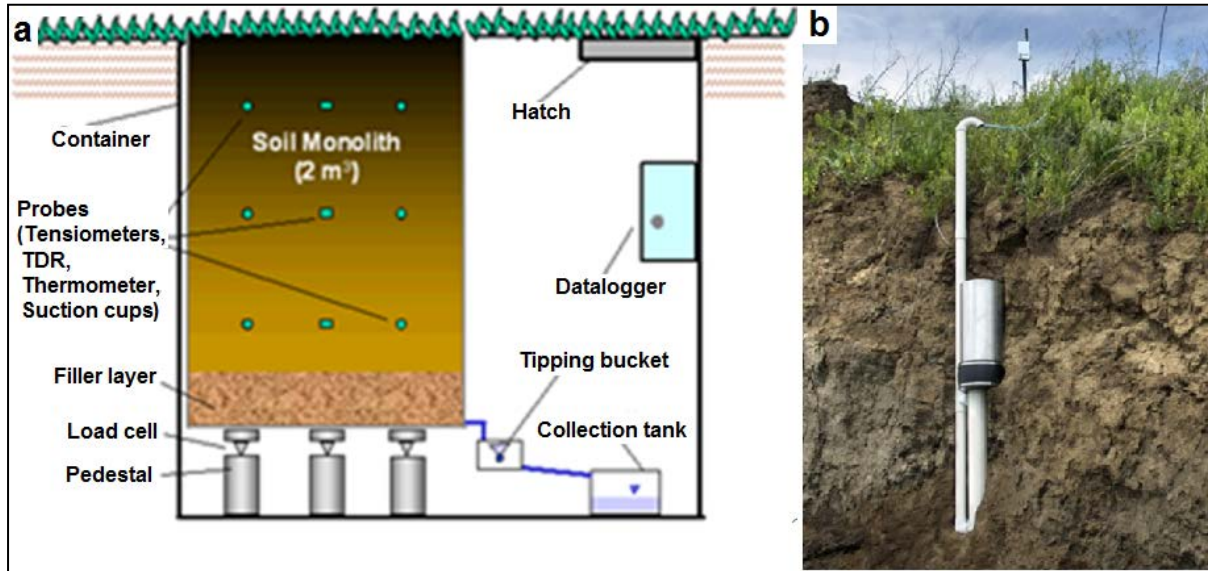
Figure 1.1: Two main types of lysimeters (a) Weighing lysimeter (Meissner and Seyfarth 2004) and, (b) Decagon G3 drain gauge (static tension lysimeter). A detailed diagram of a Decagon G3 drain gauge with labelled parts, is given on Figure 1.2.

Weighing lysimeters are good at getting the water balance right, as it can measure all the components of the soil water balance equation (Equation 1.1), and solute leaching is determined by analysing the draining component. The ET is measured daily or even at a shorter time interval, as changes in soil mass and related to water losses after accounting for precipitation and drainage because on weighing lysimeters runoff and lateral flow are considered to be zero.

$$\Delta S = P + I + ET + R + D_r + L_i + L_o \qquad (1.1)$$

where: ΔS is change in soil water, P is precipitation, I is infiltration, ET is evapotranspiration R is runoff, D_r is drainage, L_i is lateral inflow, and L_o is lateral outflow.

There are several studies that have used weighing lysimeters to evaluate NO_3^- leaching in various crops. Goss et al. (2010) reviewed nitrate (NO_3^-) leaching losses from various studies conducted on lysimeters around the globe, and they found that climatic factors, tillage practices and N sources were most influential on N leaching. For example, high rainfall received during crop establishment and after harvesting in the fallow period before planting another crop was associated with high leaching rates (Martin et al. 1994, Owens et al. 1995, Dietrich et al. 2016). Tillage practices also were found to influence the amount of leaching, as a no till system was found to reduce total NO_3^- leaching by 21% compared to conventional tillage systems in the first year of cropping (Goss et al. 1993). Gu et al. (2015) used two different sources of fertilisers (manure and urea) which were applied at a rate of 90 and 180 kg N ha^{-1} on a lysimeter, and two irrigation regimes of 350 and 500 mm were used on wheat (*Triticum aestivum* L.) grown over three seasons. They found that under stressed irrigation of 350 mm per season there was no drainage in both fertiliser source treatments, but with normal irrigation of 500 mm, 3.4 to 15.3% of applied N was leached. The depth of leaching was deeper with urea after three year, as nitrate-nitrogen (NO_3-N) was observed in the 1.0-2.0 m soil depth, yet with manure NO_3-N leaching was only detected at the 0.0-0.75 m depth. Increased leaching with high rates of inorganic fertiliser and drainage has been reported by several authors irrespective of crop type or sequence used (Boll et al. 1992, Poss et al. 1995, Young et al. 1996, Goss et al. 2010). Goss et al. (2010) concluded that weighing lysimeters have helped in shaping the knowledge of the amount of NO_3-N loss in soils, and how it is correlated to soil type, draining amount and fertiliser source.

Notwithstanding the potential accuracy of weighing lysimeters, matching of the lysimeter soil conditions to adjacent field soil conditions is difficult (O'Kane and Barbour 2003, Gee et al. 2009). There are reports of artificial soil conditions created in lysimeters, for example, a saturated bottom layer. The saturated soil creates anaerobic conditions which may cause denitrification of NO_3^- (Bergström 1990). As the size of a lysimeter increases, back filling becomes difficult. Normally, an intact soil core is required to mimic the real field conditions, but back filling of large field weighing lysimeters disturbs the soil. Unfortunately, the soil disturbance during repacking of lysimeters results in increased mineralisation when settling in, which

overestimates NO_3^- leaching from the soil for a new installation (Lord and Shepherd 1993). The other weakness of weighing lysimeters is that they do not account for lateral flow (Weihermüller et al. 2007), especially on heavy textured soil where it is dominant. The sides of the lysimeter are usually straight preventing lateral flow, but allow the establishment of preferential flow paths (Schoen et al. 1999). Hence, there is need for caution when interpreting weighing lysimeter data.

1.2.1.2 Wetting front detector

A wetting front detector (WFD) is another type of a passive lysimeter (Figure 1.2). It can indicate soil moisture front during irrigation, as it has an indicator that can pop up when soil water content saturates and collects in the funnel buried in the soil profile (Stirzaker 2005).
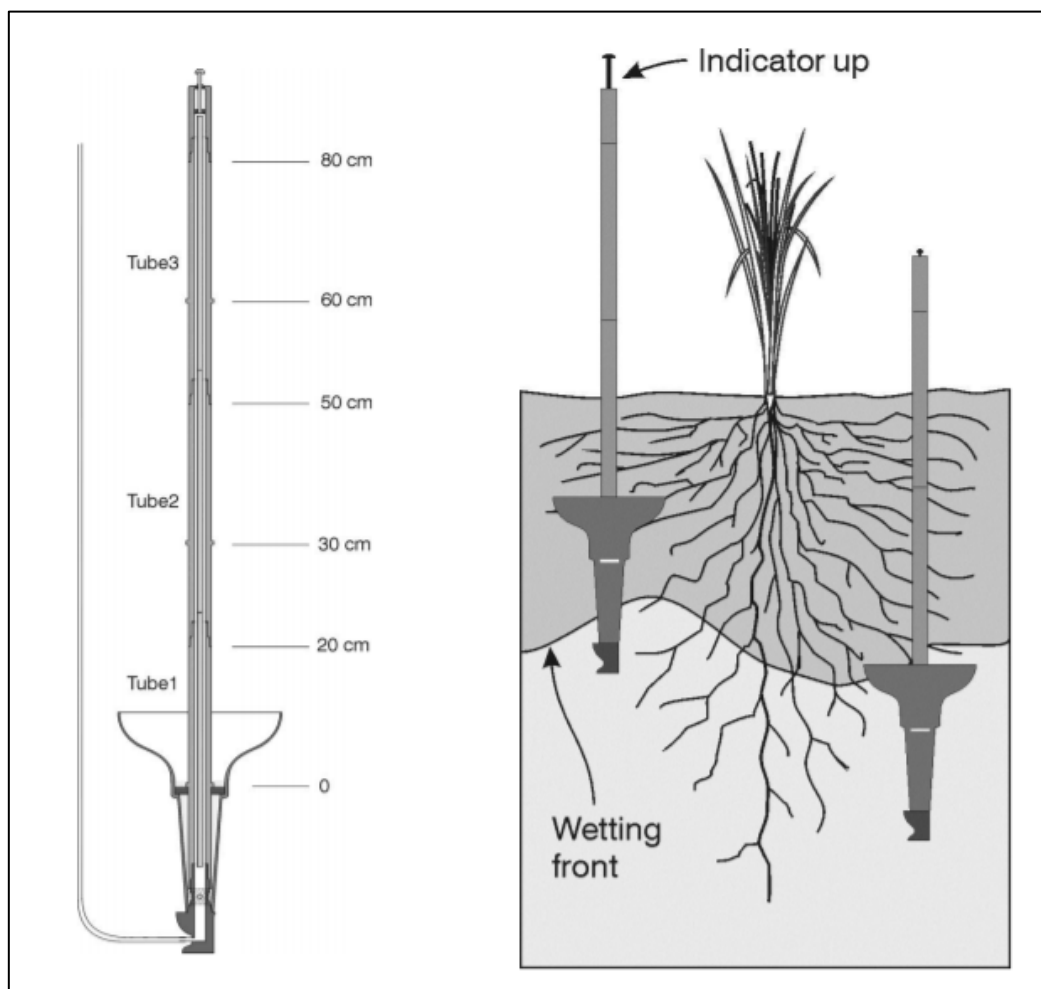
Figure 1.2: a. Schematic side view of a wetting front detector (WFD), b. WFDs installed in a field at various depths to monitor wetting front when irrigating (Agriplas 2014).

Wetting front detectors can be used to aid irrigation water scheduling since they can specify when to stop irrigation by popping up when placed under the root zone (Annandale et al. 2011). A water sample can also be collected and analysed for salt and NO_3^- concentration, which make WFDs suitable for studying soil solute movement at various depths (Stirzaker 2005). However, they cannot measure the leaching loads, as the solute flux is difficult to measure (Van der Laan 2009). Van der Laan et al. (2010) highlighted that WFDs can be used to estimate solute concentration in the draining water from the soil macropores, but they were unable to measure the solute concentration in the soil micropores.

1.2.2 Active tension lysimeters

1.2.2.1 Wick drain gauge

Static tension lysimeters use constant tension to imbibe leachate, for example the use of a fiberglass wick on a drain gauge. The water sample is collected as a result of suction generated by the wick and gravitational pull (Holder et al. 1991). The level of soil unsaturation produced by the wick depends on wick length and diameter, soil type and flux intensity (Zhu et al. 2002, Mertens et al. 2007). There are various types of wicks such as fiberglass, nylon, glass rope, and rock wool (Brown et al. 1986, Ben-Gal and Shani 2002). Fiberglass wicks are normally used in N dynamics studies because they do not adsorb the NO_3^- (Weihermüller et al. 2007).

Drain gauges have been found to be good at collecting leachate (Gee et al. 2009), and can have advantages over weighing lysimeters in some cases. For example, the Decagon G3 drain gauge (Decagon Devices, Inc., Pullman, USA) has been found to have good sample collection on medium textured soil, but not on light and heavy textured soils (Gee et al. 2009). In a drain gauge, the wick is placed in the divergence control tube (DCT) black ring below the diatomaceous earth (Figure 1.2a). The wick produces a suction that maintains an unsaturated soil condition,

which allows water to continuously flow into the drain gauge, unlike the most weighing lysimeters where the bottom layer is saturated (Gee et al. 2009). Since the DCT's opening has a known surface area (506.7 cm^2), the drainage can be calculated by dividing volume collected and the surface area, and drainage is divided by collection time to obtain a flux. Being able to measure the flux makes the drain gauge ideal in N leaching studies, as the flux is difficult to measure using suction cups and wetting front detectors (Van der Velde et al. 2005, Van der Laan 2009, Van der Laan et al. 2010, Van der Laan et al. 2012). The collected water sample settles in the tube which is below the DCT, and the conductivity, temperature and depth (CTD) sensor located in the reservoir under the DCT will capture the temperature (^{o}C), electrical conductivity (EC in mS cm^{-1}) and drainage (mm) (Decagon Devices Inc. 2015).
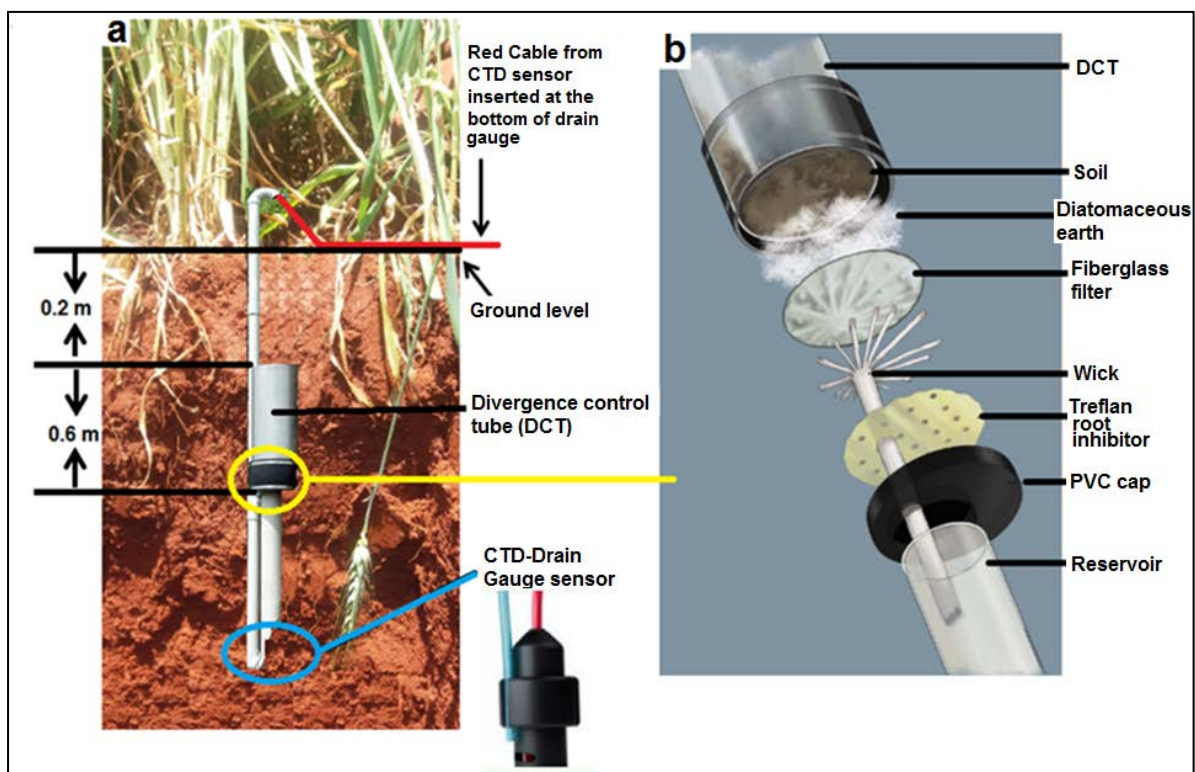
Figure 1.3: a) Decagon G3 drain gauge installation schematic diagram, b) enlarged divergence control tube (DCT). Adapted from Decagon Devices Inc. (2015).

Basso and Ritchie (2005) used tubes inserted into a fine loamy soil profile, the tubes were like a DCT but without a wick, planted with a maize (*Zea mays* L.) and alfalfa (*Medicago sativa* L.) rotation. The study evaluated NO_3-N leaching for six years. Inorganic fertiliser (urea), manure and compost were applied at 260 kg ha^{-1}, 18 t ha^{-1} and 30 t ha^{-1}, respectively. The treatments with manure had the highest NO_3-N leaching of 113.5 kg ha^{-1}, followed with compost at 65.0 kg ha^{-1}, and lastly urea with 58 kg ha^{-1}. The manure treatment had the highest NO_3-N leaching because of high mineralisation early in the season, which was greater than plant uptake and led to more leaching. For urea treatments, the applications were split and resulted in lowering the NO_3-N leaching by half, whereas the compost is slow to mineralise, so resulted in lower NO_3-N leaching than manure treatments. Although un-wicked drain gauges have been proven to work, there are also reports of convergence of water into the DCT under unsaturated conditions, or divergence when conditions are saturated which can bias the collected sample (Gee et al. 2009).

1.2.2.2 Suction cups

Suction cups are another type of static tension lysimeters (Figure 1.3), and are widely used worldwide (Zotarelli et al. 2007, Gu et al. 2016). The suction from suction cups can be as high as 50 to 80 kPa (Weihermüller et al. 2007). Van der Laan et al. (2010) pointed out that suction cups most likely reflect the NO_3^- concentrations in the soil mesopores. But the addition of such a high suction has been a basis for unresolved debate among authors, as the suction creates unnatural soil conditions that influence water and solute flow (Weihermüller et al. 2007). However, the effect and extent of matric potential created by suction cups used to be unknown (Hart and Lowery 1997), and some speculated that they collected water samples from big pores only and not from the finer pores (Hansen and Harris 1975, Hart and Lowery 1997). Weihermüller et al. (2005) illustrated how suction cups extract water samples using the HYDRUS model, and proved that the area where sample was extracted increased in soil with high hydraulic conductivity, but reduced when infiltration rate was high. The authors also observed that the activity domain of the suction cups was influenced with duration of extraction.

Suction cups can show the leachate concentration, but are not capable of estimating the flux (Weihermüller et al. 2007, Van der Laan 2009). Zotarelli et al. (2007) evaluated the NO_3^- concentrations from suction cups, soil cores, and weighing lysimeters on various vegetable crops. Suction cups obtained the lowest NO_3^- concentrations. Despite the concentration differences, all the methods displayed the same leaching pattern on sandy soils. Nonetheless, the suction cups are easy to install, monitor, and maintain. Suction cups are also cheap, which has promoted their wide adoption and use (Weihermüller et al. 2007).
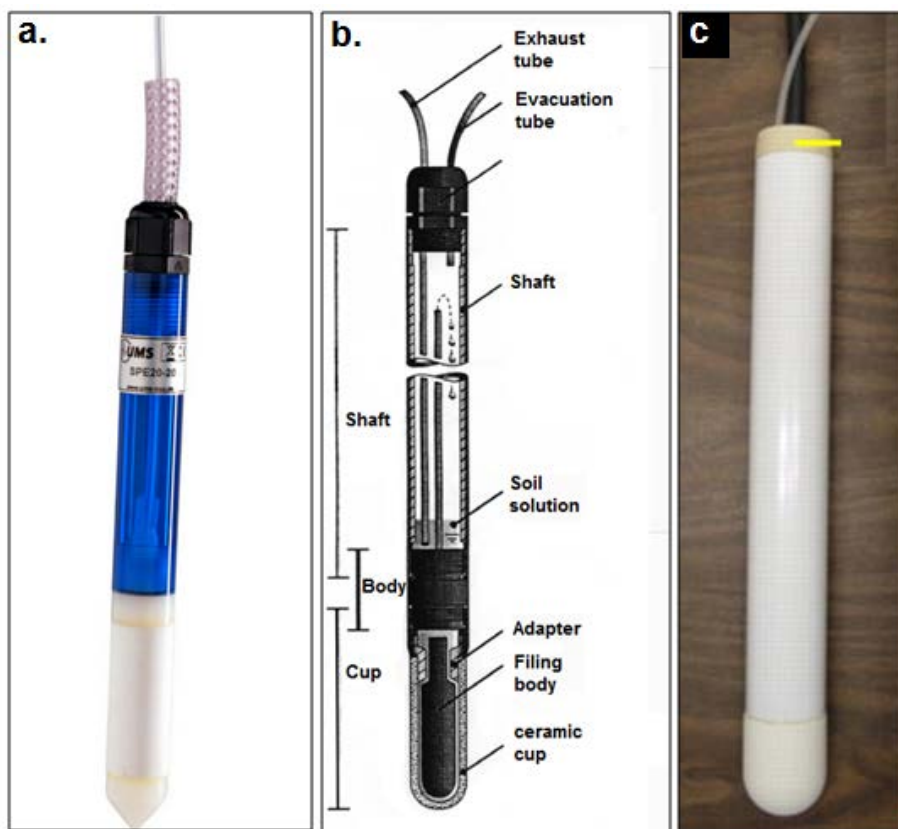
Figure 1.4: (a) SPES20 (Teflon) suction cups, (b) schematic diagram for a SPES20 and (c) ceramic suction cup.

1.2.3 Concluding remarks on lysimeters

Weighing lysimeters provide more information on the soil water balance and N movement than any other types of lysimeters. Hence, new methods or equipment are verified against a weighing lysimeter. Lysimeter measurements may not be

conclusive, therefore, the deep drainage data has to be compared with numerical modelling outputs for validation (O'Kane and Barbour 2003). For example, weighing lysimeters can influence the water and N movement, and in such cases, adjustments are required especially when the depth does not allow full root development and free drainage of water. Van der Laan et al (2014) highlighted the need for continuous NO_3^- data collected from suction cups, drain gauge, and weighing lysimeters to improve simulation with various models to increase confidence and improve quantification of N dynamics on cultivated soils.

1.3   Conservative tracer techniques

Several N chemical transformations occur naturally in the soil profile, which makes it difficult to establish the potential N leaching of the soil. In such cases, bromide (Br^-) is used as a conservative tracer as it does not undergo any transformation (Onken et al. 1977, Clay et al. 2004, Wishkerman 2006). Gilley et al. (1990) observed that Br^- was not adsorbed onto soil sediment of various soil types in soil columns under laboratory conditions, hence allowing it to be used extensively to mimic NO_3^- movement in the soil.

Bromide is a cheap, non-degradable, soluble salt, and non-toxic to mammals at low concentrations (Maw and Kempton 1982, Flury and Papritz 1993). It can be quantitatively measured at very low concentrations (Gilley et al. 1990), which makes it an attractive tracer, and most cultivated soils have a low Br^- background concentration. Flury and Papritz (1993) reported a critical concentration of 1 mg Br^{-1} L^{-1} to be safe for human consumption, and this threshold concentration is seldom reached or surpassed in most field experiments.

Low plant uptake of Br^- make correction factors unnecessary in most soils, therefore, it is mostly used to characterise soil flow rates (Tilahun et al. 2004, Tilahun et al. 2006). Bromide is not an essential element used during plant growth and development, although some studies have reported luxury uptake depending on crop type (Wishkerman 2006). Other studies reported Br^{-1} uptake by plants with low

background concentrations (0.06-0.031 mg kg^{-1}), and this was shown to increase with fertiliser application containing traces of Br$^-$, or when sodium bromide (NaBr) was used as tracer in water and solute studies (Gan et al. 1998, Yates et al. 2003). Tilahun et al. (2006) used Br$^-$ as a 'worst case scenario' to simulate NO$_3^-$ leaching, and a total of 8.1% (10.9 kg ha^{-1}) of the total Br$^-$ applied was taken up by maize (*Zea mays* L.), plants. Although an uptake range of 8-10% of the applied Br$^-$ was reported in several studies (Gish and Jury 1982, Iragavarapu et al. 1998) on maize, the results from other studies report different Br$^-$ uptake depending on crop type. For example, Br^{-1} uptake of less than 3.5% of the applied Br^{-1} (197 kg ha^{-1}) was observed in oats (*Avena sativa* L.), alfalfa (*Medicago sativa* L.) (Iragavarapu et al. 1998), and in wheat (*Triticum aestivum* L.) it was less than 2% (Jury et al. 1982).

Of particular interest, experiments conducted in South Africa confirmed similar Br$^-$ and NO$_3^-$ movement in the soil (Tilahun et al. 2004). Smith and Davis (1974) illustrated that Br$^-$ and NO$_3^-$ had identical flow patterns in the subsoil (0.61-0.76 m) as they have similar charge, although notable differences were found in the upper soil layers (0.0-0.15 m), it was attributed to high NO$_3^-$ microbial activity in top layers than in the subsoil. Therefore, such work elaborates that Br$^-$ movement can be used to represent potential N leaching.

Recently, there has been evidence that Br$^-$ reacts with soil organic matter (SOM) during the humification process through halogenation to form Br$^-$ complexes (Cortizas et al. 2016). The process of halogenation of SOM is catalysed by haloperoxidases (HPO), and in the case of Br$^-$, they are called bromo-HPO (Ballschmiter 2003). Although the process is prevalent when lignin in the SOM is decomposed into humic substances and react with bromo-compounds to form aliphatic and aromatic organo-brominated forms (Leri and Myneni 2012, Leri and Ravel 2015), substantial amounts only accumulate after a long period (thousands of years) in cultivated soils (Cortizas et al. 2016) because of low background Br$^-$ concentrations. Halogenation process cannot affect localised Br$^-$ tracer experiments running for short periods, one to two seasons. Leri and Myneni (2012) concluded that the Br$^-$ reactivity with SOM compromises its usefulness as a hydrological tracer,

but it is still widely used as a conservative tracer in soil columns or field plots (Patra and Rego 1997, Wang et al. 2010, Dusek et al. 2015, Bero et al. 2016).

1.4 Use of stable isotopes to determine fertiliser use

1.4.1 Understanding fertiliser N use efficiency (FNUE)

Quantifying fertiliser N use efficiency (FNUE) is essential to improve the N uptake by plants and limit the N losses (Baligar et al. 2001, Fageria and Baligar 2005, Delgado et al. 2006, Edmonds et al. 2009). Fertiliser N use efficiency is the ratio of plant N uptake compared to applied N. In other words, FNUE is used when the N is derived from fertiliser. The ratio is useful to explain N utilisation, although it does not show the source of N, for instance N derived from mineralisation. Kundu and Ladha (1995) reported that soil reserves supply 50 to 80% of the plant N requirement and the remainder will be supplied from inorganic fertiliser N. Some of the applied inorganic N can be immobilised, volatilised or leached, hence, more information is required to quantify N that is mineralised and supplied to the plants. As a result, the FNUE can be calculated by tracing and analysing stable isotopes ($^{14}N/^{15}N$), which will be able to differentiate various N sources (fertiliser, mineralised or fixed N) (Kriszan et al. 2007, Flores et al. 2011). If N sources are accounted for, then individual N processes like mineralisation can be quantified.

1.4.2 Using stable isotopes in N studies to understand N dynamics

Nitrogen exists in different atomic masses that are ^{13}N, ^{14}N, ^{15}N, ^{16}N and ^{17}N but occurs naturally and abundantly in the atmosphere as ^{14}N and ^{15}N. The natural abundance ratio of $^{14}N/^{15}N$ is 99.634:0.366, and any deviation from this ratio can be traced with changes in ^{15}N abundance as being increased/enriched or decreased/depleted, and it is calculated using Equation 1.2 (Peterson and Fry 1987). The variation in ^{15}N abundance is expressed in δ units (parts per thousand - ‰) and measured using a mass spectrometer (Handley and Raven 1992). The soil N transformations are enzyme mediated processes and discriminate heavier ^{15}N in the soil (Mordelet et al. 1996, Högberg 1997, Robinson et al. 1998), and ^{15}N accumulates or depletes depending on how N is transformed. Therefore, monitoring

[15]N abundance in the soil gives an indication of soil N transformation processes and how they occur in the soil (Handley and Raven 1992). These variations in soil natural abundance ratios can be detected in plants, as they do not discriminate ^{15}N when extracting any form of N from the soil media (Evans 2001, Vose 2013). Furthermore, the leaching kinetics of ^{14}N and ^{15}N was tested in undisturbed soil columns and no significant differences were observed for the same amounts allowed to leach through the same soil profile (Clay et al. 2004), which means that changes in soil ^{15}N abundance is correlated to N transformation not the difference between leaching rates of ^{14}N and [15]N.

$$\partial X\%_0 = \frac{R_{sample} - R_{standard}}{R_{standard}} \times 1000 \qquad (1.2)$$

Where $\delta X = {}^{15}N$ or ^{13}C and R represents $^{15}N/^{14}N$ or $^{13}C/^{14}C$

Natural ^{15}N abundance technique has been mostly applied in ecological studies to monitor N movement in forest soil profiles (Högberg 1997, Adams and Grierson 2001, Watzka et al. 2006, Priyadarshini et al. 2015), but the technique can also be applied to field crops (Bedard-Haughn et al. 2003, Choi et al. 2003, Wrage et al. 2005, Zhou et al. 2013, Lemesle et al. 2016). For example, Choi et al. (2003) and Wei et al. (2013) used ^{15}N stable isotopes to evaluate the distribution of $\delta^{15}N$ values in plants applied with inorganic fertiliser or compost, and observed that plants grown in composted soils had higher $\delta^{15}N$ values compared to those grown with inorganic fertilisers. In another study, Kriszan et al. (2007) analysed $\delta^{15}N$ values from a lysimeter study grown with grass for 22 years, and found that $\delta^{15}N$ values were correlated to type of fertiliser and N losses. Mordelet et al. (1996) observed that most vegetation was depleted and the soil was enriched as depth increased, they reported +2.5, +5.2 and +6.1‰ in the 0-10, 10-20 and 20-40 cm depths, respectively.

In spite of considerable work that has been done with stable isotopes on field crops focusing on effects of different management practices on soil ^{15}N and plant ^{15}N distribution, the results have been inconsistent and difficult to interpret (Kriszan et al. 2007). The plant $\delta^{15}N$ variation was suggested to show different growth patterns which can be correlated to N uptake by plants (Adams and Grierson 2001, Evans

2001), and to certain extent gives information on N metabolic pathways within the plants. During plant N metabolism, there is discrimination of ^{15}N that leads to enrichment or depletion of δ^{15}N values. Such fluctuation of δ^{15}N values in different plant parts is also related to plant N demand, and N applications during periods of high N demand not only optimise FNUE, but also limit N leaching (Wienhold 2007, Flores et al. 2011, Giagnoni et al. 2016, Tuan et al. 2016).

1.5 Use of crop models to determine leaching loads

Currently, there is an impetus to facilitate crops to fully exploit applied N, for reducing cost and pollution caused by N losses to the environment. Soil water, crop rotations, tillage, soil microbes, SOM and climatic factors regulate the behaviour of soil N dynamics (Probert et al. 1998). For example, several authors have demonstrated that well managed irrigation scheduling can reduce deep drainage and associated leaching loads (Annandale et al. 2011, Poch-Massegú et al. 2014, Liu et al. 2015). Even though N cycle processes are known, there is still poor understanding of how N moves in the soil profile (Van der Laan 2009, Van der Laan et al. 2014, Roux et al. 2016), and to accurately calculate leached N.

Hence, ways to accurately estimate and predict N leaching are required, yet they remain elusive to researchers. In a review paper, Van der Laan et al. (2014) pointed out the unavailability of a commonly used method to evaluate N losses, and they also highlighted the significant role that modelling can play in predicting N movement in the soil. As model outputs depend on quality of data, calibration and validation are prerequisites before they can be confidently used. But calibrations often fall short because there is no standard method that can accurately measure N leaching (Van der Laan 2009, Van der Laan et al. 2011, Van der Laan et al. 2014).

1.5.1 Overview of models used to simulate soil N leaching

Since several crop models simulate crop growth, they tend to simulate above ground parameters better that below ground ones, which contribute to in-accurate estimates of N losses (Van der Laan et al. 2014). Despite the importance of N loss information,

a few models have N modules that simulate soil N dynamics considering all N transformation processes (McCown et al. 1996). The most commonly used models include the Agricultural Production System sIMulator (APSIM) (Keating et al. 2003b), the Decision Support System for Agrotechnology Transfer (DSSAT) (Jones et al. 2003), the Denitrification-Decomposition (DNDC) (Li et al. 2006), the Cropping Systems Simulator (CropSyst) (Stöckle et al. 2003) and the Root Zone Water Quality Model (RZWQM) (Hanson et al. 1999). Most models were developed in environments different to where they will be used, which make parameterisation, calibration, and validation essential to get meaningful results.

Understanding the mechanisms that govern N movement in the model is important to simulate N losses accurately. For example, Li et al. (2006) reported over-estimation of NO_3^- leaching with the original DNDC model because it failed to retard NO_3^- movement, and adopting the Langmuir Equation (Li et al. 2006) to cater for adsorption and desorption of NH_4^+ improved simulated NO_3^- concentrations to agree with observed tile drain concentrations. Furthermore, after running the same model, Li et al. (2014) observed increasing N losses with increased fertilisation and irrigation water application rates. However, it is not practically possible to do field trials for all possible water and N application rates because of resource and time scarcity. These and other problems consolidate the need for crop modelling to assist estimating N loss, and therefore, best N management.

Addiscott and Wagenet (1985) and Feyen et al. (1998) reviewed various solute leaching approaches, and highlighted the challenges of limited datasets to test models over a wide range of environments other than for which they were developed. Data unavailability cripples modelling efforts in South Africa, and comprehensive long term data sets for parameterisation and validation process must be collected (Van der Laan et al. 2014). Silva et al. (2005) also proved the need for long term N leaching monitoring, as annual and biannual NO_3^- leaching patterns depended on various factors. Therefore, continual monitoring is the best solution (Van der Laan et al. 2014), so that seasonal leaching trends can be ascertained. However, the necessary data to make direct and specific meaningful management

guidelines on N is unavailable for several crops and production regions in South Africa, and crop modelling can be used as a guide to estimate N losses for a wide range of agro-ecosystems. In this review, the APSIM model will be discussed further as it was the model used in this study.

1.5.2 Agricultural Production Systems sIMulator (APSIM)

APSIM is a mechanistic crop model, and it is extensively used (Asseng et al. 2002, Ahmed et al. 2016). The model has been under continual construction and upgrading, but it was notably redesigned to incorporate subroutines for crop growth, soil water and soil N, two decades ago (McCown et al. 1995). APSIM has been used on over 30 crops, and in complex cropping systems, such as crop rotations (Wang et al. 2002; Keating et al. 2003).

When simulating soil water and solute movement, two main sub modules can be used which are SoilWat (Soil and Water) and SWIM3 (Soil Water Infiltration and Movement version 3) (Huth et al. 2012). SoilWat inherited most of its functionality from the CERES (Crop Environment REsource Synthesis) model (Jones et al. 1986), and from infiltration and runoff algorithms derived for the PERFECT model (Littleboy et al. 1992). SoilWat uses a cascading tipping bucket approach simulating upward and downward movement of water and solutes (Reddy 1983), and requires an 'efficiency factor' to regulate the amount of solute leaving each soil layer under unsaturated transient flow (Huth et al. 2012, Van der Laan et al. 2014). SWIM3 is available in APSIM from version 7.3 and above (Huth et al. 2012). It simulates water and solute movement on a daily time step, by solving numerically the Richards's Equation for soil water movement and the convection-dispersion equation for solute movement (Holzworth et al. 2014). Although simulating N leaching using SWIM3 is supposed to yield better results, at least in theory, the cascade approach is used widely. The tipping bucket approach is more commonly used because it is simpler and easier to parameterise than, especially previous versions of SWIM that required large site-specific data sets (Huth et al. 2012).

APSIM can also be used to simulate N dynamics, as it can predict various N transformations in the soil. APSIM's SoilN subroutine is used to simulate soil N processes in greater detail than other generic crop models because it has a liable organic N pool which was added to the original CERES N routine (Probert et al. 1998; Dimes and McCown 1992; Thorburn et al. 2005). As shown on Figure 1.3, there are various pools of organic matter in APSIM which are presented as pool 1 (BIOM), pool 2 (HUM), inert OM (INERT) and pool "i" (FOM), and are cycled between the surface plant residues, fresh plant material and soil mineral N. These modifications enable APSIM to simulate N dynamics and N leaching, as they take into account most of the N processes. Stewart et al. (2006) used APSIM to simulate water and NO_3^- leaching in sugarcane fields. The rate and time to irrigate regulated deep drainage and leaching, and APSIM showed increasing N losses with excess irrigation and high fertiliser rates. Nonetheless, it is still uncertain how the model will predict N leaching under South African wheat cropping systems.
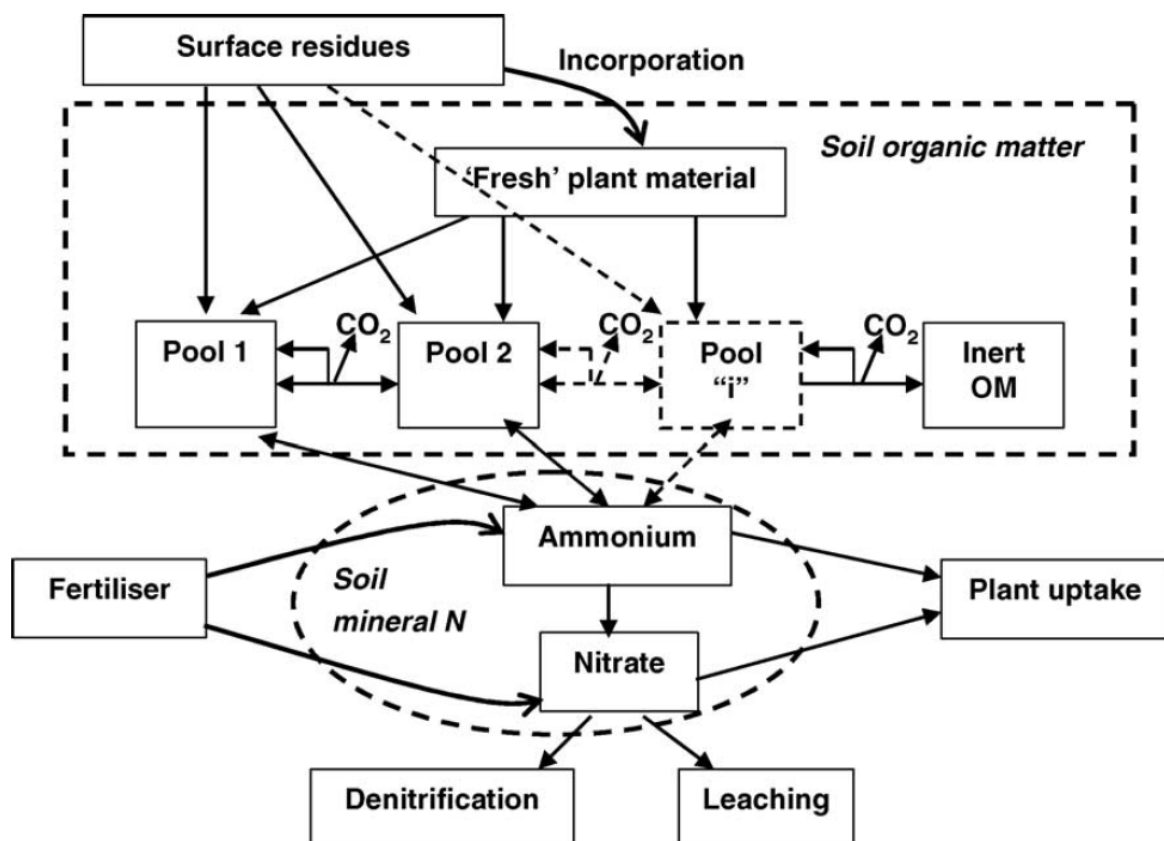
Figure 1.5: A simplified model of soil carbon (C) and nitrogen (N) processes and transformations used to describe C and N dynamics, showing surface residues, soil organic matter and mineral N in the soil, with

varying numbers (1 to ''i'') of sub-pools within the soil organic matter pool (Thorburn et al. 2005).

APSIM has a simple user interface, and is relatively easy to parameterise and get started. Besides being user friendly, APSIM has a stable, reliable and easy to maintain code receiving constant updates. APSIM was created for semi-arid tropical regions of Australia and Africa (McCown et al. 1995), which make it ideal for application to South African conditions. However, APSIM was mainly designed to simulate crop management options under dryland conditions, but it has been successfully used to simulate crop and N dynamics under irrigated cropping systems (McCown et al. 1996, Thorburn et al. 2001, Power et al. 2011).

Although models are useful and provide insights into different management options, caution must be taken when making deductions and applying these models beyond the environmental limits of calibration (Holzworth et al. 2011). For instance, when simulating extreme drought, salinization, and acidification, careful analysis of model outputs is advised. Some processes are not simulated at all in APSIM, such as nitrite leaching (NO_2^-) or NO_3^- adsorption even after liming, which reduce the confidence of the simulated output (Huth et al. 2012, Van der Laan et al. 2014).

The model also requires skilled personnel to be applied extensively, and it is considered intellectual property, therefore, it is maintained and distributed by Agricultural Production Systems Research Unit (APSRU) only, an affiliate of Commonwealth Scientific and Industrial Research Organisation (CSIRO) in Australia (Meinke et al. 1996). Such controlled access can be beneficial in keeping the integrity of the code, but can be detrimental to fast paced code improvement and development which may compromise user experience.

1.6   Conclusions

Fertiliser use continues to increase, which makes it mandatory to invest considerable effort to curb N losses and improve FNUE. Previously developed techniques, such as use of lysimeters and conservative tracers, provide measured data required as model inputs, but such datasets are not long enough to observe the trends of N movement. Nonetheless, this literature review has highlighted the need to improve the quality of datasets through continuous monitoring of soil N concentrations and water content. On the other hand, measured data can be used as input data in models. Integrating the methods will help improve the understanding of N dynamics, as a result, accurate N leaching predictions will be possible to consolidate crop management practices that reduce N losses. Although use of stable isotopes seems promising, the method has to be mastered and developed further for it to be applied with confidence on various field crops.

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CHAPTER 2: EVALUATING THE PERFORMANCE OF A COMMERCIAL DRAIN GAUGE AGAINST A FIELD WEIGHING LYSIMETER TO MEASURE DEEP DRAINAGE AND NITROGEN LEACHING

2.1 Introduction

Nitrogen (N) is the most applied element in crop production (Raun and Johnson 1999, Silgram and Shepherd 1999, Smil 1999). The cereal crops maize (*Zea mays* L.), wheat (*Triticum aestivum* L.) and rice (*Oryza sativa* L.) are the world's most produced crops and account for most of the applied N (Ladha et al. 2005). Although cultivars suited for high N rates have been bred, they still fail to recover and utilise all the applied N (Raun and Johnson 1999, Smil 1999). Hence, N losses have to be managed, as farming activities have often resulted in declining water quality and eutrophication, although it is still unclear on exactly how these activities contribute to non-point source (NPS) pollution to aquatic systems (Rossouw and Görgens 2005, Görgens et al. 2012). Nitrogen from cultivated land is lost through runoff, leaching, volatilisation and denitrification. Considering all ways that N can be lost, N leaching is considered among the major pathways in which it is lost from the soil (Delgado et al. 2006, Sainju et al. 2016), and the main cause of groundwater pollution with nitrate (NO_3^-) (Gheysari et al. 2009). Therefore, leaching in cultivated lands has to be quantifiable, so as to find mitigatory measures.

Nitrogen leaching has been measured using various types of lysimeters, though with limited success. Martin et al. (2001) defined a lysimeter as any device used to measure and study water or solute movement in the soil profile. Commonly, two main types of lysimeters are used, which are: passive tension (for example, wetting front detectors) and active tension (for example, suction cups or wick tension lysimeters). Despite the various types of lysimeters that are in use, there is still no widely acceptable and reliable method used to quantify N leaching accurately (Van der Laan 2009, Van der Laan et al. 2014). The major challenge is that to either estimate or calculate N leaching, N concentration and flux are required (Van der

Laan et al. 2010), with flux being challenging to measure and high uncertainties surrounding the measured pore water NO_3^- concentrations. Previously, several studies conducted using suction cups failed to fully estimate solute flux accurately (Gee et al. 2009, Van der Laan 2009).

Suction cups and weighing lysimeters are most commonly used in solute movement studies (Martin et al. 2001, Fisher 2012, Yang et al. 2014). Field weighing lysimeters are usually expensive to install and maintain (Bowman et al. 2002), and they are bulky and permanently fixed which limit their application. Besides being flexible and portable, suction cups and wick tension lysimeters, like ceramic cups and commercial drain gauges (for example, Decagon G3 drain gauge), provide cheaper alternatives, as they can be used at several research sites to measure water drainage and estimate N leaching. A commercial drain gauge has now been designed to measure both the solute concentration and flux, but its accuracy needs to be ascertained. Therefore, further testing of the equipment is essential.

In this study, the performance of a commercial drain gauge (G3) in measuring drainage and nitrate-nitrogen (NO_3-N) leaching was compared against a weighing lysimeter by assessing drainage outputs under an irrigated winter wheat crop.

2.2 Materials and Methods

The experiment was conducted at the University of Pretoria Hatfield Experimental Farm (25°44'58.53'' S, 28°15'31.60''E, and elevation 1371 m) (Appendix 4), and the profile soil properties of the site are given on Table 2.1. The trial site, measured 400 m^2 with several installed instruments (Appendix 5). After repairing the weighing lysimeters, new equipment was installed consisting of: a rain gauge (Texas Electronic Inc., Dallas, Texas, USA) and a new load cell (Load Cell Services, South Africa), for each lysimeter. A commercial drain gauge (Decagon G3 drain gauge, Decagon Devices, Inc., Pullman, USA) was purchased in August 2015, and was installed five metres away and to the east of the field weighing lysimeters. The base of the drain gauge divergence control tube (DCT) was inserted into the soil in such a

way that the measurement depth was at 0.9 m. The DCT was installed using the undisturbed soil core approach (Figure 1.1).

Table 2.1: Selected soil properties of the lysimeter and field trial soil at the University of Pretoria Experimental Farm.

Parameter	UOM[a]	Lysimeter Trial Depth (m)			Field Trial Depth (m)		
		0.00-0.20	0.20-0.40	0.40-0.60	0.00-0.20	0.20-0.40	0.40-0.60
Organic carbon	%	1.12	0.70	0.54	0.63	0.61	0.51
Organic matter	% wt	1.7	1.9	2.2	1.5	1.5	1.5
pH (water)	log($[H^+]$)	6.6	6.9	7.1	6.1	6.6	5.8
Total N	mg kg^{-1}	29.0	24.0	28.0	11.4	6.9	11.4
NO_3-N	mg kg^{-1}	13.0	11.0	9.0	7.7	5.1	9.5
NH_4-N	mg kg^{-1}	16.0	13.0	19.0	3.6	1.8	1.9
Sand	%	64.0	57.0	58.0	72.0	64.6	57.7
Silt	%	13.0	18.0	13.0	3.5	4.7	6.0
Clay	%	23.0	25.0	29.0	24.7	30.7	36.3
Texture	Class	SCL[b]	SCL	SCL	SCL	SCL	SC[c]

UOM[a] – unit of measurement, SCL[b] – sandy clay loam, SC[c] – sandy clay

In addition, various sensors were also inserted in specific places within the lysimeter trial. Four MPS-6 Decagon soil water potential and temperature sensors, four GS3 soil water content, soil temperature and electrical conductivity sensors and four SPES20 suction cups (UMS Germany) were installed at depths of 0.15, 0.30, 0.50, 0.70 m in the two lysimeters, and all the sensors were individually calibrated by the manufacturer. Similarly, suction cups and capacitance water content sensors were installed close to the drain gauge, two meters away and to the north from the weighing lysimeters. Fibre-glass side panels were installed on all sides surrounding the drain gauge to a depth of 0.30 m with 0.10 m left protruding out of the ground to prevent lateral flow and runoff.

The entire trial site, weighing lysimeter and drain gauge, had the same agronomic management practises. Before planting, soil samples were taken and analysed and used to formulate a fertiliser recommendation for the site. Optimum fertiliser was applied at a rate of 200 kg N ha^{-1} and 25 kg P ha^{-1} based on soil analysis results. Wheat cultivar PAN 3400 was planted on 30 June 2016. Plots were kept weed free by applying bromoxynil (3,5-Dibromo-4-hydroxybenzonitrile) at 1.0 L ha^{-1}, MCPA (2-methyl-4-chlorophenoxyacetic acid) at 2.2 L ha^{-1}, and pinoxaden (8-(2,6-diethyl-p-tolyl)-1,2,4,5-tetrahydro-7-oxo-7H-pyrazolo[1,2-d][1,4,5]oxadiazepin-9-yl 2,2-dimethylpropionate) at 0.8 L ha^{-1} 43 days after planting (DAP), which were all tank mixed and applied at once. During the growing season and after scouting, the plots were also kept pest and disease free. Pyrinex 480 EC (chlorpyrifos) was applied at 2.0 L ha^{-1} to control bollworms (*Helicoverpa armigera*) and aphids (*Diuraphis noxia*), and orius 250 EC (1,3 dichloropropene) was applied at 0.75 L ha^{-1} to control powdery mildew (*Erysphe gramis f.sp tritici*). High density drip irrigation with lines and emitters spaced at 0.40 m was installed. The soil moisture sensors placed at 0.15 and 0.30 m were used to schedule irrigation, and 21 irrigation cycles were applied during the study. The crops were irrigated when plant available water was reduced to 50%. The frequency and amounts applied for each irrigation cycle are provided in Figure 2.1.
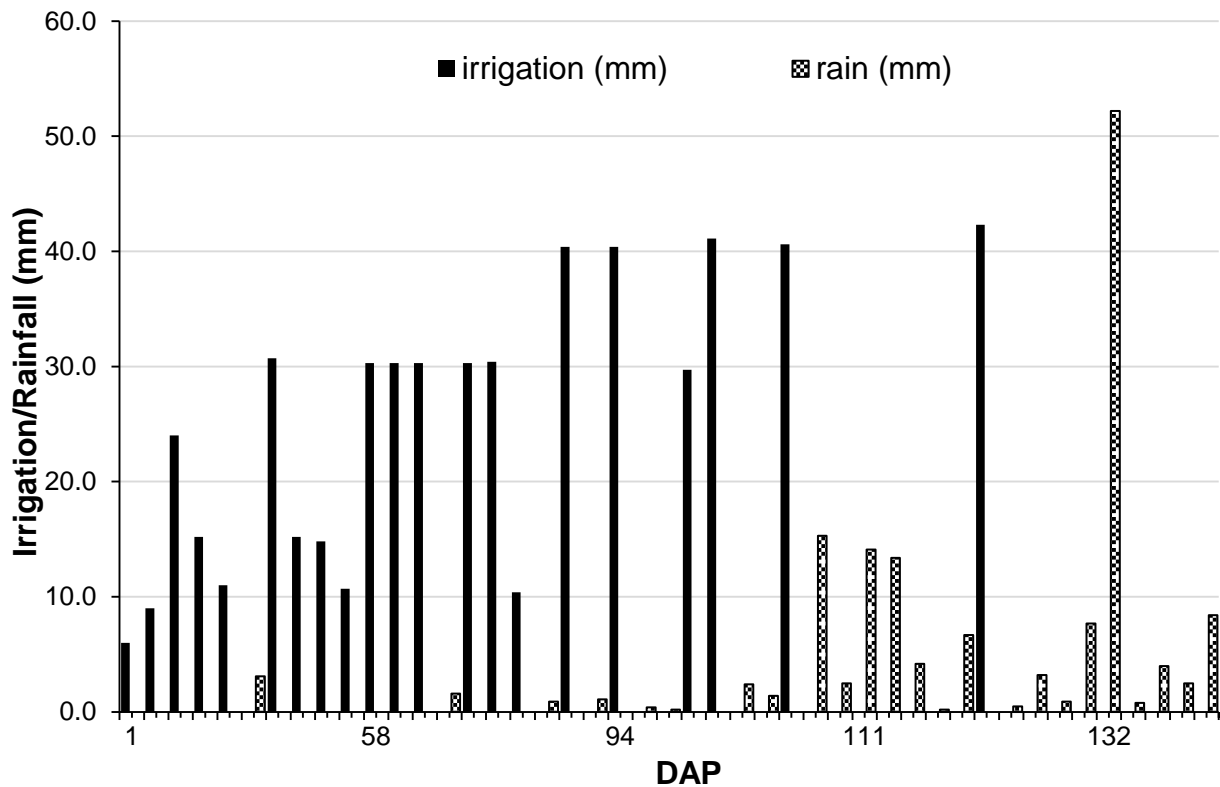
Figure 2.1: Irrigation applied and rainfall received (mm) on the lysimeter trial from 1 July to 18 November 2016 [1 to 141 days after planting (DAP)].

Weather data was collected using an automatic weather station (AWS) positioned at the University of Pretoria Experimental Farm, which was 50 m away from the trial site. The weather variables recorded were: maximum and minimum air temperature (^{o}C), maximum and minimum relative humidity (%), average wind speed (m s^{-1}), solar radiation (MJ m^{-2}) and rainfall (mm). The weather data are summarised in Table 2.2.

Soil water samples were collected at regular intervals from the drainage gauge, lysimeter drainage and suction cups (approximately 24 hours after every irrigation cycle or rainfall event). The water samples were analysed for NO_3-N concentration using RQeasy Nitrat Reflectometer (Merck, Darmstadt, Germany). The daily drainage data was compared to average drainage using standard deviations at 95% confidence interval.

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2.3 Results

Daily drainage (mm) and soil water content ($m^3 m^{-3}$), and NO_3-N levels (mg L^{-1}) after irrigation are presented in Figures 2.2 to 2.5, and averaged weather data are presented in Table 2.2. Generally, the weather conditions were suitable for growing wheat, despite the relatively high maximum temperatures recorded in October, and the grain yield was not affected with the crop producing 8.2 t ha^{-1}.

Table 2.2: Monthly weather data from July to November 2016.

Month	Average Maximum Air Temp (°C)	Average Minimum Air Temp (°C)	Average Daily Wind Speed (m s^{-1})	Cumulative Solar Radiation (MJ m^{-2})	Cumulative ET_o[a] (mm)	Cumulative Rainfall (mm)	Average Daily VPD[b] (kPa)
Jul	20.6	4.2	1.5	339.8	84.7	3.1	1.0
Aug	25.1	6.6	1.5	427.4	115.1	0.0	1.5
Sep	27.8	12.3	2.1	425.8	143.7	3.6	1.9
Oct	30.1	14.3	2.3	526.1	177.4	60.8	2.1
Nov	28.7	15.6	2.1	478.4	148.5	105.6	1.6

ET_o[a] – evapotranspiration, VPD[b] – vapour pressure deficit

Once the plant roots reached the maximum crop canopy, there was no drainage from the drain gauge, so only 1 to 70 DAP were considered. Figure 2.2 shows the daily drainage data from the drain gauge and lysimeters 1 and 2 with three distinct peaks. The drain gauge measured higher drainage than lysimeters 1 and 2, as shown by the three peaks, between 15 and 50 DAP. For the second drainage event, all the lysimeters had similar drainage, but lysimeter 1 measured slightly less drainage.
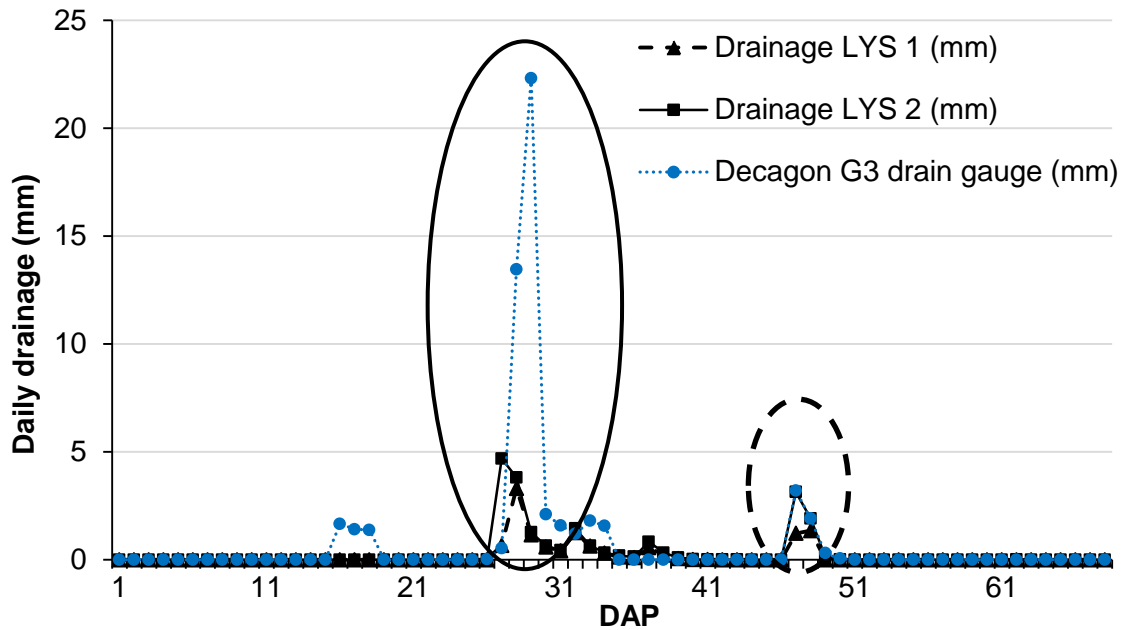
Figure 2.2: Daily drainage from lysimeter 1 and 2 (LYS 1 and 2) and the drain gauge measured from 1 to 70 days after planting (DAP). The big peak in the solid line ellipse is enlarged on Figure 2.3a, whereas another peak in the dashed line ellipse is enlarged on Figure 2.3b.

From 26 to 34 DAP, both lysimeters recorded drainage, but the drain gauge measured the highest draining volume, followed by lysimeter 2 as shown in Figure 2.3a. As can be seen in Figure 2.3b, from 46 to 51 DAP all the lysimeters drained, and the drainage patterns were similar from both lysimeters and the drain gauge. Related draining patterns can be attributed to all systems reaching saturation point thereby allowing both lysimeters and the drain gauge to drain. On all the draining days, the amounts that drained were not significantly different (using standard deviation error bars), except on 47 DAP, but the reason for this difference is not known.
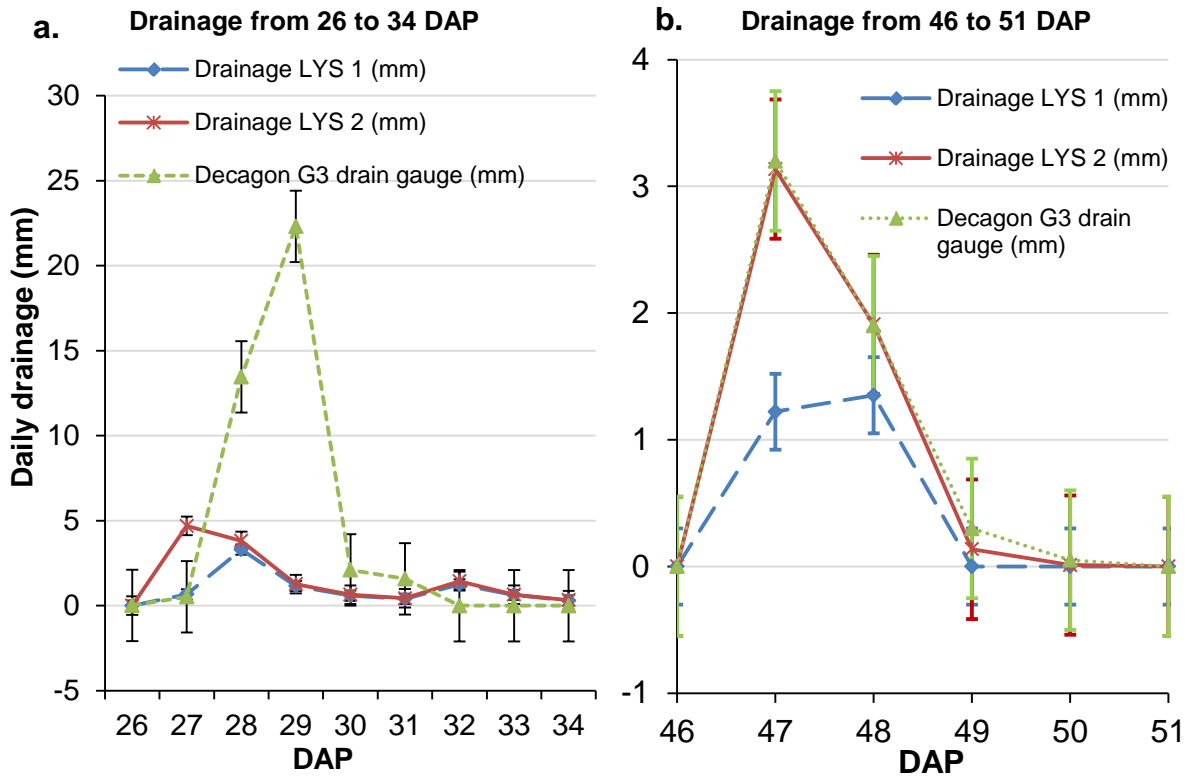
Figure 2.3: Daily drainage from lysimeters 1 and 2 and the drain gauge measured from (a) 26 to 34 days after planting (DAP) and (b) 46 to 51 DAP.
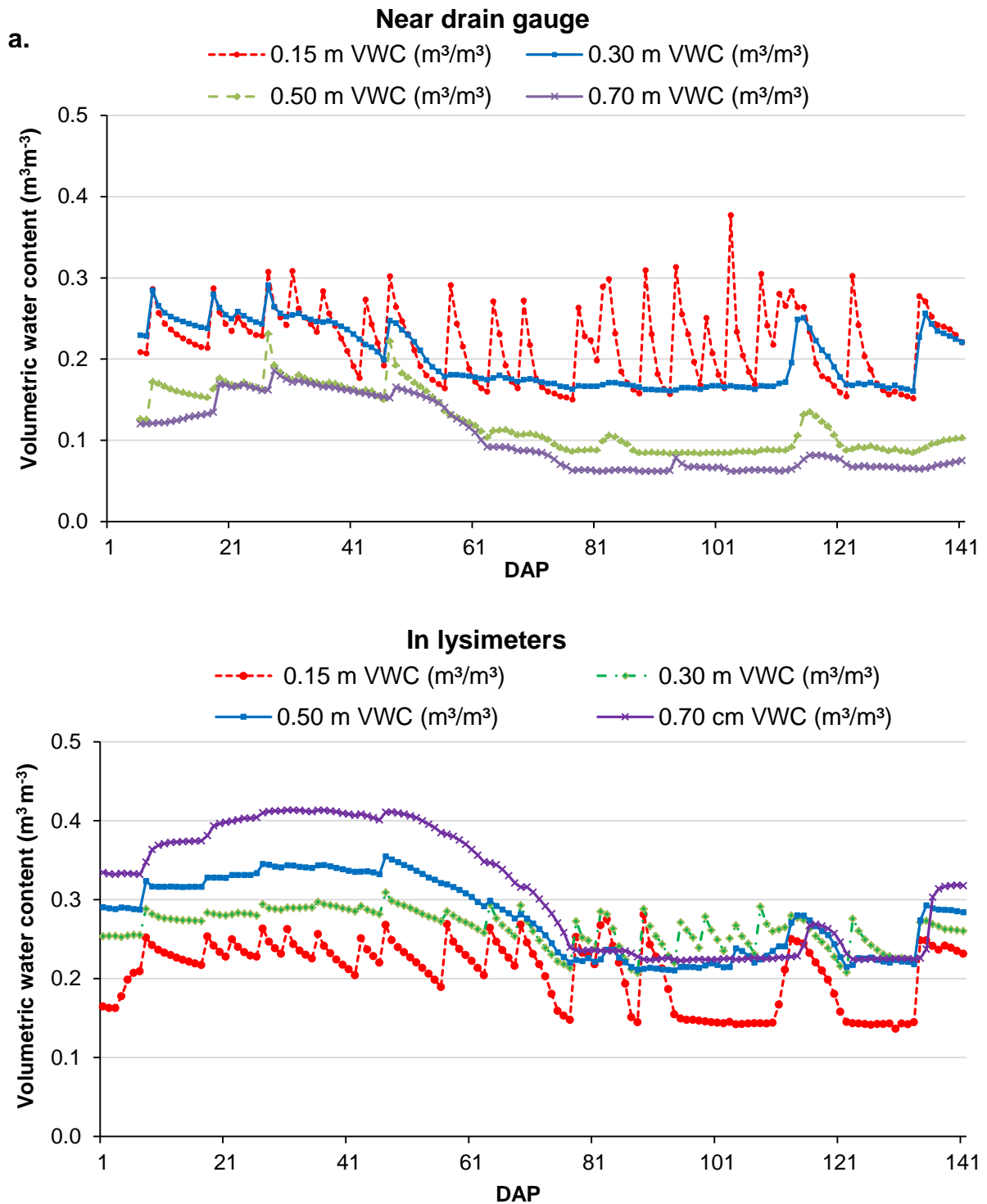
Figure 2.4: Daily volumetric water content (m³ m⁻³) data collected using capacitance sensors installed at 0.15, 0.30, 0.50 and 0.70 m depths in the soil profile for (a) the drain gauge and (b) lysimeters 1 and 2 (averaged) from 1 to 141 days after planting (DAP).

Figure 2.3a shows volumetric water content data measured close to the drain gauge. At a depth of 0.15 m, soil water content was fluctuating rapidly because of irrigation and crop water uptake, but this layer remained the wettest. Deeper in the soil profile from 0.30 to 0.70 m, the soil water content decreased with depth. Whereas, water content recorded in the lysimeters at various depths (Figure 2.3b) is inverted when compared to Figure 2.3a (much wetter with depth). The soil water content inversion clearly shows that the bottom layer of the lysimeter needs to be saturated before drainage can occur. In the lysimeters, at 94 to 110 DAP and 122 to 133 DAP the sensor in the 0.15 m was unresponsive. Since the data was averaged for lysimeter 1 and 2, small changes could have been evened out by averaging and lost the actual response of the sensor. In addition, the unresponsiveness could have also been caused by very dry soil conditions.

The NO_3-N concentrations collected at all depths on 18 DAP (Figure 2.4a) shows a different flow pattern between the drain gauge and the lysimeters. Suction cups installed close to the drain gauge had free draining soil that showed highest NO_3-N concentrations at the 0.30 m depth, but were lower at 0.50 m and lowest concentrations were at 0.70 m. However, the NO_3-N concentration measured with the lysimeter SCs was highest in the 0.15 m layer and decreased to around 100 mg L^{-1} in the 0.30 m zone, and then increased at 0.50 m to about 200 mg L^{-1}, declining again at 0.70 m. Although the NO_3-N concentration measured in the drain gauge was 25 mg L^{-1}, the NO_3-N was undetectable from the draining lysimeters (the RQeasy Nitrat Reflectometer cannot measure NO_3-N concentrations of less than 1.1 mg L^{-1}). Higher soil NO_3^-N concentrations 18 DAP are attributed to fertiliser application at planting and the mineralisation of the disturbed soil, but this is shown to be reduced intensely 48 DAP due to a bigger crop with deeper roots and increased plant N uptake. Generally, the NO_3-N was moving slower on the lysimeters compared to the drain gauge region.
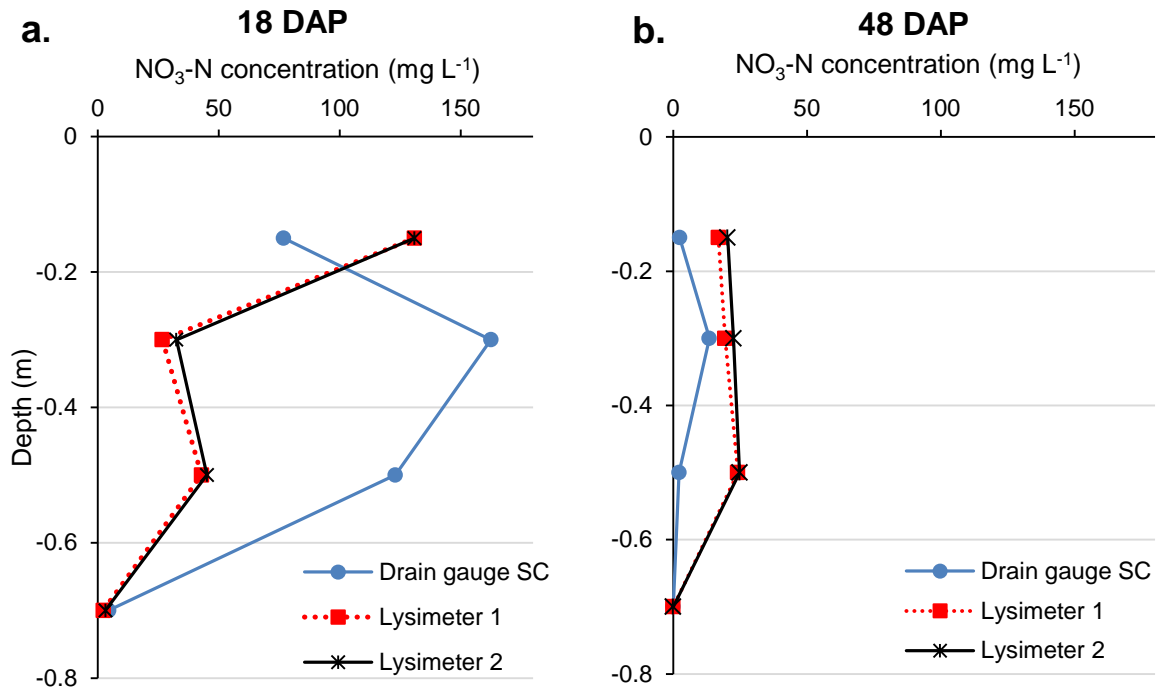
Figure 2.5: Suction cup nitrate (NO$_3^-$) concentrations measured at 0.15, 0.30, 0.50 and 0.70 m depths on (a) 18 days after planting (DAP) and b. 48 DAP.

In Figure 2.4b, the measured NO$_3$-N concentrations 48 DAP near the drain gauge were low, with all levels below 10 mg L^{-1}, except for the 0.30 m depth which was a bit higher. The NO$_3^-$N concentration measured on the lysimeters was almost similar at all depths, except for 0.70 m at which NO$_3$-N was undetectable. However, the NO$_3$-N concentrations measured in the lysimeters at 0.15, 0.30 and 0.50 m were greater than those measured above the drain gauge at these depths.

Table 2.3: Total drainage and leached nitrate-nitrogen (NO$_3$-N) from the drain gauge and weighing lysimeters.

Drainage (mm)	Total drainage (mm)	Average NO$_3$-N concentration (mg L^{-1})	Total NO$_3$-N leached (kg ha^{-1})
Lysimeter 1	12.0	<1.1	<0.1
Lysimeter 2	20.0	<1.1	<0.2
Drain gauge	54.1	46.1	24.9

The drain gauge measured a total NO$_3$-N load of 24.9 kg ha^{-1} being leached (Table 2.3). The high N leaching was caused by higher drainage with higher NO$_3$-N concentrations on the drain gauge compared to the weighing lysimeters.

2.4 Discussion

The drain gauge water content decreased with increasing soil depth, but the trend was reversed on the lysimeters. Nitrate concentration generally increased with depth but became lower again at very deep layers on the drain gauge and the lysimeters. Overall, the water content and NO$_3$-N concentration distribution seem to agree with the observed draining trends.

Early drainage was only observed from the drain gauge, but it was delayed on both lysimeters. The lag in draining on weighing lysimeters was because saturated lower soil layers first needed to form before drainage could take place, which was supported with the volumetric water content data above 0.4 m^3 m^{-3}. At a depth of 0.70 m, the soil was saturated from 1 to 60 DAP. Once saturation conditions are maintained, water could have been redistributed by capillary flow, thereby maintaining relatively higher water content at 0.30 and 0.50 m depths on the lysimeters. The saturated conditions created anaerobic conditions which may have limited the loss of NO$_3$-N leaching, but promoted gaseous N loss as nitrous oxide

(N$_2$O), nitrogen oxide (NO$_x$) and dinitrogen gas (N$_2$) by denitrification process (Delgado et al. 2006, Cameron et al. 2013). Increased denitrification could have caused NO$_3$-N concentration to be below the detectable limit of 1.1 mg L^{-1} in the lysimeters. Further research is required to confirm the processes that are occurring at the bottom of the lysimeter by installing redox potential sensors.

From 26 to 34 DAP, as irrigation was constantly being applied to support increasing crop growth, significantly higher drainage was measured on the drain gauge. Higher drainage recorded in the drain gauge compared to the lysimeter can also be attributed partly to the wick and diatomaceous earth (Gee et al. 2009, Decagon Devices Inc. 2015), which created a constant suction (11 kPa) resulting in a higher drained volume. A wick hastens water movement from the divergence control tube to be collected as drainage, as it can still sample in unsaturated conditions, which would restrict prolonged saturated conditions in the bottom layer (Landon et al. 1999, Czigány et al. 2005, Weihermüller et al. 2007).

The draining water and NO$_3$-N concentrations discrepancy on the lysimeters suggest occurrence of by-pass flow, which occurs in most structured soils (Cresswell et al. 1992, Nye and Tinker 2000). Since lysimeters were refilled it could have created atypical conditions allowing quick flow of water to the bottom soil layers along the side walls, when compared to an undisturbed soil core in the drain gauge divergence control tube. Quick water flow (by-pass flow) without properly wetting the top soil layers was exhibited with higher soil water content in the lysimeter bottom soil profiles, while upper soil layers remained drier. By-pass flow has been reported on lysimeter studies (Reeder 1986, Young et al. 1996, Bowman et al. 2002), and was noted to cause fast wetting of the bottom layers before the top layers become saturated. Ordinarily, water is expected to flow in the soil following tipping bucket approach, where higher soil layer must be saturated to allow moisture to move to deeper layer.

There were a few limitations for this study, mainly related to the installation and design of the weighing lysimeter. Firstly, refilling the lysimeter disturbed the soil

profile which created compacted layers as it settles over years, and it permitted by-pass flow that influenced NO_3-N movement and breakdown. Secondly, both weighing lysimeters have a small draining valve, which could have restricted free drainage. Meanwhile, restricted drainage resulted in little drainage that may have caused water redistribution by capillarity in the bottom soil layers on lysimeter. In addition, there is a need to monitor the drain gauge drainage against a weighing lysimeter over several seasons or multiple years to confidently verify the performance. However, the collected data set was adequate to prove that the drain gauge is useful, and it has a big potential to measure N leaching.

2.5 Conclusion

Although the weighing lysimeters' drainage was comparable to a drain gauge's drainage after several irrigation cycles, the NO_3-N concentrations in the lysimeter were significantly different to the drain gauge. The weighing lysimeter N concentrations will have to be further assessed to check if its design was contributing to lowered NO_3-N leaching and increased denitrification. The drain gauge has a great potential to be used to quantify NO_3-N leaching, as it is portable and can be deployed at various N leaching hotspots. There is still need to test the drain gauge extensively on various crops, soils and during several seasons to check seasonal performance.

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CHAPTER 3: DETERMINATION OF NITROGEN FERTILISER USE EFFICIENCY USING STABLE ISOTOPE ANALYSES

3.1 Introduction

Poor nitrogen (N) recovery, a ratio of N uptake versus N applied, in annual crops of 50% of the applied fertiliser is often reported in literature (Baligar et al. 2001, Fageria and Baligar 2005, Foyer et al. 2016). Low N recoveries are linked to increasing N losses that will not only raise production costs, but also enhance the risk of N pollution. Therefore, ways to increase N recovery and reduce N losses to the environment must be devised. In commercial agriculture, N supply is usually dominated by applied N from fertilisers and often supplemented by soil organic matter mineralisation. If the contribution of both soil organic N mineralisation or the applied fertiliser can be precisely quantified, N recovery can be improved by adequately meeting the plant N demand in space and time which minimises excess N in the root zone.

Timing N applications to meet plant N demand and uptake will lead to better N management. But given the dynamic nature and behaviour of N in the soil, it makes the quantification of various N sources difficult to determine (Dobermann 2005, Fageria and Baligar 2005, Dawson et al. 2008, Edmonds et al. 2009), or even quantify the contribution of each source when calculating fertiliser N use efficiency (FNUE) (Moll et al. 1982). Despite considerable research directed to improve N management by minimising N losses in agro-ecosystems, the progress has been minimal (Gardner and Drinkwater 2009).

In order to understand and quantify the contribution of various N sources, stable isotopes can be used to trace various N sources and their fate on various field crops (Bedard-Haughn et al. 2003). Therefore, ^{15}N natural abundance ($\delta^{15}N$) analysis account for the small differences of $^{14}N{:}^{15}N$ ratio between sources and sinks in the soil, water and plant, and can be calculated using Equation 3.1. The natural stable

[15]N abundance has been used on several N studies (Awiti et al. 2008, Wei et al. 2013, Busari et al. 2016), yet δ^{15}N use is still limited compared to carbon (C) isotopes studies due to analytical problems and complexity of the N cycle (Hobbie et al. 2000, Adams and Grierson 2001, Wienhold 2007). The difference in δ^{15}N is caused by isotope fractionation in soil N processes which are influenced by soil microbes that prefer lighter ^{14}N to heavier ^{15}N in enzymatic regulated N transformations within the soil profile (Mordelet et al. 1996, Kriszan et al. 2007, Nakamura et al. 2012, Wei et al. 2013). Commonly, all the enzymes involved in the N transformation discriminate ^{15}N except for nitrogenase which is involved in N fixation and located in legume nodules (Adams and Grierson 2001). As a result of ^{14}N preference, the soil δ^{15}N become enriched and leaves a signature in the soil (Handley and Raven 1992), so it can provide a basis for monitoring ^{15}N abundance as a tracer of soil N processes and sources (Choi et al. 2003, Wei et al. 2013).

In this study, stable ^{15}N isotope abundance in the soil at different depths and in various plant parts was evaluated, so as to determine the fate of applied fertiliser N, and to quantify FNUE in an irrigated wheat crop. Alternatively, this work provided a preliminary study to understand soil-plant N relations that will be verified by running Agricultural Productions System sIMulator (APSIM), and to find a plant part with δ^{15}N values that can be used to estimate plant N% and plant δ^{15}N values essential to calculate FNUE.

3.2   Materials and Methods

A field trial site consisting of six plots was used for this study (Appendix 4), and the profile soil properties of the site are on Table 2.1. The dimensions of each plot were 2.0 x 2.0 m (length x width) (Appendix 6). Only three of the six plots were fertilised, but all the plots received similar agronomic practices, and they were irrigated according to crop water requirements based on capacitance sensor measurements inserted in the soil profile at a depth of 0.15 m. The crop was irrigated when the soil water content at 0.15 m measured by capacitance sensors had reached 0.20 m^3m^{-3}, about 50% of plant available water. The irrigation volumes applied are given in detail on Appendix 1, which shows dates and amount of irrigation applied on the fertilised

and unfertilised plots. Total irrigation water applied was 550 and 610 mm on the unfertilised and fertilised plots, respectively. High density drip irrigation was used with drip lines and emitters spaced at 0.40 m. Soil samples were taken and analysed before planting, and used as the basis for fertiliser application. The fertilised plots received 200 kg N ha^{-1} in four equal splits, on 1, 29, 41 and 70 days after planting (DAP), of 50 kg N ha^{-1}, and 25 kg P ha^{-1} was also applied to these plots in one application at planting. Lime ammonium nitrate (LAN) with 28%N was applied to supply N, and di-ammonium phosphate (DAP) supplied both P at 10.5% and N at 3.5%. Both LAN and DAP was supplied by Omnia Fertilisers, South Africa. Wheat cultivar PAN3400 was planted on the 30th of July 2016. The plots were kept weed, pest and disease free.

A soil baseline of natural ^{15}N abundance (δ^{15}N) was established from the surface at 0.00 m up to a depth of 0.80 m before planting and after harvesting. Initially, the sampling depth interval was 0.05 m from soil surface to 0.20 m, and increased to 0.20 m between 0.20 and 0.80 m depths. Each soil sample was air dried after collection, and was split into two batches each of approximately 0.05 kg after mixing and grinding lightly. The first batch was acid washed with 1% hydrochloric acid (HCL), and they were left for 24 hours to remove any carbonates on the sediment. After washing with acid, the sediment was rinsed three times with distilled water, and placed in an oven to dry for 72 hours at 60°C. The second batch did not receive any chemical treatment, and samples were placed into 5 ml micro test tubes before weighing. Following drying, 65-70 mg of sediment, both acid and non-acid washed, was weighed and placed in tin capsules that were pre-cleaned in toluene for isotopic analysis. Plant samples were dried and homogenized and aliquots of 1.0 to 1.1 mg were weighed for isotopic analysis. All isotopic results were referenced to Vienna Pee-Dee Belemnite for carbon (C) isotope values, and to air for N isotope values. A laboratory running standard (Merck Gel: δ^{13}C = -20.57‰, δ^{15}N = 6.8‰, C% = 43.83, N% = 14.64) and blank sample were run after every 5 unknown samples. The reproducibility of the results was 0.05‰ for both N and C. Stable isotopic analysis (δ^{15}N and δ^{13}C) was carried out using a Flash EA (1112 Series) elemental analyser coupled to a Delta V Plus stable light isotope ratio mass spectrometer via a ConFlo

IV system (all equipment supplied by Thermo Fischer, Bremen, Germany), housed at the Stable Isotope Laboratory, Mammal Research Institute, University of Pretoria.

Results were expressed in delta notation using a per mille scale as follows:

$$\delta X\ ‰\ = \frac{\text{Rsample}}{\text{Rstandard}} \times 1000 \qquad (3.1)$$

where $\delta X = {}^{15}N$ or ${}^{13}C$ and R represents ${}^{15}N/{}^{14}N$ or ${}^{13}C/{}^{12}C$ respectively

Initially, LAN and DAP were analysed for stable isotope abundance and had a $\delta^{15}N$ weight average of -2.1‰, and destructive plant sampling was done at tillering, flowering and physiological maturity. Plant material was separated into roots, senesced leaves, green leaves, flag leaves, and grains depending on sampling date and growth stage. Plant samples were ground, and a sample of 1.0–1.1 mg was weighed for each of the six plots. The plant samples were also analysed for $\delta^{15}N$ using a mass spectrometer as described previously for soil. The data were analysed using student's t-test and the means were separated using standard errors at the 95% confidence interval. A regression analysis was also performed to establish correlations between $\delta^{15}N$ values and plant N%.

Plant N derived from fertiliser (Ndff) given in Equation 3.2 was calculated using plant stable isotopes $\delta^{15}N$ values (Vose 2013).

$$\text{Ndff}\ = \frac{\text{Nu} - \text{Nt}}{\text{Nu} - \frac{\text{Nf}}{n}} \qquad (3.2)$$

Where: Nu   = atom ${}^{15}N$‰ in unfertilized plants

Nt   = atom ${}^{15}N$‰ in fertilized plants

Nf   = atom ${}^{15}N$‰ in the fertiliser

n   = the plant discrimination factor between ${}^{14}N$ and ${}^{15}N$.

Assuming no discrimination between ${}^{14}N$ and ${}^{15}N$, then n = 1 (Vose 2013).

Generally three assumptions at root-soil interface are considered which are a) negligible fractionation occurs on plant N uptake, b) no intra-plant $\delta^{15}N$ variation

occurs among plants with similar treatment, and c) whole-plant $\delta^{15}N$ do not differ significantly from the source $\delta^{15}N$ value (Evans et al. 1996).

To calculate the FNUE, Equations 3.2 to 3.4 were used.

Total N uptake (kg ha^{-1}):

$$\text{N uptake} \;=\; \frac{[\text{Yield dry matter (kg ha}^{-1}) \times \text{plant N\%]}}{100} \qquad (3.3)$$

Fertiliser uptake (kg ha^{-1}):

$$\text{Fertiliser N yield (FNU)} \;=\; \frac{[\text{N uptake (kg ha}-1) \text{ x \% Ndff]}}{100} \qquad (3.4)$$

Fertiliser N use efficiency (FNUE):

$$\%\text{FUE} \;=\; \frac{\text{Fertiliser N yield}}{\text{Applied N rate}} \;\times\; 100 \qquad (3.5)$$

3.3 Results

Figure 3.1a shows the $\delta^{15}N$ values in the soil profile increased from 0.00–0.05 m to 0.20–0.40 m for both fertilised and unfertilised plots and decreased for 0.40–0.60 m and 0.60–0.80 m. At tillering, $\delta^{15}N$ values were higher than at physiological maturity for both fertilised and unfertilised plots. An exception was observed for the 0.15–0.20 m and 0.20–0.40 m depths where the fertilised plots had slightly higher $\delta^{15}N$ than unfertilised plots, but for all the other depths the unfertilised plots $\delta^{15}N$ values were always greater.

Figure 3.1b shows $\delta^{15}N$ values increased from 0.00–0.05 m to 0.40–0.60 m in the soil profile after harvesting for both fertilised and unfertilised plots, and decreased slightly for 0.60–0.80 m. Although $\delta^{15}N$ values at 0.20 to 0.60 m were higher slightly than the deepest layer of 0.6–0.8 m, they were not significantly different for both fertilised and unfertilised plots. When comparing Figure 3.1a and 3.1b for the 0.20–0.40 m depth, the $\delta^{15}N$ values before planting were higher than values obtained after harvesting for both fertilised and unfertilised plots. The peak $\delta^{15}N$ values were in the 0.20-0.40 m layer before planting, but this peak shifted to 0.40-0.60 m layer after harvesting which potentially indicates movement of N to deeper soil layers, or microbial processes discriminating against ^{15}N at these depths.
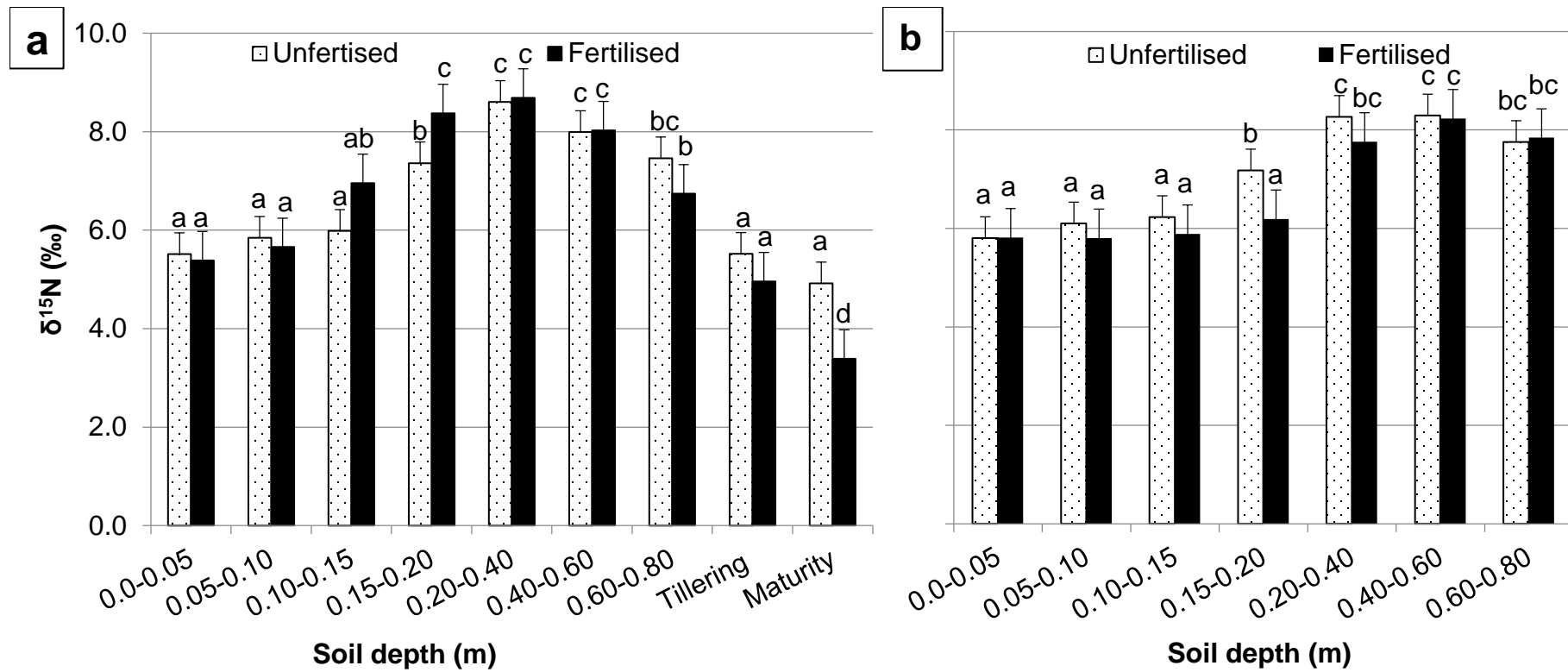
Figure 3.1: The δ15N values for soil samples taken from fertilised and unfertilised plots a. before planting and b. after harvesting. Residual soil bound on plant roots after pulling out the plants at tillering and physiological maturity was also analysed and the values are shown on Figure 3.1a.
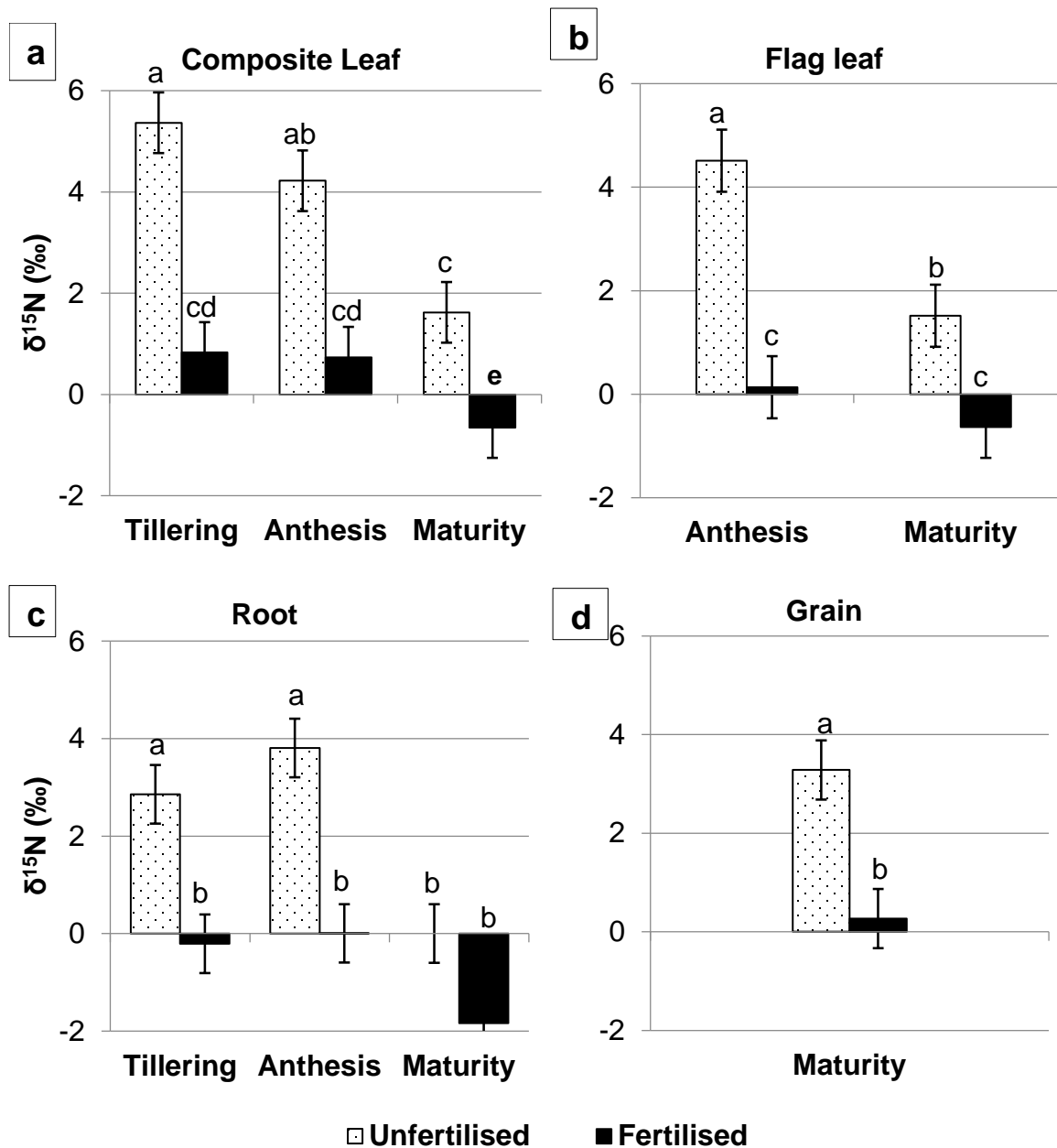
Figure 3.2: The δ^{15}N values for (a) composite leaf, (b) flag leaf, (c) root and (d) grain. The wheat was harvested at tillering, anthesis and maturity from the fertilised and unfertilised plots and separated into different plant parts before analysis.

In Figure 3.2 there was a clear distinction of δ^{15}N values on the fertilised and unfertilised plots. The δ^{15}N values on unfertilised plots were always enriched significantly higher than on fertilised plots for all the plant parts that were considered. The roots on the fertilised plots were depleted (low δ^{15}N values) than unfertilised plots and in all other plant parts. Figure 3.1a and 3.1b shows δ^{15}N values decreasing

as the plants gets old, however in the roots the trend of $\delta^{15}N$ values increases as the plants mature on unfertilised plots and more depleted on fertilised plots.
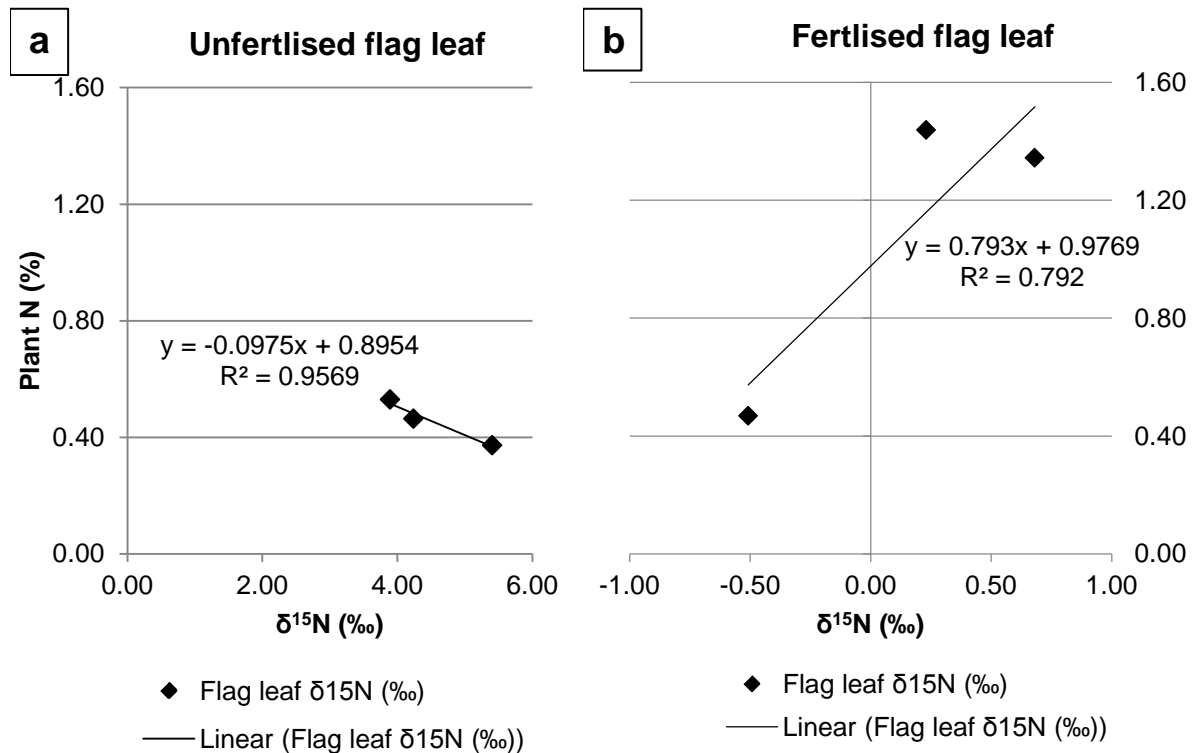
Figure 3.3: The correlation between the total plant nitrogen (N) and flag leaf $\delta^{15}N$ for (a) unfertilised plots and (b) fertilised plots at anthesis.

Figure 3.3 and 3.4 shows the correlation between the flag leaf $\delta^{15}N$ values and plant N% at anthesis and physiological maturity. Although the data set used to derive the correlations was limited (only three data points), there are useful trends that were noted from the data set. A positive correlation, $r^2 = 0.96$ and $r^2 = 0.79$, was observed between flag leaf $\delta^{15}N$ values and plant N% on both unfertilised and fertilised plots at anthesis. Flag leaf $\delta^{15}N$ values proved to be related to plant N source and plant N%. However, a decline of plant N% was observed on unfertilised plots with increasing flag leaf $\delta^{15}N$ values at anthesis, while plant N% increased as flag leaf $\delta^{15}N$ increased when fertilised. At physiological maturity (Figure 3.4), the correlation between flag leaf $\delta^{15}N$ and plant N% was strongly positive for both unfertilised ($r^2 = 0.99$) and fertilised plots ($r^2 = 0.91$).

Figure 3.4: The correlation between flag leaf δ^{15}N and plant nitrogen (N) for (a) unfertilised plots and (b) fertilised plots at physiological maturity.

Table 3.2 shows the Ndff and FNUE values that are above 50% indicative of a well-managed agricultural system. Detailed information about the calculations is given by Equations 3.1 to 3.5, and further information is also given on Appendix 2.

Table 3.1: Calculated fertiliser use efficiency using depleted nitrogen fertiliser.

Parameter	Calculated Value
$\delta^{15}N$ in the fertiliser (‰)	-2.1
N derived from fertiliser (%)	61
Total above ground N uptake (kg ha^{-1}):	222.6
Fertiliser N yield (kg ha^{-1}):	135.5
Fertiliser N use efficiency (%)	68

3.4   Discussion

Stable isotopes were able to differentiate between the soil N reserves and applied fertiliser N. Different plant parts on the unfertilised plots showed more positive $\delta^{15}N$ values which were similar to observed baseline $\delta^{15}N$ values, but decreased as the plants matured. The flag leaf $\delta^{15}N$ values at physiological maturity had a strong correlation with final plant N% for both fertilised and unfertilised treatments. As a result of $\delta^{15}N$ values distinction between the soil N reserve and fertiliser N, the calculated FNUE was 68%.

The trend of $\delta^{15}N$ enrichment as depth increased was observed from soil surface to 0.4 m depth, and the $\delta^{15}N$ values then dropped significantly when depth continues to increase to 0.8 m depth. The root volume and density is highest in the 0.2 to 0.4 m for most annual crops, therefore, a heavy root density provide a large surface area where N processes occurs, and fractionation is more likely to happen because it is the most active region. Increased microbial biomass has been reported in this zone (Giagnoni et al. 2016), which may have caused a more positive $\delta^{15}N$ values. The increasing $\delta^{15}N$ enrichment was also reported by Mordelet et al. (1996), but these values vary spatially and temporally and can be cultivar specific. However, the averaged $\delta^{15}N$ values for all depths in the unfertilised plot was 12% lower before planting compared to average $\delta^{15}N$ values after harvesting meaning that $\delta^{15}N$ increased. In fertilised plots, the average $\delta^{15}N$ values for all the depths before

planting and fertiliser application were higher by 33% compared to stable isotopes values after harvesting. More positive $\delta^{15}N$ values in unfertilised plots is an indication of soil processes occurring in the soil such as mineralisation and nitrification (Högberg 1997, Choi et al. 2003a, Yun and Ro 2009) which are microbe mediated processes that have a bias against heavy ^{15}N. Other transformation processes such as denitrification would be ruled out since the soil profile was not water logged. Although it can be argued that the top layers can experience anaerobic conditions soon after irrigation, the instances were short and far spaced to influence denitrification as a result of good irrigation scheduling. In deep soil layers, the soil organic carbon (C) as well as organic N declines, which results in low $\delta^{15}N$ values because of reduced mineralisation. An increase of $\delta^{15}N$ values at these depths could imply leaching of ^{15}N from upper layers with high microbial biomass.

The rhizosphere soil bound to the roots collected at tillering and anthesis showed $\delta^{15}N$ values to be significantly different from the surrounding bulk soil. In other related studies the rhizosphere was found to have more microbial communities relative to the bulk of the soil (Giagnoni et al. 2016), implying more N processes such as mineralisation and nitrification occur more in this region that results in more positive or enriched $\delta^{15}N$ values. The $\delta^{15}N$ discrepancy with the rest of the soil suggests lower levels of mineralisation in the rhizosphere which is uncharacteristic, but it is still not clear why the less positive $\delta^{15}N$ were experienced during tillering and physiological maturity in this zone. There may also be a possibility that an increased N demand and indiscriminate ^{15}N uptake (Evans 2001) at flowering masked the corresponding potential enrichment of $\delta^{15}N$ values, regardless of high mineralisation rates. Such a difference shows how this zone can be intensively monitored, using stable isotopes, to determine the various activities that can influence the N transformations in the rhizosphere, and how different N forms are preferred and taken up by plants.

The composite leaves and flag leaf $\delta^{15}N$ values in the unfertilised plots decreased as the plant matured, except for the roots. At tillering, similar $\delta^{15}N$ values in the leaf and soil were observed on unfertilised plots suggests that plant N demand was low, and

N was being derived from the soil plant available N to satisfy the crop N requirements, hence the similar $\delta^{15}N$ values. At anthesis, critical N shortage could have been created, as the root $\delta^{15}N$ was highest at anthesis, but it was drastically reduced to almost nil at physiological maturity. The unfertilised plants may have run out of organic N which was being obtained from soil mineralisation during the grain filling stage, as a result, $\delta^{15}N$ values declined at anthesis and physiological maturity. Another possible reason for the $\delta^{15}N$ decline may be attributed by N stress on unfertilised plots that would normally trigger N assimilation and re-translocation, as such processes result in less positive $\delta^{15}N$ values due to heavy ^{15}N discrimination (Robinson et al. 1998, Flores et al. 2007) in the older leaves during the grain filling period, hence the grain became $\delta^{15}N$ enriched at the expense of composited leaves and flag leaf. The grain $\delta^{15}N$ enrichment was caused by an accumulation of amino acids, which were derived from protein hydrolysis of the enriched $\delta^{15}N$ leaves during the grain filling period (Kichey et al. 2007). However, the fertilised plots were only slightly enriched because the depleted fertiliser $\delta^{15}N$ contributed more of the required N during the protein synthesis during the grain filling stage.

In fertilised plots, depleted $\delta^{15}N$ values depicted that fertiliser was the dominant source at physiological maturity, for composite leaves, flag leaves and roots during the grain filling stage. Considering other harvesting stages and plant parts, the $\delta^{15}N$ in fertilised plots were slightly positive, and it showed that the plants were still taking some N from the soil organic N. At physiological maturity, measured $\delta^{15}N$ values suggest that most N was coming from applied fertiliser. In addition, $\delta^{15}N$ values were able to distinguish between the two sources of N that were used, as Dalal et al. (2013) also managed to use the stable isotope method to differentiate among various N sources under no till in a wheat crop.

Discrimination of ^{15}N within the root system after N uptake cannot be ruled out, as ammonium (NH_4^+) N forms are assimilated in the plant root before they are translocated to other plant parts. The root N assimilation resulted in enriched $\delta^{15}N$ at tillering and anthesis when compared to the composited leaves on unfertilised plots. The increasing enrichment of $\delta^{15}N$ indicates increased N assimilation in the roots

and availability of NH_4^+ N form. Since soil N reserves were availed for plant uptake after mineralisation, the N form taken up by plants was mainly in the NH_4^+ form. Mostly, NH_4^+ N forms are reduced in the roots to prevent ammonia (NH_3) toxicity, an intermediate substrate in the glutamine synthatase–glutamate synthatase (GS-GOGAT) pathway. In this reaction, GS-GOGAT, glutamine-synthatase is known to discriminate against ^{15}N (Evans 2001). However, as the inorganic N declined sharply just after anthesis, the $\delta^{15}N$ values were reduced to almost zero in the roots at maturity confirms the running out of soil organic N available for uptake in the unfertilised plots. This supports the theory given by Evans (2001) and Vose (2013) that plant ^{15}N discrimination during uptake is of little relevancy when N source is limiting. Therefore, the differences of $\delta^{15}N$ observed were due to N source.

There was a strongly positive relationship between the flag $\delta^{15}N$ and plant N% for both the fertilised and unfertilised plots. The strong positive relationships established at anthesis and physiological maturity were related to N source and plant N%; hence, we can use the flag leaf $\delta^{15}N$ correlation equation to determine plant N% and N source rather than whole plant analysis. However, there was poor correlation between the $\delta^{15}N$ values and the roots, composited leaves and grains. In other studies, the composited plant $\delta^{15}N$ was correlated to N source and was used successfully as an indicator for distinguishing organic and in-organic produced plants (Flores et al. 2007, Flores et al. 2011), but the method required taking of whole plant samples which can be time consuming and costly other than using a single correlated plant part to pinpoint N sources. The flag leaf $\delta^{15}N$ values will help answer the question of the amount of fertiliser N uptake and the other N component derived from mineralisation processes. Although useful relationships were derived from the limited data set, this study probes for further research to verify the patterns. Such information is crucial to further give insights on N availability, so that adjustments or refinements can be made to site specific fertiliser recommendations.

In this study, the N derived from fertiliser and FNUE were above the commonly reported values of less than 50% in wheat (Baligar et al. 2001, Fageria and Baligar 2005, Foyer et al. 2016). Despite low N uptake figures being consistently reported

across the globe, there are some few isolated reports that have reported wheat N uptake of more than 90% (Van Cleemput et al. 1981, Fillery and McInnes 1992, Corbeels et al. 1999). High N recovery can reduce residual N in the soil which is likely to be lost thorough N leaching, and stable isotope methods can be used to explore ways to quantify and improve FNUE.

3.5 Conclusion

The stable isotope natural abundance method was able to distinguish between soil-derived N sources and applied fertiliser N. Application of stable isotopes was also able to show when the N supply in the unfertilised soil became limiting. Therefore, by tracing N use in plants using stable isotopes, especially the flag leaf, there is an opportunity to establish peak N demand in plants and to improve FNUE and reduce N losses from the root zone. The FNUE was 68%, although it was better than the commonly reported values in literature, potential N loss of 32% from unused fertiliser still poses a major risk of pollution to the environment.

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CHAPTER 4: EVALUATION OF APSIM TO SIMULATE WATER, BROMIDE AND NITROGEN DYNAMICS IN WHEAT CROPPING SYSTEMS

4.1 Introduction

In the sub-tropical and semi-arid regions of sub-Saharan Africa, commercial agriculture thrives under irrigation. However, strict adherence to irrigation scheduling must be maintained (Annandale et al. 2011), as improper irrigation and erratic rainfall often results in over application of water. Water application in excess of the soil water holding capacity can result in a loss of nitrogen (N), either via leaching or in runoff, but other processes such as volatilisation and denitrification can also occur (Delgado et al. 2006, Edmonds et al. 2009, Liu et al. 2015). Leaching losses are affected by various factors, including irrigation method (for example, furrow, drip or sprinkler), N type and N application rate. For instance, if urea is applied, losses by volatilisation can be high in soils with high pH and in cases when it is not fully incorporated into the soil (Nye 1986, De Datta 1987, Choudhury and Kennedy 2005). But, with nitrate- or ammonium-based fertilisers, the ammonium (NH_4^+) ions are adsorbed in soils with high cation exchange capacity (CEC) and are not easily lost, whereas nitrates (NO_3^-) pose a greater risk of loss, as they are highly soluble (Thorburn et al. 2010, Phogat et al. 2013, Salazar et al. 2014). Hence, understanding and quantifying the N losses, especially through leaching, is essential to succeed with sustainable crop production.

The high N dynamics complexity and spatial variability of measurements make crop models useful research tools to answer specific hypotheses (Boote et al. 1996, Sinclair and Seligman 1996), and they can also synthesise or explain trends occurring in agroecosystems. However, the adoption and use depends on the model complexity and testing in various environments (Addiscott et al. 1995). Confidence in models is drawn from the parameterisation and validation process, and if a range of application of the model, for example when N leaching can be ascertained. Conservative tracers such as bromide (Br^-) or chloride (Cl^-) can be used as they do

not undergo chemical transformations as N does (Tilahun et al. 2004, Wishkerman 2006, Oelmann et al. 2007, Bero et al. 2016). Once the potential N leaching of the soil is established and parameterised, then modelling N leaching outputs under varying conditions are simulated with more certainty. Although N dynamics in soils are not fully understood (Van der Laan 2009, Van der Laan et al. 2014), modelling of N leaching together with measured soil water and NO_3^- data can improve knowledge on N dynamics in a specific system. Since it is unfeasible to conduct field trials for all promising water and N application rates to ascertain N losses, crop modelling can be used as an alternative tool to predict N losses and optimise management practises.

Among several crop models reported in literature, the Agricultural Production System sIMulator (APSIM) model is widely used to simulate plant growth and soil water and N dynamics (McCown et al. 1995, Keating et al. 2003). The model has a simple, empirical tipping bucket approach used to simulate water and N movement called SoilWat (soil and water) module (Huth et al. 2012). Additionally, APSIM has the soil water infiltration and movement (SWIM) module, which simulates water and solute movement using Richards' Equation and the convective-dispersion equation (Huth et al. 2012, Brown et al. 2014, Holzworth et al. 2014). SoilWat is usually preferred to SWIM3 because of low input requirements required to initialise simulations. Since APSIM model has a robust N dynamics module and was extensively applied on wheat systems (Asseng et al. 1997, Asseng et al. 1998, Asseng et al. 2000, Asseng et al. 2002, Mohanty et al. 2012, Zhao et al. 2014, Ahmed et al. 2016), it was ideal for modelling N leaching on wheat cropping systems in our study.

The objective of this study were to establish the N leaching potential using Br^- as a conservative tracer for the Hutton sandy clay loam soil (Soil Classification Working Group, 1991). Another objective was to evaluate the performance of a parameterised and calibrated APSIM model, and to predict NO_3-N leaching from the soil profile using the model.

4.2 Materials and Methods

Both lysimeter and field trial sites described in Chapter 2 and 3 were used for this study (Appendix 4 to 6). The trial sites were located at the University of Pretoria Experimental Farm, and wheat was planted on the 30th of July 2016 and harvested on the 15th of November 2016. The soil is a sandy clay loam Hutton soil (Soil Classification Working Group, 1991), and a list of selected soil properties is summarised in Table 2.1.

The crop was kept weed, pest and disease free to obtain growth parameters under optimum conditions for the APSIM crop model. Recommended agronomic practices were followed, and tensiometers and volumetric soil water content (VWC) sensors inserted at 0.15 m were used to schedule irrigation. A total of 610 and 550 mm of irrigation were applied on the fertilised and unfertilised plots, respectively, and detailed irrigation schedules for the lysimeter and field trial are given in Figure 2.1 and Table 3.1, respectively. Saturated hydraulic conductivity was measured using a Decagon dual-head infiltrometer (Decagon Devices Inc., Pullman WA, USA). Water potential sensors, wetting front detectors (WFDs), suction cups (SCs) and tensiometers, were also installed at selected depths depending on the trial site, see Table 4.1.

Table 4.1: Depth of insertion for various types of instruments in the lysimeter and field trial sites.

Depth (m)	Lysimeter Trial	Field Trial
0.15	MPS-6[a], SPES20[b], GS3[c]	CS[d]
0.25		WFD[e], SC[f], T[g], CS
0.30	MPS-6, SPES20, GS3	
0.50	MPS-6, SPES20, GS3	WFD, SC, T, CS
0.70	MPS-6, SPES20, GS3	

MPS-6[a] – soil water potential sensor, SPES20[b] – suction cup, GS[c] – volumetric water content sensor, and CS[d] – capacitance sensor (all supplied by Decagon Devices Inc., Pullman WA, USA), WFD[e] – wetting front detector (Agriplas, South Africa), SC[f] – suction cup (Soil Moisture Equipment Corp., Santa Barbara, CA, USA), and T[g] – tensiometer (Delta-T Devices, Cambridge, UK).

Phenological data that was collected during the wheat growing season included: days taken from sowing to germination, tillering, flowering, anthesis, and physiological maturity. Other data collected were: plant above ground dry matter accumulation, grain yield, ears per m^{-2} and stem, leaf and grain N concentration. Root depth was also measured by digging a pit close to the centre of the lysimeter trial site, and the roots were visually inspected. The leaf area index (LAI) was measured using an LI-3100C area meter (Li-Cor Inc., Lincoln, Nebraska, USA) and AccuPAR LP-80 ceptometer (Decagon Devices Inc., Pullman WA, USA). Destructive sampling was done at tillering, anthesis and physiological maturity, so plant material was oven dried for 72 hours at $60^{o}C$. A moisture cup Mini GAC and GAC PLUS (DICKEY-john Corporation, Illinois, USA) was used to determine the grain moisture and adjust the oven dried grain moisture to 12.5%, the industry standard for maximum allowable moisture content of wheat grain.

The daily weather data required by the model was collected using an automatic weather station (AWS) positioned on the University of Pretoria Experimental Farm in close proximity to the trials. The parameters recorded were: maximum and minimum air temperature (^{o}C), maximum and minimum relative humidity (%), average wind speed (m s^{-1}), solar radiation (MJ m^{-2}) and rainfall (mm). Evapotranspiration (ET$_{o}$) (mm) and average vapour pressure deficit (VPD) (kPa) were estimated and calculated using the weather data, and the ET$_{o}$ and VPD for the growing season are shown in Figure 4.1.
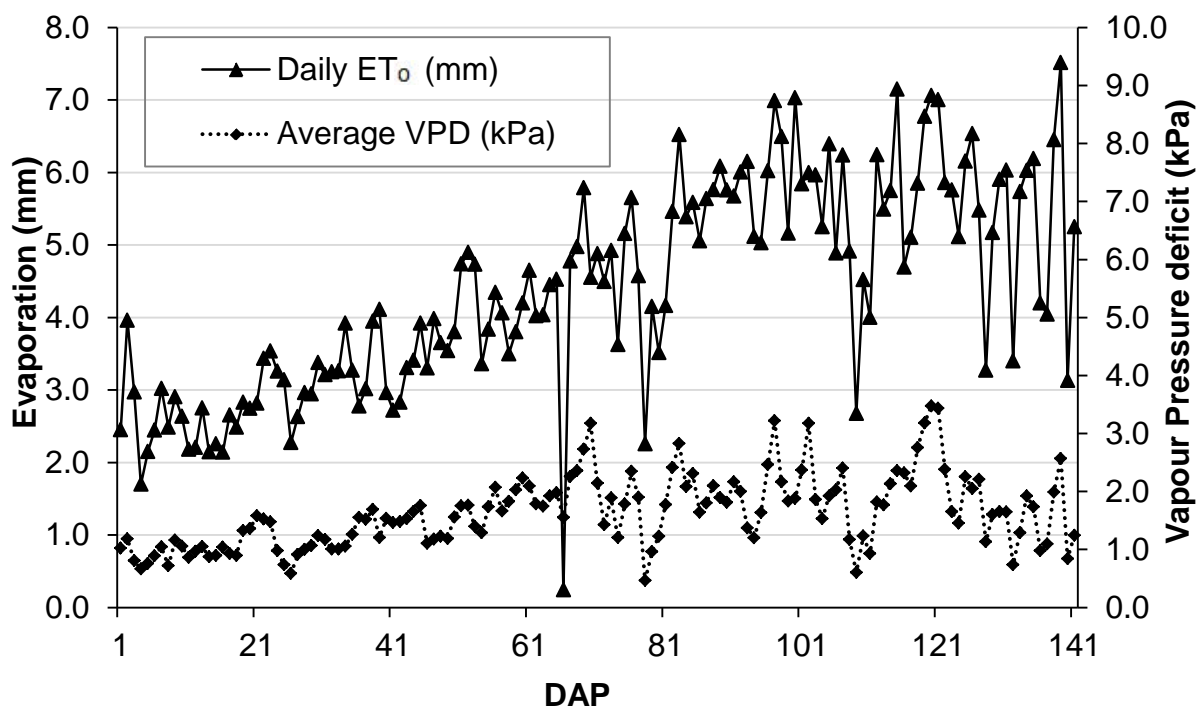
Figure 4.1: Daily evapotranspiration (ET$_{o}$) (mm) and vapour pressure deficit (VPD) (kPa) variation during the growing season on the University of Pretoria Experimental Farm.

Bromide (Br^{-}), as a conservative tracer, was applied to the field trial (fertilised and unfertilised plots) 41 days after planting (DAP) at a rate of 0.020 kg m^{-2}. The Br^{-} was dissolved in 0.5 L of distilled water, and it was applied using a hand-held sprayer. Water samples were collected 24 hours after every irrigation cycle until physiological maturity. The water samples for Br^{-} analysis were collected at 0.25 and 0.50 m depths. Collected samples were put in a plastic container and stored in a cold room at 5°C until they were analysed. Samples were analysed for NO$_3^{-}$ and selected

samples for Br^- concentration due to high cost. Bromide was analysed using ion chromatography at the Agricultural Research Council (ARC) Climate and Soil, Pretoria, South Africa, while NO_3^- concentration was analysed using an RQEasy Nitrate Reflectometer (Merck, Germany).

4.2.1 APSIM model description

APSIM version 7.7 was used, and consists of several crop models, with APSIM-Wheat being applied for this simulation (McCown et al. 1996, Asseng et al. 1998, Asseng et al. 2002, Keating et al. 2003, Holzworth et al. 2014). Using SoilWat, soil N (SOILN) and residue modules, the APSIM-Wheat can simulate plant growth on a daily time step. The SoilWat module uses a multi-layer, cascading or tipping bucket approach to simulate water and solute movement, and a mixing factor is used to determine the fraction of solute that moves to the layer beneath (Van der Laan et al. 2014). The model requires a specified drained upper limit (DUL), saturation (SAT) and water lower limit (LL15), daily meteorological data and agronomic management practices (for example, planting, tillage, fertiliser, harvest) to simulate crop growth and development and soil processes. After calibrating APSIM using the lysimeter trial data, the model was tested using the field trial data, from fertilised and unfertilised plots.

Soil water content, soil inorganic N, LAI, total above ground dry matter (TDM) and grain yield were used to assess the performance of the model. The square of the correlation coefficient (r^2), mean absolute error (MAE), index of agreement (D), and root mean square error (RMSE) were the statistical tests used. When r^2 and D were above 0.8 and MAE% was below 20%, the model was considered to be performing well (De Jager 1994). RMSE was evaluated on case-by-case basis, and usually must be less than 20% of standard deviation.

4.3 Results

Measured soil and growth parameters were results and used to calibrate the APSIM model. Saturated hydraulic conductivity was measured using a Decagon ring infiltrometer for lysimeter and field trial sites. The Soil-Plant-Air-Water (SPAW) software estimated values for soil hydraulic properties which are listed in Table 2.1 and 4.2. Cultivar specific parameters measured during the growing season are listed in Appendix 3, and all the parameters that were changed in the model are also provided.

Table 4.2: Measured and calibrated soil hydraulic properties for the field trial site.

Depth (m)	BD[a] kg m^{-3}	LL15[b] m^3 m^{-3}	DUL[c] m^3 m^{-3}	SAT[d] m^3 m^{-3}	K_s cm day^{-1}
0.00-0.15	1540	0.14	0.24	0.35	500
0.15-0.30	1560	0.14	0.24	0.35	1000
0.30-0.60	1580	0.14	0.22	0.30	1000
0.60-0.90	1580	0.14	0.22	0.30	500
0.90-1.20	1580	0.14	0.22	0.30	500
1.20-1.50	1580	0.14	0.22	0.30	500
1.50-1.80	1580	0.14	0.22	0.30	500

BD is bulk density, LL is crop lower limit, DUL is drained upper limit, SAT is saturation and K_s is saturated hydraulic conductivity. [a]Estimated using SPAW pedo-transfer functions, [b-d]Derived from observed soil moisture content data collected by capacitance sensors.

4.3.1 Bromide concentrations

Bromide was applied 41 DAP, and according to APSIM peaked at 0.25 m at 168.4 kg Br ha^{-1} 51 DAP. It took 60 days for Br$^-$ at 0.25 m depth to be less than 1 kg Br ha^{-1}

after reaching the peak concentration, and the model simulated Br⁻ movement well because the r^2 and MAE% values were in the acceptable range, however, the D value was not in the range and RMSE value was high (Figure 4.2a and Table 4.3). At 0.50 m depth, the concentration peaked at 163.2 kg Br ha⁻¹ 57 DAP, and, after peaking it took 70 days to reach less than 5 kg Br ha⁻¹. At 0.50 m depth, the r^2 and D values were in the acceptable range, whereas the MAE% was above the acceptable range by 53% and the RMSE value was high (Figure 4.2b and Table 4.3).
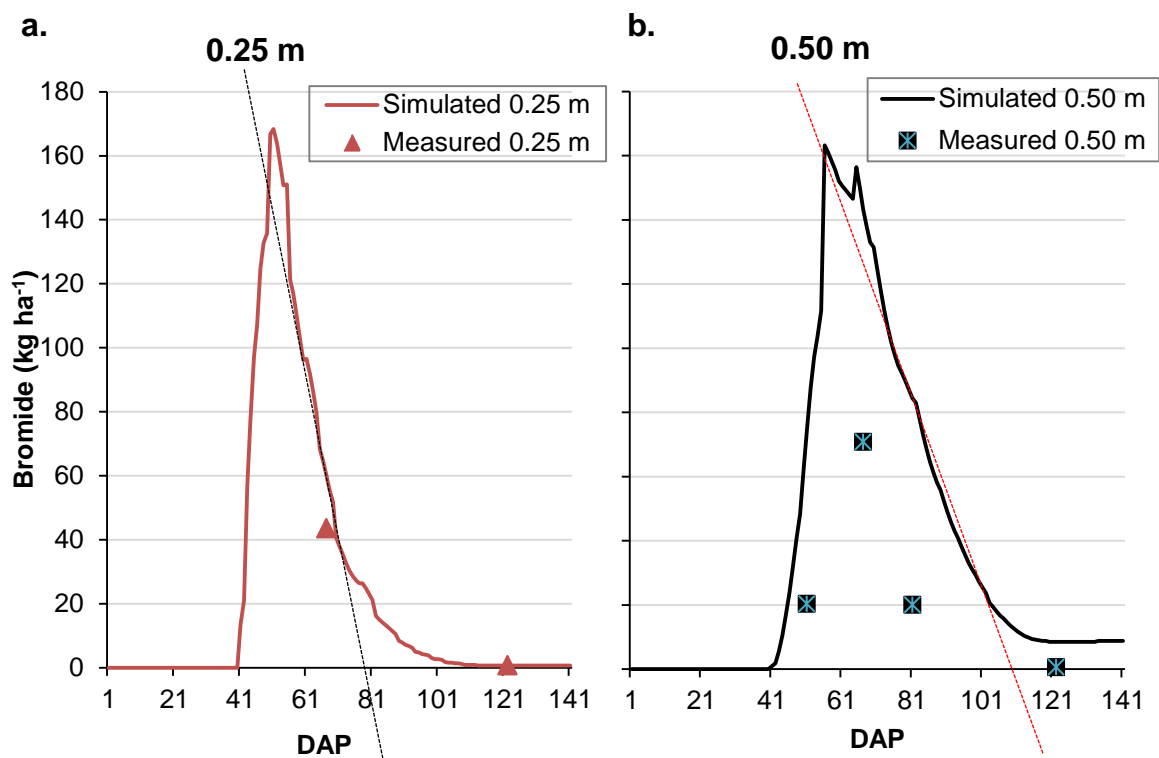
Figure 4.2: Measured and simulated bromide Br⁻ concentration at (a) 0.25 m and (b) 0.50 m. The rate of Br⁻ leaching was estimated using the declining concentration slope, with a dashed line touching many points on the declining slope.

The Br⁻ concentration was more dispersed (remained with higher concentration after peaking) at 0.50 m depth than at 0.25 m because of a lag of water movement. Water wets the topsoil first before moving to lower layers, delaying the movement of Br⁻. The movement of Br⁻ was 7.2 kg Br ha⁻¹ day⁻¹ at 0.25 m, whereas at 0.50 m it was

2.9 kg Br ha^{-1} day^{-1}, and values for Br$^-$ loss were calculated using the declining concentration slope, indicated with dashed slope on Figure 4.4. Using the model to simulate the possible Br$^-$ leaching at 0.9 m it can be equated to 26.6 to 68.0 kg ha^{-1} season^{-1}, and the leaching range (minimum and maximum) was derived from the declining slope.

Table 4.3: Statistical evaluation of measured and simulated bromide (Br$^-$) concentration in fertilised and unfertilised plots.

Depth (m)	n	r^2	D	MAE%	RMSE (kg ha^{-1})
0.25	3	0.98	0.53	8.91	11.33
0.50	4	0.86	0.89	33.22	8.09

4.3.2 Volumetric water content

Figures 4.3 (a-c) and 4.4 (a-c) shows the simulated and measured VWC at soil depths of 0.15, 0.30 and 0.50 m. APSIM was able to simulate VWC at the depths of 0.15 and 0.30 m well, as they had low MAE% values of less than 5% for both the fertilised and unfertilised plots. Although r^2 and D values at 0.15 and 0.30 m did not meet the criteria for a good simulation, the MAE% and RMSE values were in the acceptable range. However, the VWC simulation at 0.50 m in the fertilised plots was over estimated from 58 to 141 DAP, whereas in the unfertilised plots the VWC simulation only started to be over-estimated from 110 to 141 DAP. At 0.5 m, the MAE% and RMSE values met the criteria for a good simulation in fertilised and unfertilised plots, but they had poor D and r^2 values for all the simulations, except for unfertilised plots at 0.25 m which had a D value of 0.82 (Tables 4.4 and 4.5).
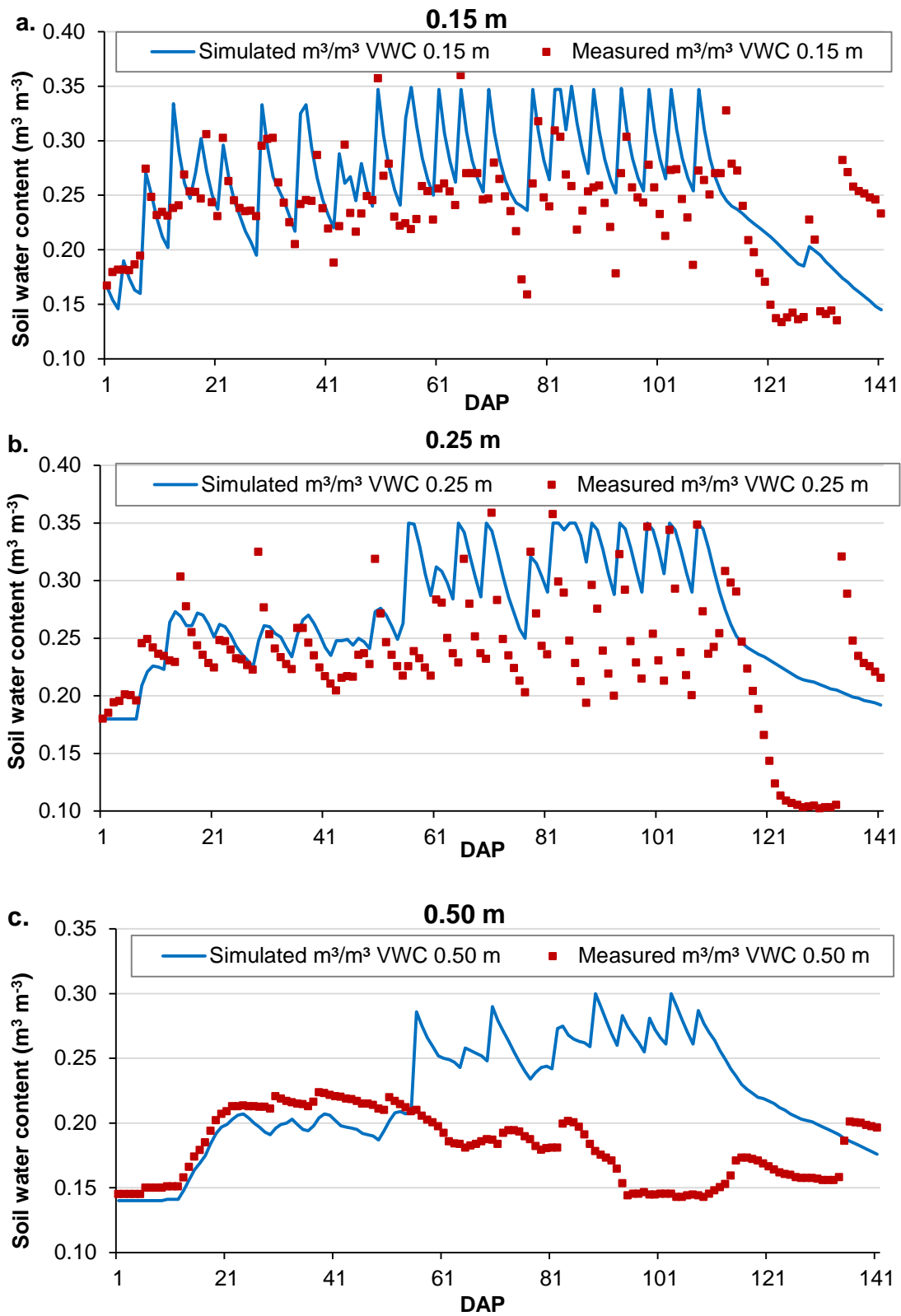
Figure 4.3: Measured and simulated volumetric water content (VWC) at (a) 0.15 m, (b) 0.30 m and (c) 0.50 m in fertilised plots.
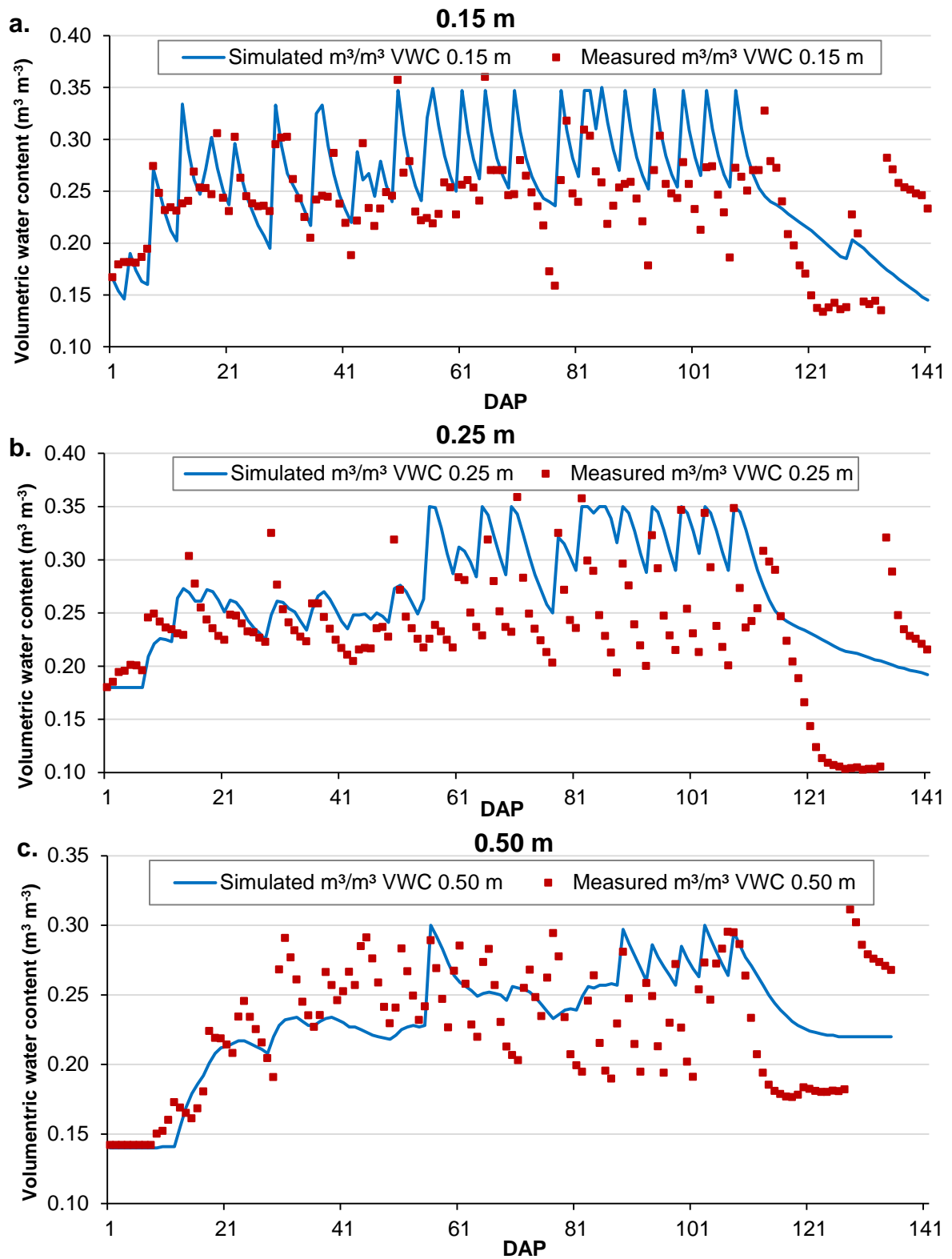
Figure 4.4: Measured and simulated volumetric water content (VWC) at (a) 0.15 m, (b) 0.30 m and (c) 0.50 m in unfertilised plots.

In all the plots, from 120 to 141 DAP the VWC sensor at all the depths were non-responsive and recorded low water content figures, which could have been caused by dry conditions of less than 0.1 m^3 m^{-3}. These dry conditions were experienced close to the physiological maturity as irrigation water is withdrawn to facilitate wheat drying off.

Table 4.4: Statistical evaluation of measured and simulated volumetric water content in fertilised plots.

Depth (m)	r^2	D	MAE%	RMSE (m^3 m^{-3})
15	0.34	0.52	4.0	0.05
25	0.31	0.51	4.9	0.06
50	0.01	0.41	5.1	0.07

Table 4.5: Statistical evaluation of measured and simulated volumetric water content in unfertilised plots.

Depth (m)	r^2	D	MAE%	RMSE (m^3 m^{-3})
15	0.01	0.48	9.2	0.11
25	0.31	0.82	2.3	0.03
50	0.33	0.71	3.1	0.04

4.3.3 Leaf area Index (LAI)

The model simulated the LAI for the fertilised plots well, but slightly over-estimated the LAI for fertilised plots, except at 85 DAP when it accurately simulated LAI (Figure 4.5). The model performed well to estimate the LAI in the fertilised and unfertilised plots as the r^2 and D values were greater than 0.8 and a low RMSE value although the D values were poor (Table 4.6).
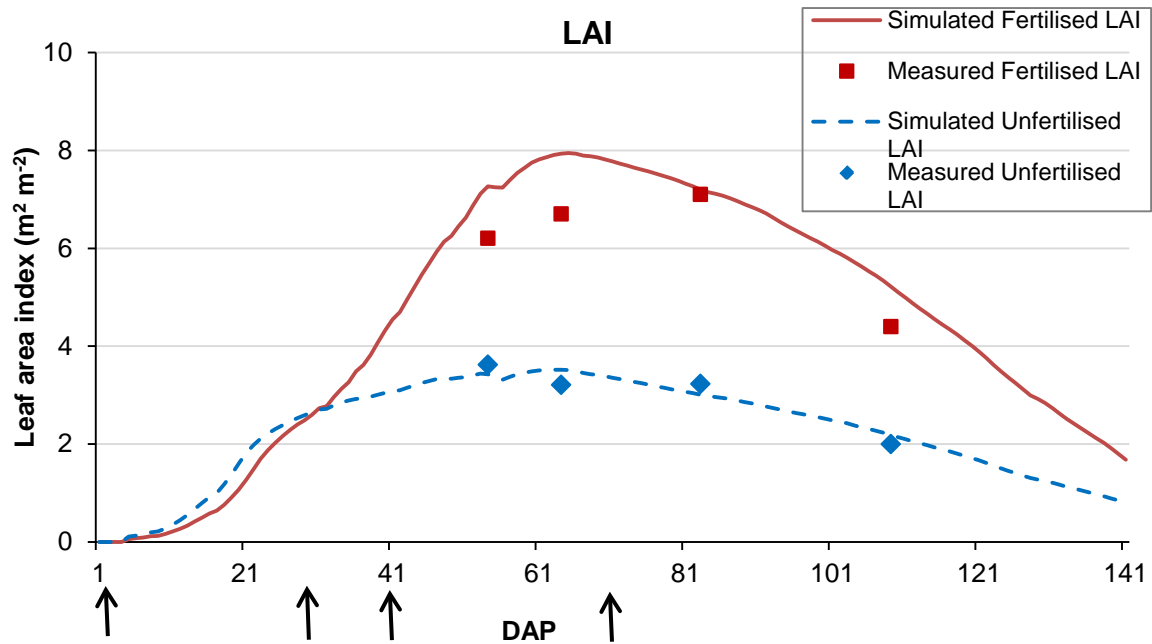
Figure 4.5: Measured and simulated leaf area index (LAI) in fertilised and unfertilised plots. The arrows indicate when fertiliser was applied to the fertilised plots (0, 29, 41 and 71 days after planting (DAP)).

The LAIs between the fertilised and unfertilised plots were initially similar, most likely due to access of mineralised N, but at 8 DAP there was a clear difference between the two treatments until 30 DAP. The high plant vigour may have been caused by mineralisation which supplied adequate N to ensure better LAI development. Mineralisation in fertilised plots and N applied at planting may have resulted in excess N in the root zone, which may have reduced LAI development, as excess N in the rhizosphere can inhibit root growth (Tian et al. 2008).

Table 4.6: Statistical evaluation of measured and simulated values for leaf area index (LAI) in fertilised and unfertilised plots.

Plot	r^2	D	MAE%	RMSE ($m^2\ m^{-2}$)
Fertilised	0.83	0.63	28.4	0.91
Unfertilised	0.86	0.97	22.8	0.23

4.3.4 Total above-ground dry matter (TDM) production and grain yield

The model was able to simulate the TDM and final grain yield well (Figure 4.6a) in fertilised plots. Although the TDM was overestimated in the early season and underestimated during the mid-season, all the model performance criteria were met (r^2, D, MAE% and RMSE), except for grain yield MAE% which was over by 9% (Table 4.7). On unfertilised plots, the TDM and grain yield was simulated well because the model performance criteria (r^2, D, MAE% and RMSE) were in the acceptable range, except for TDM MAE% which was above the threshold by 17% (Figure 4.6b and Table 4.7).

Table 4.7: Statistical evaluation of measured and simulated values for total aboveground dry matter (TDM) and grain yield on fertilised and unfertilised plots.

Plot	TDM				Grain yield			
	r^2	D	MAE%	RMSE (t ha^{-1})	r^2	D	MAE%	RMSE (t ha^{-1})
Fertilised	0.83	0.85	19.0	2.42	1.00	0.63	28.7	4.18
Unfertilised	1.00	0.95	36.9	0.38	1.00	0.98	7.7	0.11
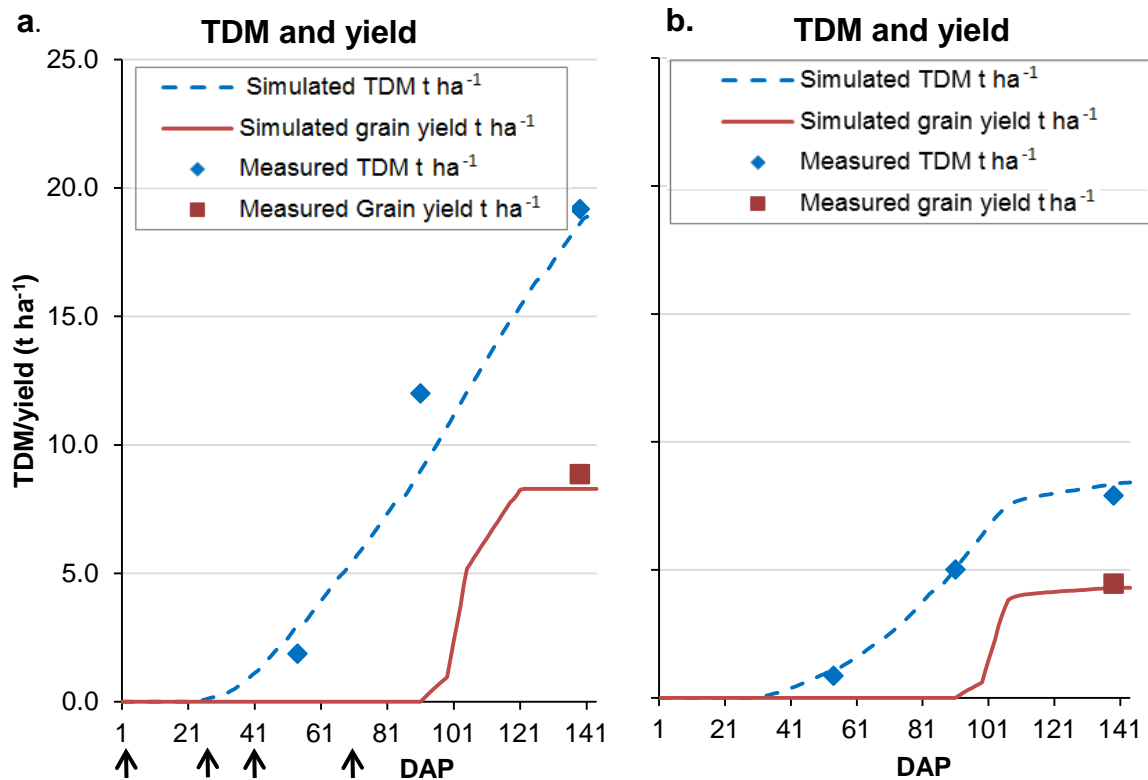
Figure 4.6: Measured and simulated total aboveground dry matter (TDM) and grain yield for the (a) fertilised and (b) unfertilised plots. Arrows indicate when the fertilised plots were fertilised at 0, 29, 41 and 71 days after planting (DAP).

4.3.5 Soil water nitrate-nitrogen concentrations

Figures 4.7 and 4.8 shows the soil NO_3-N in fertilised and unfertilised plots at 0.25 m and 0.50 m depths. Soon after planting, the SC and WFD NO_3-N concentrations were underestimated by APSIM at 0.25 and 0.50 m depths in fertilised plots, but the simulations improved as the season progressed. At the 0.25 m depth in fertilised plots, the NO_3-N concentration in WFDs was simulated well, and this may be attributed to settling which minimised overestimation due to mineralisation. Since the SCs were installed just before planting, the overestimation of NO_3-N could be due to increased mineralisation as a result of soil disturbance during installation and during seedbed preparation. In unfertilised plots, the SCs also overestimated soil NO_3-N soon after planting just like in fertilised plots, but the WFD simulated the soil NO_3-N concentration well, probably because they had settled and the N pulse from

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increased mineralisation due to soil disturbance during seedbed preparation may not have been deep enough to be detected at 0.25 and 0.50 m depths. Generally, the measured WFD NO_3-N concentration was simulated well by APSIM in both fertilised and unfertilised plots, and the measured SC NO_3-N concentrations started to agree with the simulated values after 30 DAP until harvesting. Although the statistics show that the simulations were not good (Table 4.8), a trend can be seen that the APSIM simulation were able to give the same concentrations as WFDs. Suction cup concentrations were high soon after planting, but later into the growing season the concentrations reduced and were more closely simulated.
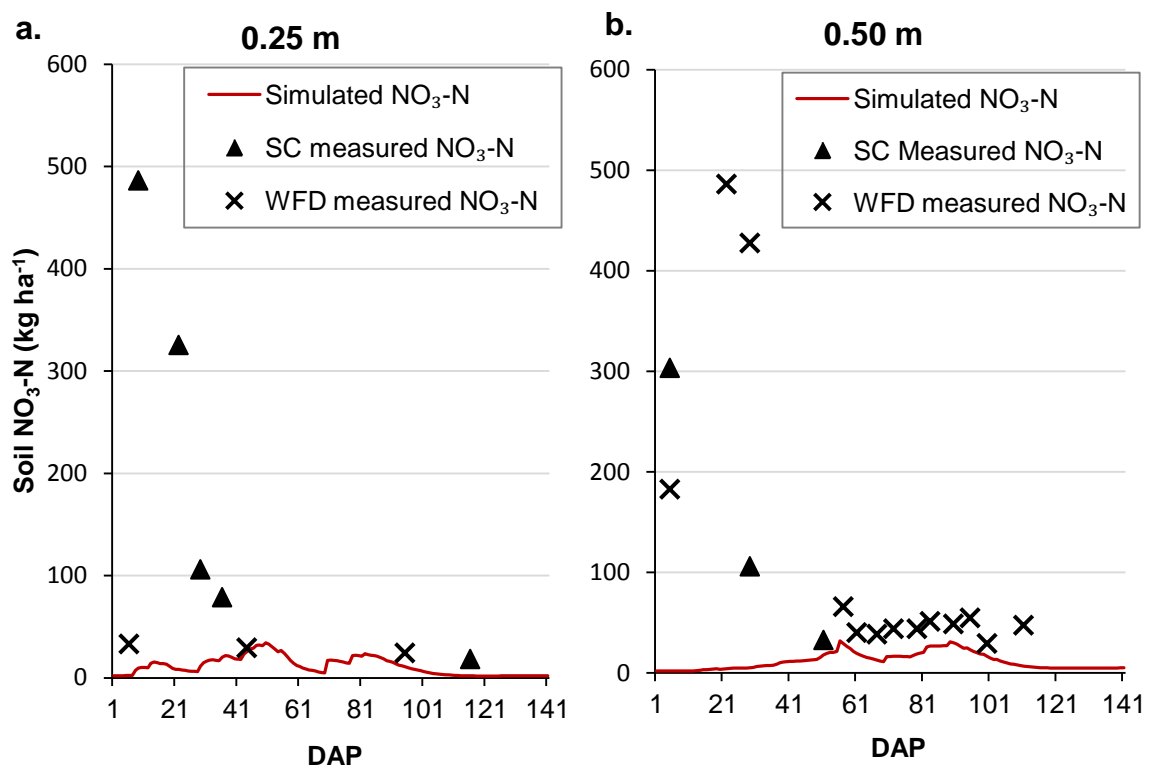
Figure 4.7: Simulated and measured soil water nitrate-nitrogen (NO_3-N) concentration in fertilised plots for (a) 0.25 m and (b) 0.50 m soil depth. Measured NO_3-N was collected by suction cups (SC) and wetting front detectors (WFD).
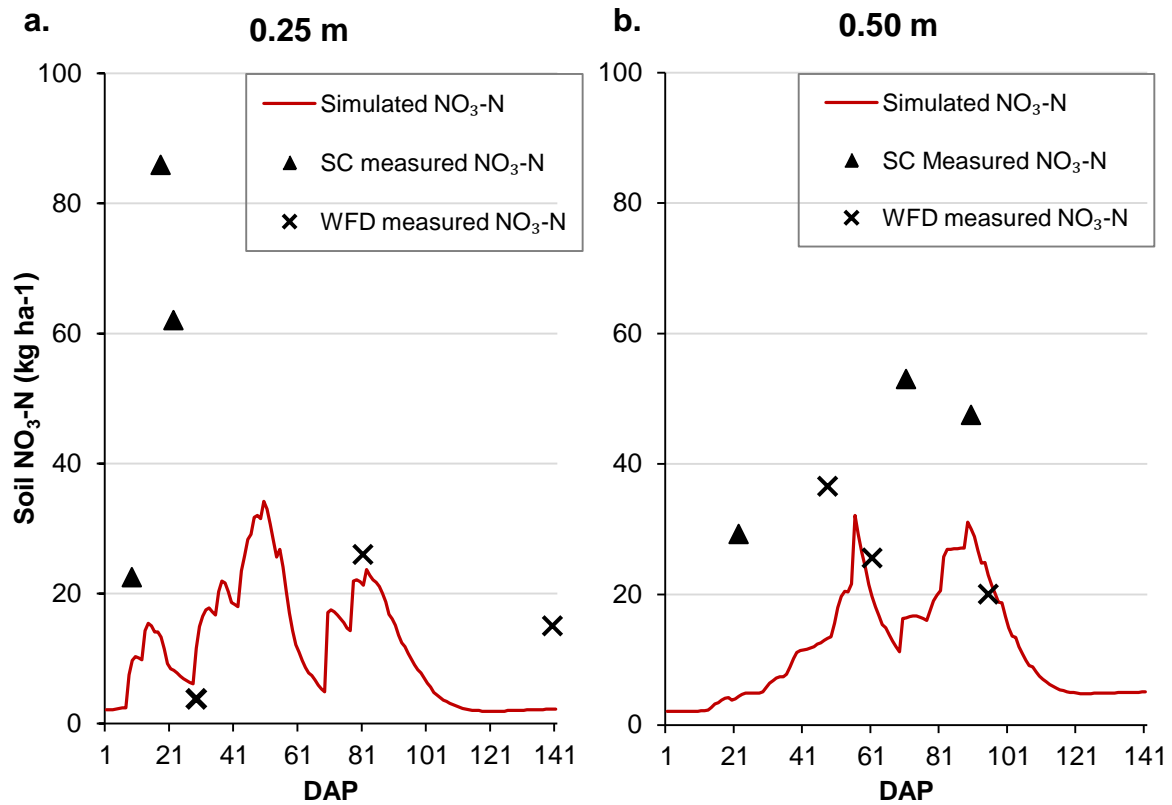
Figure 4.8: Simulated and measured soil water nitrate-nitrogen (NO₃-N) concentration in unfertilised plots for (a) 0.25 m and (b) 0.50 m soil depth. Measured NO₃-N was collected by suction cups (SC) and wetting front detectors (WFD).

Table 4.8: Statistical evaluation of measured and simulated nitrate-nitrogen (NO_3^-N) concentration in fertilised and unfertilised plots measured from suction cups (SC) and wetting front detectors (WFD).

Plot	Instrument	Depth (m)	r^2	D	MAE%	RMSE (kg ha^{-1})
Unfertilised	SC	0.25	0.33	0.50	46.4	30.42
Unfertilised	WFD	0.25	0.50	0.13	6.7	4.00
Unfertilised	SC	0.50	0.50	0.43	35.4	21.12
Unfertilised	WFD	0.50	0.50	0.31	21.1	16.50
Fertilised	SC	0.25	0.00	0.92	19.2	11.66
Fertilised	WFD	0.25	0.07	0.50	15.7	11.13
Fertilised	SC	0.50	0.68	0.90	33.9	26.01
Fertilised	WFD	0.50	0.30	0.82	32.2	38.97

4.3.6 Nitrate-nitrogen leaching

The cumulated leached NO_3-N was 22.7 kg ha^{-1} for the fertilised plots, whereas the daily leached NO_3-N reached a maximum of 1.6 kg ha^{-1} on 100 DAP (Figure 4.9a) at the 0.9 m soil depth. In fertilised plots, the third split top dressing coincided with intensified NO_3-N leaching. In unfertilised plots, the cumulative leached NO_3-N was 4.5 kg ha^{-1}, and the daily leached NO_3-N peaked at 0.2 kg ha^{-1} 61 DAP (Figure 4.9b). The leached NO_3-N peaked early in unfertilised plots, which suggested the loss of mineralised N from soil organic matter (SOM) in unfertilised plots.
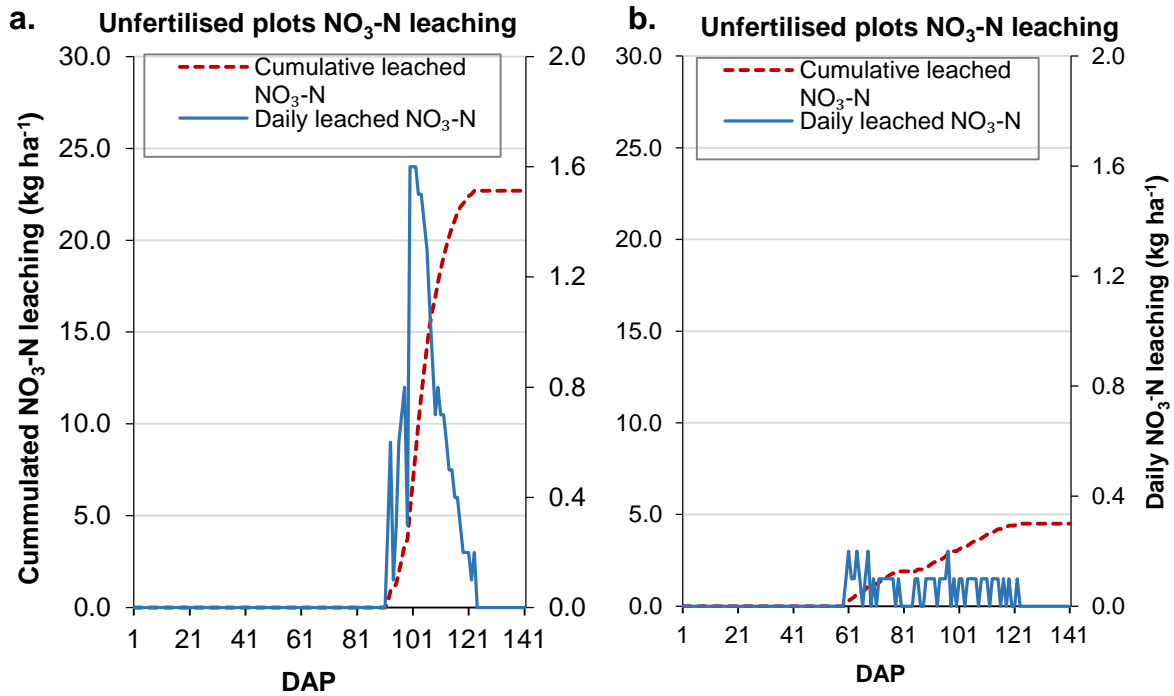
Figure 4.9: Simulated daily and cumulative nitrate-nitrogen (NO₃-N) leaching in (a) fertilised plots and (b) unfertilised plots at a soil depth of 0.9 m.

4.4 Discussion

The APSIM model was able to simulate well the TDM, grain yield, VWC and Br⁻ movement on fertilised and unfertilised plots. Although the model performed well on some parameters, high D and low RMSE values, there was poor correlation reflected by low r^2 values for Br⁻ and NO₃-N concentration in some instances, as the model did not perform well on all the statistical analyses for all considered parameters. The poor r^2 values implied that the observed and simulated values were, at most, not linearly correlated, and; therefore, the good model performance was indicated by high D and low RMSE values. The fertilised plots leached more N, and this can be reduced by determination of initial N available to crops and timing of split top dressings.

4.4.1 Bromide concentrations

The Br^- concentrations were found to be more dispersed at 0.50 m soil depth compared to 0.25 m depth. The increased Br^- dispersion was caused by diffusion process and hydrodynamic dispersion in a myriad of soil pore sizes and tortuosity in flow paths as the soil deepens (Tillman 1991, Radcliffe and Šimůnek 2010). Despite Br^- and NO_3^- being anions of almost similar molecular weight and charge, Clay et al. (2004) observed higher Br^- leaching rate when compared to NO_3-N because of different sorption characteristics. Bromide and NO_3^- have a sorption of 0.002 ± 0.036 mg kg^{-1} and 0.17 ± 0.03 mg kg^{-1} of soil, respectively, and converted Br^- leaching to NO_3-N leaching amount by reducing with 25%. The faster movement of Br^- was also observed in this study. If observed Br^- leaching potential (2.9 to 7.4 kg Br ha^{-1} day^{-1}) of the Hutton soil is reduced by 25%, then 2.2 to 5.6 kg NO_3-N ha^{-1} day^{-1} (20.2 to 51.5 kg NO_3-N season^{-1}) would be expected, and the APSIM simulated maximum NO_3-N leaching concentration was in this range. Therefore, the Br^- was able to establish the upper leaching potential of a sand clay loam Hutton soil, and they have a high risk of heavy leaching.

4.4.2 Volumetric water content

APSIM simulated VWC well for all the depths. Typically, wheat is planted in winter in South Africa and relies on irrigation. In a study done in Asia using APSIM, the VWC of wheat varieties grown in India and China were simulated well, but the model was not able to simulate water content under water stressed conditions well (Gaydon et al. 2017). Simulating episodes of water stress when water content is less than 0.1 m^3 m^{-3} has also been reported in other crop models such as Soil Water Balance (SWB), where the model was not able to simulate low water levels in maize and wheat systems (Van der Laan 2009, Van der Laan et al. 2010). Water stress did not negatively influence the results, as the crop was supplied with adequate water based on crop water requirements.

4.4.3 Leaf area Index (LAI)

Leaf area index (LAI) was simulated well. The unfertilised wheat LAI showed an early vigour for the first 30 DAP. Early vigour can be attributed to mineralisation that commenced during fallow period before planting, and due to disturbed soil and decomposed SOM after planting, which supplied adequate nutrients to the plants for the first 30 DAP. Limited N in the root zone can promote deeper roots (Jiang et al. 2017), which allows plants to have a large surface area to extract nutrients and limit the amount of N losses from the soil. Since better LAI was simulated on unfertilised plots, first N top dressing on wheat can, therefore, could target 30 DAP to support increased crop growth rates. Soil analysis results also indicated the availability of residual N fertiliser from the previous crop which could have benefited the establishing crop.

4.4.4 Total aboveground dry matter production and grain yield

The TDM and grain yield of wheat were simulated well, and the small discrepancies in observed and simulated values can be due to how radiation use efficiency (RUE) and temperature are simulated in the model. Typically, a sigmoidal growth curve is expected for crop growth, but this was not exhibited on fertilised plots because the RUE in the wheat module has a constant value which is not varied along the growing season (Zheng et al. 2014). Thus, when crops are fertilised the biomass accumulation is rapid in the early season and fail to exhibit the expected normal growth curve, whereas in unfertilised plots there is slow accumulation of biomass which allow the distinct sigmoid shape to be exhibited. In APSIM, the RUE has a default value of 1.24 g MJ^{-1} (Zheng et al. 2014), which was adjusted to 1.84 g MJ^{-1} during calibration to improve simulations.

On the other hand, the average temperature is calculated by taking an average of maximum and minimum air temperatures, but such an average may have a lower average when smaller time frames of an hour are considered, and, when seasons are changing from the cool to dry season (from July to August). Gaydon et al. (2017) also reported poor TDM and grain yield simulations for late-planted wheat in India

because of lower cardinal temperatures that are default in APSIM. As the wheat was planted in July, the average daily temperatures may not represent the shorter time frame temperature changes which can influence plant growth, and therefore simulated TDM was overestimated in the early season and underestimated mid-season. However, the variation between the measured and simulated values were small and did not affect the overall TDM and grain yield simulations, and therefore, N uptake was not compromised. Nitrogen uptake influences the amount of N that remains in the soil or leaches from the soil.

4.4.5 Soil water nitrate-nitrogen concentrations

Since the WFD was able to measure the simulated NO_3-N, it showed that the WFD can be a simple instrument that can be used to quantify the soil N status and monitor N leaching if they are allowed to settle. Van der Laan et al. (2010) reported conflicting results with this study, as they found that SC had higher NO_3-N concentrations compared to WFD, for they attributed WFD to be sampling from draining water that was by-passing the soil matrix. However, in this study water samples collected from settled WFD were simulated well with APSIM.

The measured SC NO_3-N concentration in fertilised plots was not simulated well. Since fertiliser was applied at planting, it may have contributed to increased NO_3-N movement that was detected at 0.25 and 0.50 m depths. The under-estimation can also be caused by APSIM's failure to simulate high mineralisation capacity of the trial soil, as Van der Laan et al. (2010) reported high NO_3-N in unfertilised plots because of mineralisation. Disturbing the soil also increase mineralisation (Courtaillac et al. 1998), for Kristensen et al. (2000) reported mineralisation to double in disturbed soils previously with a mono culture of maize and under no till system, and the increased mineralisation may have added to the soil NO_3-N and was detected and measured by the SCs.

4.4.6 Nitrate-nitrogen leaching

Nitrate-nitrogen leaching was 88% higher on the fertilised plots compared to unfertilised plots. The NO_3-N leaching peaked at 100 DAP in fertilised plots, which also coincided with the third N top dressing. High NO_3-N leaching was also reported in Hutton soils under sugarcane production (Van der Laan et al. 2011). They reported leaching losses of 31% of the applied fertilised on planted sugarcane field, whereas in this study it was 34% of the applied fertiliser. Considering the time taken to grow sugarcane compared to wheat, the intensity of leaching losses is higher under irrigated wheat systems as observed in this study. Although splitting the N fertiliser potentially helps in reducing the amount of NO_3-N leaching (Van der Laan et al. 2011), timing of the N top dressing can also help. From this study, the first N application at planting can be reduced or omitted, and the third top dressing can be applied earlier so that NO_3^-N leaching can be reduced. Such information from this study can be useful to farmers if N availability and mineralisation of the soil is known, otherwise, more work is required to evaluate how management practices may influence N availability and eventual fine tuning of fertiliser recommendations.

N processes depend on soil temperature, but it is estimated using air temperature in APSIM. Such an approach has a tendency of over-estimating soil N process such as mineralisation, immobilisation, nitrification and denitrification. Van der Laan et al. (2011) observed some significant differences in net mineralisation in sugarcane fields because of slight over-estimation of simulated soil temperature in winter, when they used Canegro-N model.

4.5 Conclusion

The potential NO_3-N leaching potential of the Hutton soil has a range of 20.2 to 51.5 kg N ha^{-1} season^{-1} at a soil depth of 0.9 m. APSIM was able to simulate VWC, TDM and grain yield well, and hence can be used to estimate N leaching. Well-timed fertiliser applications will reduce N leaching. Use of modelling and infield monitoring of NO_3-N movement can lead to better understanding of N dynamics, which will help to refine fertiliser recommendations and reduce NO_3-N leaching.

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GENERAL DISCUSSION

5.1 Overview

Under intensive agricultural systems, nitrogen (N) leaching is one of the major pathways that contribute to non-point source pollution in water bodies (Prasertsak et al. 2002; Van der Laan et al. 2011). Once N is applied in cultivated soils, various N sources can undergo N transformations, such as nitrification and mineralisation, which can increase the susceptibility of N loss if not taken up by the plants. Quantifying NO_3-N leaching losses in cultivated soil is difficult, as methods fail to measure or estimate leaching loads because a flux and representative concentration are required (Van der Laan 2009, Van der Laan et al. 2011, Van der Laan et al. 2014). As a result, there is no universal method used to quantify N losses, yet such information is required in order to calibrate models, which can be used as a proxy to predict losses and aid field N management decisions and, or assist in policy formulation for N use.

5.2 General discussion

The purpose of this study was to evaluate and compare different techniques that measure or estimate NO_3-N leaching load. Several techniques that were evaluated include: lysimeters, stable isotopes, conservative tracers and modelling. The first objective was to evaluate the performance of a drain gauge in measuring drainage and NO_3-N leaching against a weighing lysimeter, and the second objective was to determine the fertiliser N use efficiency (FNUE) in a wheat (*Triticum aestivum* L.) cropping system. Fertiliser-NUE determination was important because there was a need to quantify N uptake from applied fertiliser, and estimate the amount that would potentially leach out of the root zone. Third and fourth objective was to quantify the potential N leaching using conservative tracer, and to evaluate and validate the performance of APSIM after calibration.

Firstly, the drain gauge's performance was checked against a weighing lysimeter, by measuring the drainage and N leaching (Chapter 2). More frequent drainage was measured using a drain gauge compared to weighing lysimeters. Drainage collected by a drain gauge was 54.1 mm, which was 338% more than the average drainage for the two weighing lysimeters. Even though all the lysimeters recorded some drainage, the NO_3-N concentration was undetectable in the draining water, whereas the drain gauge average season NO_3-N concentration was 46.1 mg L^{-1}. As saturated soil conditions were created at the bottom of a weighing lysimeter, they caused anaerobic conditions that reduced NO_3-N loss through leaching but aggravated denitrification. The drain gauge maintained unsaturated conditions because of a wick that was put in the divergence control tube.

Secondly, stable isotopes were used to determine the FNUE (Chapter 3). Stable isotopes managed to distinguish between the N sources, derived from applied fertiliser or soil N, in the analysed plant material. The FNUE was 68%, which meant that 32% of the applied fertiliser remained unused in the soil profile. As 200 kg N ha^{-1} was applied to the fertilised plots, the fertiliser that remained in the soil profile was 64 kg N ha^{-1} or 49.6 kg NO_3-N ha^{-1}. Since the drain gauge measured 24.9 NO_3-N kg ha^{-1}, this suggests that approximately 50% of the remaining fertiliser was lost through leaching, yet the other half was still left in the root zone that could have led to more leaching, even after harvesting the crop. However, the stable isotopes method did not directly quantify NO_3-N leaching in the soil, and that the changing $\delta^{15}N$ values in the soil were difficult to interpret, as nitrification during mineralisation, denitrification or volatilisation are all reported to enrich the soil with $\delta^{15}N$ values. The stable isotopes managed to provide useful information on how much fertiliser can be applied without leaving excess residual N in the soil, which can decrease the risk of N export into water sources.

Drainage and NO_3-N concentration from the weighing lysimeter and drain gauge can be combined with stable isotopes to further explain the N dynamics. The lysimeters and drain gauge allows for the quantification of N leaching, but does not account for plants' uptake. Using the ^{15}N stable isotopes, the NO_3-N taken up by the plant was

105.4 kg ha^{-1}. Stable isotopes at plot level provided the seasonal plant requirements, whereas the weighing lysimeters showed that denitrification was the main cause of N loss under saturated soil conditions, whereas NO_3-N leaching prevailed under unsaturated soil conditions. All techniques consolidated our understanding of N movement in the soil, so that N movement in the soil can be properly modelled.

The third and fourth objectives were combined, and APSIM was calibrated on wheat for the first time in South Africa. The objectives were to determine the potential leaching using bromide (Br$^-$) conservative tracer and validate the calibrated APSIM model. There were good APSIM simulations for leaf area index (LAI), grain yield, TDM and NO_3-N that warranted more confidence in the predicted NO_3-N leaching (Chapter 4). The APSIM predicted leaching amount was agreeable with the NO_3-N measurement from a drain gauge, 22.7 and 24.9 kg ha^{-1} respectively. The leached NO_3-N was within the range that was stipulated with a Br$^-$ tracer. Since APSIM simulated LAI, grain yield, TDM and water content on fertilised and unfertilised well, the model can be used for making decisions on N management in wheat cropping systems. Although the unfertilised plots had significantly lower leached NO_3-N (4.5 kg ha^{-1}), they had 44% lower grain yield compared to fertilised plots. Lower yield of this magnitude will not motivate farmers even if the plots had lower N leaching. An appropriate compromise can be set by running several model simulations to optimise the grain yield while minimising the N leaching losses.

Soil NO_3-N was monitored using suction cups (SC) and wetting front detectors (WFD). Soon after planting, high NO_3-N concentration in the top 0.0 to 0.3 m measured by SCs and WFDs indicated increased mineralisation. Such information from SC and WFD indicated the soil N movement in the soil profile, other than relying on NO_3-N concentrations measured at a single depth, which was the case for drain gauge and the weighing lysimeter. Initial soil water NO_3-N concentration was high irrespective of fertilisation, which suggested proper timing of N applications to avoid excess amounts in the root zone.

Overall, the objectives were met. The drain gauge managed to quantify the NO_3-N leaching, whereas the stable isotopes were used to calculate the FNUE. The calibrated APSIM performed well and was used to predict leached NO_3-N in wheat cropping system.

5.3 References

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CONCLUSIONS AND RECOMMENDATIONS

The drain gauge performed well in measuring drainage and NO_3-N leaching. The wick in the drain gauge ensured unsaturated bottom boundary conditions, and represented the field conditions better than the case of saturated conditions created in the weighing lysimeter. The drain gauge can be used to quantify NO_3-N leaching, although further testing is still required on several crops and seasons to further check seasonal performance.

The stable isotopes natural abundance method distinguished between applied fertiliser N and soil-derived N taken up by the crop. There was a strong positive correlation between the flag leaf δ^{15}N values and plant N% on both the fertilised and unfertilised plots at physiological maturity, so flag leaf δ^{15}N values can be used to calculate FNUE instead of whole plant analysis. The FNUE was 68%, which meant that 32% of the applied fertiliser that was not used by the crop. Although stable isotopes analysis differentiated various N sources, it was not able to specify the main N transformation process occurring in the soil or plant. Hence, the use of labelled fertilisers is recommended to clarify when and how the N transformations occur. Since there is evidence of the crop failing to use all the applied fertiliser, crop sequences have to be carefully designed to cater for excess N leached into deep soil layers, as this can be achieved by planting deep rooted crops such as sunflowers.

The potential N leaching of the Hutton soil was estimated to range from 20.2 to 51.5 kg NO_3-N ha^{-1} season^{-1} at a soil depth of 0.9 m. A calibrated APSIM model was able to simulate soil water content, TDM and grain yield well and was used to predict N leaching. The predicted season NO_3-N leaching agreed with the measured quantities from the drain gauge, which demonstrated that modelling and infield monitoring of NO_3-N movement can be used to understand N dynamics better. Such information is essential to refine fertiliser recommendations and reduce NO_3-N leaching.

Further research is required to evaluate the methods in different agro ecological wheat growing regions in South Africa. The low leaching measured in the weighing lysimeter will require redox potential sensors to verify the mechanism of N transformation that occurs in saturated bottom layers. Further running of several APSIM simulations is also recommended to explore various N management options for various wheat growing regions in South Africa, so that the results can have a wide range of application.

SUMMARY

Nitrogen (N) is the most applied inorganic fertiliser, as most agricultural soils are deficient of this element. Nitrate-nitrogen (NO_3-N) leaching has been reported in cultivated soils around the globe, and it is one of the main ways in which above- and below-ground water sources are polluted, but there is no universal method used to quantify leaching losses. The purpose of this study was to evaluate different techniques used to measure and predict NO_3-N leaching load and to determine the fertiliser N use efficiency (FNUE).

Two trial sites, lysimeter and field, were planted on the 30th of June 2016 with wheat (*Triticum aestivum* L.) cultivar PAN3400 at the University of Pretoria Experimental Farm, Hatfield, Pretoria. Firstly, the lysimeter trial consisted of two weighing field lysimeters and a drain gauge. Volumetric and matric potential water sensors and suction cups were inserted at 0.15, 0.30, 0.50 and 0.70 m depths in the weighing lysimeters and also close to the drain gauge. The site was fertilised at 200 kg N ha^{-1}, and had high density drip irrigation installed. After every irrigation cycle, drainage was collected and measured from the bottom of drain gauge and weighing lysimeters. Apart from measuring the drainage, water samples were collected from the bottom of weighing lysimeter and drain gauge and from suction cups (SCs), for determining the NO_3-N concentration.

Secondly, the field trial site consisted of six plots each with an area of 4 m^2, into which two sets of SCs, wetting front detectors (WFDs) and capacitance sensors were installed at 0.25 and 0.50 m depths. Fertiliser was applied at a rate of 200 kg N ha^{-1}, and bromide (Br$^-$) was also applied at a rate of 0.020 kg m^{-2} as a conservative tracer, for determining the potential NO_3-N leaching. Three of the plots were fertilised, and they were completely randomised with the unfertilised plots (where no fertiliser was applied). All the plots were installed with high density drip irrigation. Soil and fertiliser samples were collected before planting and analysed for a baseline of stable ^{15}N natural abundance (^{15}N‰ or δ^{15}N values) using a mass spectrometer. Soil

samples collected after harvesting and selected plant parts taken at tillering, anthesis and physiological maturity were also analysed for stable ^{15}N natural abundance. Water samples were collected from the WFDs and SCs to determine the NO_3-N and Br^- concentration.

On both sites, phenology and leaf area index (LAI), yield and total aboveground dry matter (TDM) were collected, and an automatic weather station close to the trial sites was used to collect weather data. Phenological and growth data from the lysimeter trial was used to calibrate APSIM (Agricultural Production Systems sIMulator), and the field trial data set was used to validate the model. Water samples were analysed for Br^- and NO_3-N concentration using ion chromatography and RQEasy Nitrate Reflectometer (Merck, Germany) respectively.

The first objective of the study was to evaluate the performance of a drain gauge when compared to a weighing lysimeter, so data from the lysimeter trial was used. The drain gauge drained more frequently and in greater amounts than on the weighing lysimeters, and 46.1 mg L^{-1} of NO_3-N concentration was measured in drained water from the drain gauge, but was not detectable in the drained water from the weighing lysimeters. Undetectable NO_3-N from weighing lysimeter drainage was attributed to denitrification in the saturated bottom layers, which resulted in N being lost as nitrogen oxides other than leaching. The drain gauge NO_3-N leaching load for the season was 24.9 kg ha^{-1}.

The second objective was to use the stable ^{15}N natural abundance to determine fertiliser N use efficiency (FNUE), so data collected from the field trial was used. Fertiliser-NUE was 68%, which meant that 32% of the applied fertiliser was not utilised by the crop. Different plant parts had varying $\delta^{15}N$ values, which was caused by different fractionation during plant N metabolism. However, the flag leaf $\delta^{15}N$ values and plant N% were strongly correlated when the wheat was at physiological maturity. Therefore, a flag leaf can be used to calculate FNUE and distinguish the different N sources taken up by the plants.

Data collected from both trial sites was used to answer the third and fourth objectives. The aim was to quantify the potential N leaching using conservative tracer, and to evaluate and validate the performance of APSIM after calibration with experimental data. Using Br^- conservative tracer, potential NO_3-N leaching ranged from 20.2 to 51.5 kg N ha^{-1} season^{-1}. When the wheat was fertilised, the calibrated APSIM predicted leaching NO_3-N to be 22.7 kg ha^{-1}. Drain gauge measured and APSIM predicted NO_3-N leaching agreed well, with a small discrepancy of 2.2 kg ha^{-1}. High soil NO_3-N concentration was measured from the WFDs and SCs soon after planting although it was poorly simulated by APSIM, the simulation became better as the season progressed. Measured monitoring data of NO_3-N concentration from SCs and WFDs complemented the modelling efforts and assisted to explain the fate of N in the soil profile.

As a result of an evaluation of various techniques in this research, the drain gauge can be used to measure NO_3-N leaching, and its drainage and NO_3-N outputs can also be used to calibrate the APSIM model. Furthermore, using the stable isotopes it was established that 32% of the applied fertiliser was unused, and the fate of the unused fertiliser can be investigated using APSIM.

ACKNOWLEDGEMENTS

APPENDIX

Appendix 1: Irrigation applied to fertilised and unfertilised plots from the 1st of July to 28th of October 2016

Irrigation Date	Unfertilised (mm)	Fertilised (mm)
01-Jul-16	6	6
04-Jul-16	9	9
08-Jul-16	24	24
18-Jul-16	11	11
13-Jul-16	38	30
22-Jul-16	15	15
29-Jul-16	37	28
05-Aug-16	18	23
12-Aug-16	7	15
14-Aug-16	0	5
16-Aug-16	5	10
19-Aug-16	20	25
25-Aug-16	15	18
30-Aug-16	21	25
03-Sep-16	25	35
08-Sep-16	33	46
16-Sep-16	29	34
20-Sep-16	31	40
21-Sep-16	9	10
27-Sep-16	38	39
02-Oct-16	40	40
07-Oct-16	40	40
11-Oct-16	40	41
16-Oct-16	40	40

Appendix 2: Calculation of fertiliser nitrogen use efficiency (FNUE)

The FUE and plant N nitrogen derived from fertiliser (Ndff) given in equation 3.2 was calculated using plant stable isotopes $\delta^{15}N$ value.

$$Ndff = \frac{Nu - Nt}{Nu - \frac{Nf}{n}} \qquad (3.2)$$

where: Nu   = atom % ^{15}N in unfertilized plants =   2.42

Nt   = atom % ^{15}N in fertilized plants =   -0.32

Nf   = atom % ^{15}N in the fertiliser (for example 0.006%) = -2.08

n   = the plant discrimination factor between ^{14}N and ^{15}N.

Assuming no discrimination between ^{14}N and ^{15}N, then n = 1.

Ndff = 61%

FUE was calculated using the following equations 3.2 to 3.4.

Total N uptake or N yield (kg ha^{-1}):

$$N\ yield = \frac{[\text{Yield dry matter (kg ha}^{-1}) \times \% \text{ total N}]}{100} \qquad (3.3)$$

Dry matter yield kg ha^{-1} = 18.03 tonnes

% N for the whole plant = 1.23%

N yield = 222.6 kg ha^{-1}

Fertiliser uptake or fertiliser N yield (kg ha^{-1}):

$$Fertiliser\ N\ yield\ (FNU) = \frac{[\text{N yield (kg ha}-1) \text{ x \% Ndff}]}{100} \qquad (3.4)$$

FNU = 222.6 kg/ha * 61/100 = 135.47 kg ha^{-1}

Fertiliser N use efficiency

$$\%FNUE = \frac{\text{Fertiliser N yield}}{\text{Applied N rate}} \times 100 \qquad (3.5)$$

% FNUE = 135.47/200 = 68%

Appendix 3: Genetic coefficients for wheat cultivar, PAN3400, planted on the 1st July 2016.

Cultivar parameters	Definition	Unit	Lysimeter plots
Grains_per gram_stem	Kernel number per stem weight at the beginning of grain filling	g	34.0
Potential_grain filling_rate	Potential daily grain filling rate	$g\ grain^{-1}\ day^{-1}$	0.0060
Potential_grain growth_rate	Grain growth rate from flowering to grain filling	$g\ grain^{-1}\ day^{-1}$	0.0022
max_grain_size	Maximum grain size	g	0.035
tt_start_grain_fill	Thermal time from start grain filling to maturity	^{o}C days	500
tt_floral_initiation	Thermal time from floral initiation to flowing	^{o}C days	450
tt_flowering	Thermal time needed in anthesis phase	^{o}C days	110
tt_end_of_juvenile	Thermal time needed from sowing to end of juvenile	^{o}C days	340
vern_sens	Sensitivity to vernalisation	–	2.2
photop_sens	Sensitivity to photoperiod	–	0
flowering_day	Flowering day after sowing	day	81
maturity_day	Maturity day after sowing	day	136
grain_filling	Number of days	day	55
rue	Radiation use efficiency	$g\ MJ^{-1}$	1.84

Appendix 4: Map showing lysimeter and field trial sites. Main map in yellow is the South African map and the small insert in the main map is the enlarged trial sites.

Appendix 5: Pictures of the lysimeter trial site, a. layout of lysimeters and drain gauge, and b. lysimeter 1 and 2
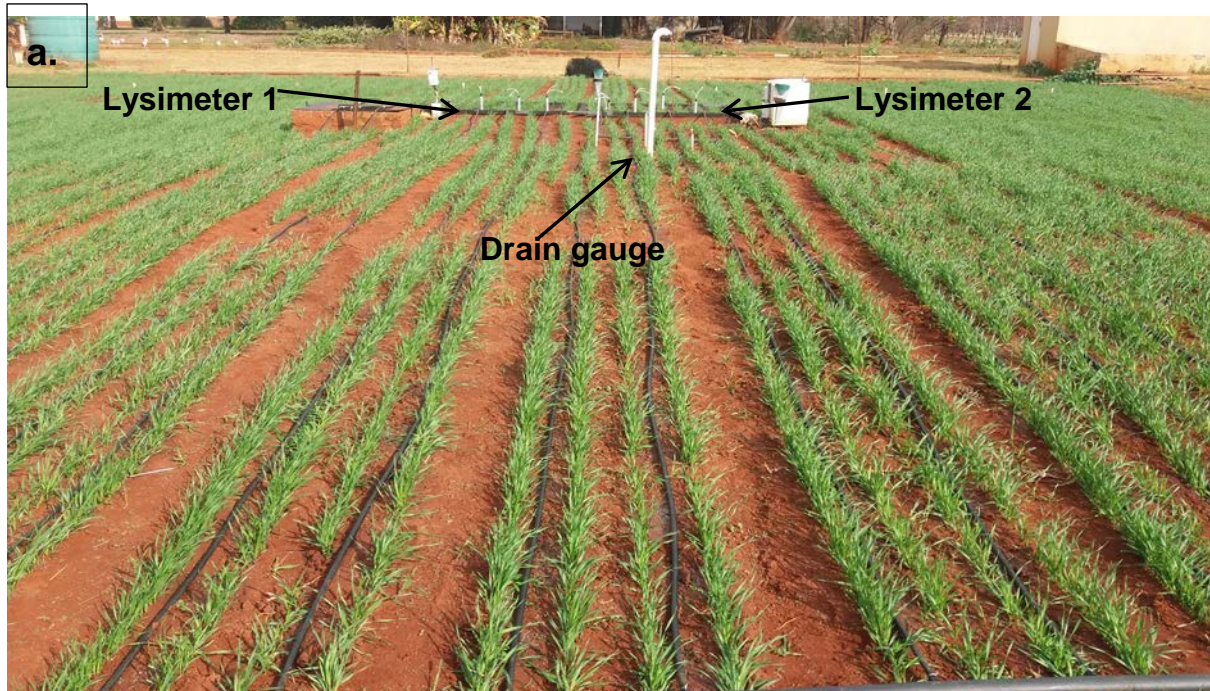
Appendix 6: Pictures of the field trial site, a. unlabelled plots were not fertilised and b. dry wheat ready for harvesting.