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Simulation of water and nitrogen dynamics in a Cerrado soil under coffee cultivation using SWAP and ANIMO models

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Simulation of water and nitrogen dynamics in a Cerrado soil under coffee cultivation using SWAP and ANIMO models

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ABSTRACT

PINTO, V. M. **Simulation of water and nitrogen dynamics in a Cerrado soil under coffee cultivation using SWAP and ANIMO models.** 2015. 123 p. Tese (Doutorado) – Centro de Energia Nuclear na Agricultura, Universidade de São Paulo, Piracicaba, 2015.

Agriculture when only focused on production leads to an unsustainable use of inputs with negative consequences to the environment and human health. One consequence of the excessive use of fertilizers is the pollution of surface and underground water resources in agricultural eco-systems and their boundaries. The Brazilian Cerrado has been suffering the transformations of the intensive agriculture during the last decades. Due to the poor fertility of soils, in general very sandy and of low pH, the use of agricultural inputs is intensified and the nutrient downward transport by leaching becomes a serious problem in different regions. Information about the current use practices of fertilizer use in the Cerrado environment must be gathered for a healthy transition of this biome. Models based on physical and chemical processes are useful tools to simulate water and nutrient dynamics in agricultural systems, including the related losses due to adopted managements. They have the potential to evaluate different scenarios to predict outcomings of such practices. Among the available models for such processes, SWAP (Soil, Water, Atmosphere and Plant model) has been used under several agronomic conditions to describe hydrologic processes, and ANIMO (Nitrogen in Agriculture model) to simulate N cycling in agricultural systems. Our study presents an application of SWAP to adult perennial coffee crops along one productive cycle, with focus on deep drainage losses and irrigation management in a representative Brazilian Cerrado management system. The SWAP/ANIMO combination was used in this study to simulate N absorption by coffee plants and N leaching in the form NO_3-N, as a result of an intensive fertilizer management practice. The ANIMO program was calibrated in relation to one N treatment, of 400 kg ha^{-1} $year^{-1}$, and was evaluated with independent data of NO_3-N in soil solution of another treatment of 800 kg ha^{-1} $year^{-1}$. The yearly water balance (WB) obtained from SWAP was similar to that obtained through a sequential climatologic WB of Thornthwaite and Matter. However, the monthly deep drainage values obtained by SWAP as compared to the WB values presented differences with a determination coefficient of 0.77 in a linearization of the results. Irrigation scenarios with intervals of 3(IF_3), 5(IF_5), 10 (IF_{10}) e 15 (IF_{15}) days between water applications were simulated by SWAP and compared with the irrigation management practiced in the farm where the experiment was carried out. These simulations showed for longer intervals (IF_{15}) drainage losses were smaller, water productivity higher, as well as relative productivity. Measurements of N absorption by plants obtained experimentally were similar to ANIMO simulations. Sensitivity analyses of the model showed that leaching and soil solution concentration of NO_3-N are sensitive to soil pH and temperature of the decomposition processes. We conclude that the combination of SWAP with ANIMO was efficient for the description of the N cycle in a Cerrado soil-plant-atmosphere system.

Keywords: Water balance. Nitrogen balance. Modeling. Brazilian savannah.

RESUMO

PINTO, V. M. **Simulação da dinâmica da água e do nitrogênio em um solo de Cerrado cultivado com café utilizando os modelos SWAP e ANIMO**. 2015. 123 p. Tese (Doutorado) – Centro de Energia Nuclear na Agricultura, Universidade de São Paulo, Piracicaba, 2015.

A agricultura focada apenas na produção leva ao uso insustentável de recursos resultando em consequências negativas para o meio ambiente e a saúde humana. Uma consequência do uso excessivo de fertilizantes é a contaminação dos recursos hídricos subterrâneos e superficiais em ecossistemas agrícolas e nos seus arredores. Devido o solo da região do Cerrado ser pobre em nutrientes, predominantemente arenoso e com alta acidez, o uso de insumos agrícolas é intensificado e o transporte químico de nutrientes via lixiviação é um problema para a agricultura intensiva nas diferentes regiões. Informações sobre as atuais práticas de uso de fertilizantes e seus efeitos no ambiente de Cerrado precisam ser coletadas para reduzir os impactos da agricultura nesse ecossistema. Modelos baseados em processos físicos e químicos são ferramentas úteis para simular a dinâmica da água e nutrientes no meio agrícola e as perdas associadas aos manejos adotados, com potencial para avaliar diferentes cenários de previsão dos resultados dessas práticas. Entre os modelos baseados em processos, o SWAP (modelo Solo, Água, Atmosfera e Planta) tem sido utilizado com sucesso em várias condições agronômicas para descrever processos hídricos, e o ANIMO (modelo de nitrogênio na agricultura) para simular o ciclo do nitrogênio em sistemas agrícolas. Nosso estudo apresenta uma aplicação do SWAP para culturas de café perenes maduras ao longo de um ciclo produtivo, com foco nas perdas por drenagem e no manejo da irrigação em um sistema típico do Cerrado Brasileiro. A combinação dos modelos SWAP/ANIMO foi utilizada nesse estudo para simular a absorção de N pelas plantas de café e a lixiviação do nitrogênio na forma de nitrato (NO_3-N) resultante de uma prática de manejo de fertilizantes intensiva. O ANIMO foi calibrado para o cenário correspondente à aplicação de 400 kg ha^{-1} ano^{-1} de fertilizante mineral, e foi avaliado com dados independentes de NO_3-N na solução do solo medidos em parcelas de outro tratamento que receberam 800 kg ha^{-1} ano^{-1}. O balanço hídrico anual obtido pelo SWAP foi semelhante ao obtido pelo balanço sequencial climatológico, de Thornthwaite e Matter. No entanto, os valores mensais de drenagem profunda obtidos pelo SWAP e comparados com os resultados do balanço climatológico apresentaram diferenças, com um coeficiente de determinação de 0,77 na linearização dos resultados. Cenários de irrigação com intervalos de 3 (IF_3), 5 (IF_5), 10 (IF_{10}) e 15 (IF_{15}) dias entre aplicações de água foram simulados utilizando o SWAP e comparados com a prática de manejo da fazenda onde o estudo experimental foi realizado. As simulações dos cenários com o SWAP mostraram que as irrigações com intervalos mais longos (IF_{15}) apresentam menores quantidades de perdas por drenagem, maior produtividade da água e produtividade relativa da cultura. As medidas de absorção de N pelas plantas obtidas experimentalmente foram similares às estimativas do modelo ANIMO. As analises de sensibilidade do modelo mostraram que as previsões da lixiviação e concentração de NO_3-N na solução do solo são sensíveis às variáveis pH do solo e temperatura de referência dos processos de decomposição. Conclui-se que a combinação dos modelos unidimensionais baseados em processos SWAP/ANIMO foi eficaz na descrição do ciclo do N avaliado no sistema solo-planta do Cerrado.

Palavras-chave: Balanço hídrico. Balanço de nitrogênio. Modelagem. Cerrado.

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LIST OF SYMBOLS

Symbol	Description (unities)
$\%F_{hu}$	Percentage of material decomposed directly into humus and biomass (%)
$\%F_{fp}$	Percentage of fast reaction part (%)
$\%F_{sp}$	Percentage of slow reaction part (%)
σ_N^{max}	Maximum transpiration stream concentration factor (-)
θ	Volumetric soil water content ($cm^3\ cm^{-3}$)
θ_r	Residual volumetric soil water content ($cm^3\ cm^{-3}$)
θ_s	Saturated volumetric soil water content ($cm^3\ cm^{-3}$)
θ_s^+	5% upper limit of saturated volumetric soil water content ($cm^3\ cm^{-3}$)
θ_r^+	5% upper limit of saturated volumetric soil water content ($cm^3\ cm^{-3}$)
θ_s^-	5% lower limit of saturated volumetric soil water content ($cm^3\ cm^{-3}$)
θ_r^-	5% lower limit of saturated volumetric soil water content ($cm^3\ cm^{-3}$)
α	Shape parameter in soil water retention curve (cm^{-1})
α^+	5% upper limit of shape parameter in soil water retention curve (cm^{-1})
α^-	5% lower limit of shape parameter in soil water retention curve (cm^{-1})
λ	Shape parameter in soil water retention curve (-)
λ_{dsl}	Shape parameter in soil water retention curve of intermediate and deeper soil layers (-)
Δp	General designation for “parameter variation”
ΔV	General designation for “N cycle process variation”
Δz	Soil thickness (m)
Δz_1	Thickness of Surface layer (m)
Δz_2	Thickness of intermediary layer (m)
Δz_3	Thickness of deep layer (m)
Δz_{top}	Thickness of top soil compartment (m)
Δz_{res}	Thickness of the reservoir for additions (m)
ρ_s	Soil dry bulk density ($kg\ m^{-3}$)
ρ_{d1}	Dry bulk density (Surface layer) ($kg\ m^{-3}$)
ρ_{d2}	Dry bulk density (Intermediate layer) ($kg\ m^{-3}$)
ρ_{d3}	Dry bulk density (Deeper layer) ($kg\ m^{-3}$)
η	Relative partial sensitive index (-)

A_d	Coefficient of temperature for dissolved organic transformation (J mol^{-1})
A_n	Coefficient of temperature for organic matter transformation and nitrification (J mol^{-1})
AP_{03-13}	Average precipitation in Barreiras during 2003-2013 (mm)
AP_{r10}	Average precipitation in Barreiras reduced in 10% (mm)
AP_{r20}	Average precipitation in Barreiras reduced 20% (mm)
B_i	Monthly drainage values obtained by Bortolotto et al. (2012) (mm)
c_{OM}	Organic content in the material (%)
c_{NH4-N}	Ammonium content in the material (%)
c_{NO3-N}	Nitrate content in the material (%)
c_{Nhu}	Humus N concentration (kg kg^{-1})
c_{DOM}	N concentration in dissolved organic matter (kg kg^{-1})
c_{Nex}	N concentration in root exudates (kg kg^{-1})
c_{Nfp}	N concentration in fast reaction part of materials added (kg kg^{-1})
c_{Nsp}	N concentration in slow reaction part of materials added (kg kg^{-1})
c_{wNH4}	Ammonium concentration in rainwater (kg m^{-3})
c_{wNO3}	Nitrate concentration in rainwater (kg m^{-3})
c_{dNH4}	Ammonium concentration in atmospheric air (kg m^{-3})
c_{dNO3}	Nitrate concentration in atmospheric air (kg m^{-3})
$c_{NH_4}(t)$	Liquid concentration of ammonium (kg m^{-3})
C/N	Relation carbon and nitrogen (-)
d	Index of agreement (-)
DS	Development stage (-)
ET_p	Potential evapotranspiration (mm)
ET_a	Actual evapotranspiration (mm)
E_p	Potential evaporation (mm)
E_a	Actual evaporation (mm)
EXC	Water excess (mm)
F_i	Monthly drainage value obtained by SWAP (mm)
i_c	Interception coefficient (-)
I	Irrigation (mm)
ID	Irrigation depth (mm)
IF_i	Irrigation frequency
IF_3	Irrigation frequency with three days intervals
IF_5	Irrigation frequency with five days intervals

IF_{10}	Irrigation frequency with ten days intervals
IF_{15}	Irrigation frequency with fifteen days intervals
IF_{Farmer}	Farmer irrigation management
J_i	General designation for "model predicted value"
h	Soil water pressure head (cm)
h_1	Soil pressure head value where roots water extraction ceases due to anoxia (cm)
h_2	Soil pressure head value at which the constant maximum root extraction begins (cm)
h_3	Soil pressure head value at which the constant maximum root extraction ends (cm)
h_{3h}	Soil pressure head value at which the constant maximum root extraction ends under high plant transpiration (cm)
h_{3l}	Soil pressure head value at which the constant maximum root extraction ends under low plant transpiration (cm)
h_4	Soil pressure head of wilting point (cm)
H_a	Humidity (kPa)
k_{gr}	Extinction coefficient for solar radiation (-)
k_{dif}	Extinction coefficient for diffuse light (-)
k_{dir}	Extinction coefficient for direct visible light (-)
k	Decomposition rate constant (y^{-1})
k_{hu}	Decomposition rate constant of humus (y^{-1})
k_{DOM}	Decomposition rate constant of dissolved organic matter (y^{-1})
k_{ex}	Decomposition rate constant in root exudates (y^{-1})
k_{fp}	Decomposition rate constant of slow reaction part of materials (y^{-1})
k_{sp}	Decomposition rate constant of slow reaction part of materials (y^{-1})
k_{li}	Coffee litter decomposition rate constant (y^{-1})
k_n	Nitrification rate (y^{-1})
k_{nr}	Nitrification rate of reference (y^{-1})
k_d	Denitrification rate (y^{-1})
K	Soil hydraulic conductivity (m d^{-1})
K_s	Saturated soil hydraulic conductivity (m d^{-1})
K_{sr}	Saturated hydraulic conductivity in soil root zone (m d^{-1})
K_c	Crop factor (-)
LAI	Leaf area index (ha ha^{-1})
LAI_0	Leaf area index at the initial plant development stage (ha ha^{-1})
$LAI_{50\%}$	Leaf area index at 50% of plant development stage (ha ha^{-1})

$LAI_{75\%}$	Leaf area index at 75% of plant development stage (ha ha^{-1})
$LAI_{100\%}$	Leaf area index at 100% of plant development stage (ha ha^{-1})
MaP_{30}	Maximum historical precipitation in Barreiras (mm)
MiP_{30}	Minimum historical precipitation in Barreiras (mm)
M_{200}	Nitrogen management with application of 200 kg N $ha^{-1}y^{-1}$
M_{400}	Nitrogen management with application of 400 kg N $ha^{-1}y^{-1}$
M_{600}	Nitrogen management with application of 600 kg N $ha^{-1}y^{-1}$
M_{800}	Nitrogen management with application of 800 kg N $ha^{-1}y^{-1}$
n	Shape parameter in soil water retention curve (-)
n^-	5% lower limit of shape parameter in soil water retention curve (-)
n^+	5% upper limit of shape parameter in soil water retention curve (-)
N	Number of observations (un)
NSE	Nash Sutcliffe model efficiency parameter (-)
N_{org}	Input amount of organic nitrogen (kg ha^{-1} y^{-1})
$NA_{1/2d}$	N application frequency every second day
$NA_{1/1w}$	N application frequency once a week
$NA_{1/2w}$	N application frequency each fifteen days
$NA_{1/1m}$	N application frequency once a month
$NA_{7/12m}$	N application seven times during the year
$NA_{3/12m}$	N application three times during one year
O_i	General designation for “experimentally observed value”
$\overline{O}$	General designation for “average experimentally observed value”
pH	Soil pH (-)
pH_1	Soil pH of surface layer (-)
pH_2	Soil pH (Intermediate and deeper layers) (-)
p_1	Diffusion coefficient of soil surface layer (-)
p_2	Diffusion coefficient of intermediate and deeper layers (-)
p	General designation for “parameter”
$P_{Default}$	Precipitation amount used in SWAP/ANIMO validation (mm)
P	Precipitation (mm)
P_i	Canopy water interception (mm)
P_r	Plant residues (kg ha^{-1})
Q	Drainage (mm)
Q_i	Drainage flux simulated with those standard parameter values (mm)
Q_i’	Drainage flux simulated with parameter variation (mm)

Q_d	Downward drainage flux (mm)
Q_{cr}	Upwards drainage flux (mm)
Q_{dI}	Downward drainage flux due to irrigation (mm)
Q_{dP}	Downward drainage flux due to precipitation (mm)
RAD	Solar radiation (kJ m^{-2})
RO	Run-off and run-on (mm)
R_d	Rooting depth (m)
RR_d	Relative root depth (-)
R_y	Root density (-)
R_{y0}	Relative root density in soil surface at RR_d = 0 (-)
$R_{y0.6}$	Relative root density at RR_d = 0.6 (-)
$R_{y1.0}$	Relative root density at RR_d = 1.0 (-)
s_{NH4}	NH_4 sorption coefficient (m^3 kg^{-1})
s_{1NH4}	NH_4 sorption coefficient for soil surface layer (m^3 kg^{-1})
s_{2NH4}	NH_4 sorption coefficient for soil surface layer (m^3 kg^{-1})
S	Soil water extraction rate by plant roots (cm^3 cm^{-3} d^{-1})
SLA	Specific leaf area (m^2 kg^{-1})
SCA	Plant soil cover (m^2)
S_w	Wind speed (m s^{-1})
t	Time (d)
t_p	Planting date (JD)
t_c	Transitional date between periods (JD)
t_h	Harvesting date (JD)
T_p	Potential transpiration (mm)
T_a	Actual transpiration (mm)
T_{a1}	Cumulative transpiration in first period (mm)
T_{a2}	Cumulative transpiration in second period (mm)
T_{air}	Air temperature (ºC)
T_{ref}	Soil reference temperature for organic transformations (ºC)
U_{p1}	Cumulative uptake for first period (kg ha^{-1})
U_{p2}	Cumulative uptake for first period (kg ha^{-1})
V	General designation for “N cycle process”

W_s	Soil water storage (mm)
WP_{I+P}	Water productivity (kg m^{-3})
Y_a	Actual yield (t ha^{-1})
Y_p	Biological productivity of coffee (t ha^{-1})
z	Vertical coordinate (m)
Z_r	Depth of initial root zone (m)

LIST OF ABBREVIATIONS

S.D.	Standard deviation
STD	Standard combination of van Genuchten parameters
CWB	Climatologic water balance
WB	Water balance
DOM	Dissolved organic matter
AWC	Available Water Capacity
VG	van Genuchten
LEPA	Low Energy Precision Application
EMBRAPA	Brazilian Agricultural Research Corporation
INMET	National Institute of Meteorology
SWAP	Soil, water, atmosphere and plant model
ANIMO	Agricultural nitrogen model
RMSE	Root mean square error
RDM	Root dry matter
DHRC	Lower boundary of the soil layer with highest root concentration
NUpE	Nitrogen efficiency uptake

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1 Introduction

The demand for food production has increased and agriculture frontiers advanced in the Brazilian territory. During the last decades, the Brazilian savannah (Cerrado) was explored by agriculture under specific management practices, established in parts by scientific and technological advances (LOPES; GUILHERME; RAMOS, 2012), which allowed the crop cultivation in areas which were thought to be improper due to soil and weather conditions.

Rada (2013) concluded that Brazil can significantly improve its position as a supplier of commodities if the Cerrado agriculture increases its efficiency and farmers start using advanced technology and management practices in the technical frontier.

For coffee cultivation in the Cerrado, several actions have been made by institutions like Embrapa, which is responsible for new technologies of rational water use as, for example, the controlled water stress used for cultivation management and the Wastewater Cleaning System used for coffee fruit processing (COSTA; BESSA; FERREIRA, 2014). Bruno et al. (2011) and Neto et al. (2011) looked for the best application moment and dose of nitrogen for a coffee cultivation in a Cerrado area and their studies are examples for an efficient use of resources in agriculture.

Water and fertilizer efficient use are relevant themes for coffee cultivation in the Cerrado and more scientific studies are needed with the aim to promote an efficient cultivation in this region. Significant information regarding water dynamics and nitrogen losses due to management practices are important for achieving these objectives.

The recent advance in computational technology contributed for the construction of models that became an advantage as a tool in scientific studies. Today models can be used for identification of gaps in scientific knowledge, for generating and evaluating hypotheses, for planning experimental research, and, moreover, can be used to establish most influent parameters that control systems (MATHEUS; STEPHENS, 2002). Simulation models are also able to evaluate future scenarios, to predict specific situations and the outcomes of a system due to actions. The commented characteristics of modeling are desirable for studies in agriculture, which are full of risks and influences of weather, management, pests and diseases.

Models in their majority can be classified as empiric or process-based, or they can tend to be more of one or other (or both) classifications. Process-based models simulate in detail the physical and biologic processes that describe the behavior of studied systems.

Empiric models are simpler and are based on relations of correlation, without describing the system completely (ADMS et al., 2013). The process-based models although more comprehensive in processes description, generally require more input data and information. However, process-based models are more susceptible to be applied for different study conditions, since they are composed by general formulations, common in all terrestrial systems, and can be adjusted to specific situations.

The hypothesis to be investigated in this study is that a combination of one-dimensional process-based models is effective to simulate the dynamics of water and nitrogen in a highly fertirrigated coffee farming system in the Cerrado.

The specific objectives are:

1. Adjust SWAP and ANIMO models to a fertirrigated coffee cultivation system of the Cerrado and simulate the dynamics of water and nitrogen.
2. Calibrate SWAP and ANIMO models and evaluate the sensitivity of the simulated processes to the input parameters and variables.
3. Evaluate the effectiveness of SWAP/ANIMO combination to simulate nitrogen plant uptake, nitrate soil concentration, and nitrate leaching.
4. Evaluate the potential of SWAP and ANIMO models to generate scenarios of irrigation and fertilizer management.

1.1 Introdução

Aumenta a exigência pela produção em quantidade de alimentos e o cultivo agrícola avança para novas áreas no território Brasileiro. Nos últimos anos o ecossistema Cerrado tem sido explorado pela agricultura sob manejos específicos, estabelecidos em partes pelo avanço científico e tecnológico (LOPES; GUILHERME; RAMOS, 2012), que permitiram o cultivo agrícola em áreas antes caracterizadas como impróprias devido às condições de solo e clima.

Rada (2013) sugere que o Brazil pode aumentar significativamente a sua posição na competição global pelo fornecimento de “commodities” agrícolas aumentando a eficiência da agricultura no Cerrado se houver melhorias nas técnicas de manejo e aproximação da tecnologia empregada por agricultores àquela da fronteira tecnológica.

Para o cultivo do café no Cerrado, muitos esforços têm sido feitos por instituições como a Embrapa no Cerrado central, a qual é responsável por novas tecnologias de uso racional da água, podendo-se citar, por exemplo, o estresse hídrico controlado como manejo de cultivo e o sistema de limpeza de Águas Residuárias usado no processamento dos frutos de café (COSTA; BESSA; FERREIRA, 2014). Bruno et al. (2011) e Neto et al. (2011) buscaram o melhor momento de aplicação e dose de nitrogênio para o café do Cerrado, e são exemplos de medidas para um manejo eficiente de recursos na agricultura.

O uso eficiente da água e de fertilizantes são temas relevantes para o desenvolvimento da cafeicultura no Cerrado. No entanto, são necessários mais estudos com propósitos de promover a sustentabilidade desse cultivo no Cerrado. Informações significativas a respeito da dinâmica da água nesses sistemas e de processos de perdas de nitrogênio ligados ao manejo de fertilizantes são temas importantes para alcançar estes objetivos.

O avanço da tecnologia computacional contribuiu para que os modelos computacionais se tornassem uma ferramenta de suporte vantajosa em estudos científicos. Hoje os modelos podem ser usados na identificação de colunas no conhecimento científico, para gerar e testar hipóteses, com o objetivo de projetar experimentos e, além disso, podem ser usados na determinação dos parâmetros mais influentes de um sistema (MATHEUS; STEPHENS, 2002). Modelos de simulação são também ferramentas capazes de gerar cenários para o futuro, prever situações e respostas de um sistema a uma ação. Essas características da modelagem são importantes especialmente para a agricultura, a qual é permeada por riscos e influências do clima, do manejo agrícola, de pestes e doenças.

Os modelos podem ser classificados como empíricos ou baseado em processos, ou tender mais para uma das duas classificações. Os modelos baseados em processos simulam com detalhe os processos físicos e biológicos que descrevem o comportamento de um sistema. Os modelos empíricos são mais simples e baseiam-se em relações de correlações, sem descrever um sistema completamente (ADMS et al., 2013). Os modelos baseados em processos apesar de mais compreensivos na descrição dos processos, requerem maior número de dados de entrada e informações. No entanto, os modelos baseados em processos são mais susceptíveis a serem aplicados em diferentes condições, pois são compostos por formulações gerais, comuns nos sistemas terrestres e aceitam a incorporação de dados locais, podendo ser adequados a situações específicas.

A hipótese desse estudo é que uma associação de modelos unidimensionais baseados em processos físicos é eficaz para simular a dinâmica da água e do nitrogênio em um sistema de cultivo de café do oeste da Bahia.

Com o propósito de avaliar esta hipótese, este estudo tem os seguintes objetivos:

1. Adequar os modelos SWAP e ANIMO ao um sistema de cultivo de café fertirrigado do Cerrado e simular a dinâmica da água e do nitrogênio.
2. Calibrar o SWAP e o ANIMO e avaliar a sensibilidade dos processos simulados aos dos parâmetros de entrada dos modelos e variáveis.
3. Avaliar o potencial da combinação SWAP/ANIMO para simular a absorção de nitrogênio pelas plantas, a concentração de nitrato no solo, e a lixiviação de nitrato.
4. Avaliar o potencial dos modelos SWAP e ANIMO para gerar cenários de manejo de irrigação e manejo de fertilizantes.

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2 Deep drainage modeling for a fertigated coffee plantation in the Brazilian Cerrado

Abstract

Modeling in agriculture represents an important tool to understand processes as water and nutrient losses by drainage, or to test different conditions and scenarios of soil and crop management. Among the existing computational models to describe hydrological processes, SWAP (Soil, Water, Atmosphere and Plant model) has been successfully used under several conditions. This model was originally developed to simulate short cycle crops and its use also to cover longer cycles, e.g. perennial crops, is a new application. This report shows a SWAP application to a mature coffee crop over one-production cycle, focusing on deep drainage losses in a typical soil-plant-atmosphere system of the Brazilian savanna (Cerrado). The estimated annual deep drainage Q = 1019 mm obtained by SWAP was within 99% of the value determined by the climatologic water balance of 1010 mm. Monthly results of SWAP for Q compared to the estimative using the climatological method presented a determination coefficient of 0.77. A variety of coffee fertigation scenarios was simulated using SWAP and compared to farmer's management scenario, leading to the conclusion that larger irrigation intervals result in lower Q losses, better water productivity and higher crop yield.

Keywords: Brazil, SWAP, deep drainage, water productivity, Cerrado

2.1 Introduction

The savanna ecoregion (Cerrado) prevails in central Brazil, also reaching the northeast part of the country and including part of the state of Bahia. The Cerrado domain in Bahia is highly suitable for irrigated agriculture due to the great availability of surface and underground water resources. According to Brazil's National Grain Supply Company (CONAB), western Bahia is an important food (grain) provider and holds, for example, the highest coffee yield under Cerrado conditions in the country. However, there are some concerns in respect to the modern agriculture practiced in this producer region. Due to the ineffective land management during the last decades, the irrigated farms concentrated at specific areas and, therefore, conflicts over water use already took place in western Bahia (LIMA, 2011). At the same time, management practices applied by farmers are not sustainable in terms of fertilizer and water usage, especially due to the lack of scientific studies that support their decisions (BRUNO et al., 2011).

Numerical modeling applied to agriculture is a useful tool to simulate biophysical processes and can be used to obtain short-term results and future predictions under defined scenarios. The information generated is helpful for establishing a more sustainable agriculture as well as supporting strategies for the mitigation of pollution, named by Strauch et al. (2013) as the “Best Management Practices”. The hydrological model SWAP (Soil, Water, Atmosphere and Plant) is one of the existing algorithms used worldwide for a variety of soils, crops and climatic conditions (CHIRICO et al., 2013; CRESCIMANNO; MORGA; VENTRELL, 2012; EITZINGER et al., 2004; KAMBLE et al., 2013; MA et al., 2011; NOORY et al., 2011). The model has shown consistent results when applied to maize crops in sub-tropical climates (PINHEIRO et al., 2013) and to soybeans and common beans in tropical climates (SCORZA JUNIOR; SILVA; RIGITANO, 2010; DURIGON et al., 2012). SWAP was successfully validated already under several climatic and environmental conditions as cited Ines et al. (2006). More recent studies with this model found close agreement between measured and simulated values (MISHRA et al., 2013; SINGH; REN; KANG, 2010; UTSET et al., 2007; VAZIFEDOUST et al., 2008; VERMA; GUPTA; ISAAC, 2012).

This study aimed to use SWAP to evaluate the deep drainage of a Cerrado coffee plantation and analyze irrigation scenarios in view of water productivity and conservation, minimizing environmental impacts. Values of SWAP input parameters were acquired from a one-year experimental database coming from a study performed on a mature coffee crop growing in central Brazil (BORTOLOTTO et al., 2011; 2012; BRUNO et al., 2011).

The computer simulations focused on improving water usage and understanding of water dynamics in a sandy soil typical of the Brazilian Cerrado, an area intensively used to grow perennial crops. We studied several scenarios of irrigation to improve water productivity for the chosen area.

2.2 Materials and methods

2.1.1 The Soil, Water, Atmosphere and Plant model (SWAP)

The model SWAP was developed more than 40 years ago and was gradually upgraded reaching its last version SWAP 3.2 (KROES et al., 2008). This last version of the model had the source code restructured, numerical stability improved, macropore process integrated, and simplification of precipitation and evapotranspiration inputs included (VAN DAM et al., 2008).

SWAP makes use of Richards' equation in one dimension added by the sink terms (S) to calculate the water movement in the soil matrix, as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial \left[\mathrm{K}(h) \left(\frac{\partial h}{hz} + 1 \right) \right]}{\partial z} - S\left(h\right) \tag{2.1}$$

where θ (cm^3 cm^{-3}) is the volumetric soil water content, t (d) time, S (cm^3 cm^{-3} d^{-1}) the soil extraction rate by plant roots, K (cm d^{-1}) the soil hydraulic conductivity, h (cm) the soil water pressure head and z (cm) the vertical coordinate taken positively upwards. SWAP uses Richards' equation for describing water flux in the unsaturated and saturated zones of the soil and solves the equation (2.1) numerically, using the relations between θ, h and K, with the Mualem-van Genuchten relations $\theta(h)$ and $K(h)$ (MUALEM, 1976; VAN GENUCHTEN, 1980).

The upper boundary conditions in SWAP are determined according to the rates of potential evapotranspiration ET_p (mm), irrigation I (mm) and precipitation P (mm) of the area under study. Daily ET_p is calculated with the Penman-Monteith equation (MONTEITH, 1965; 1981) using meteorological data of air temperature T_{air} (ºC), solar radiation RAD (kJ m^{-2}), wind speed S_w (m s^{-1}) and air humidity H_a (kPa).

The water balance is determined as in equation (2.2):

$$\pm\Delta W_s = P + I - ET_a \pm RO - P_i \pm Q \qquad (2.2)$$

where W_s (mm) is the soil water storage in a defined elemental soil volume, ET_a (mm) the actual evapotranspiration, RO (mm) the run-off and run-on, P_i (mm) the canopy water interception and Q (mm) the soil water drained at the lower boundary, equal to $-Q_d$ or $+Q_{cr}$. The percolation Q_d is downwards and Q_{cr} the upwards, when the capillary rise is present. Q_d can still be subdivided into the components Q_{dI}, due to irrigation, and Q_{dP}, due to the rainfall. Actual evapotranspiration is calculated considering the reduction of root water uptake when there is water or salinity stress, and the reduction of soil water content due to the soil surface drying. The actual transpiration T_a (mm) is obtained as follows:

$$T_a = \int_{-R_d}^{0} S(z)d\,\mathrm{z} \qquad (2.3)$$

where the lower integration limit R_d is rooting depth and S the root water flux, which is related to the potential transpiration T_p (mm). During water stress, $S(z)$ is described in SWAP as proposed by Feddes, Kowalik and Zaradny (1978). In this function, the root water uptake is regulated by the critical pressure head values h_1 (point where water extraction ceases due to anoxia), h_2 (begin of constant maximum root extraction), h_3 (end of constant maximum root extraction), h_4 (wilting point, where root extraction ends). The actual evaporation is determined by Darcy's relation and empirically either according to Black, Gardner and Thurtell (1969) or to Boesten and Stroosnijder (1986), to be selected by the SWAP user. The bottom boundary condition is adjusted by the user and can be, for example, prescribed with pressure head values of the bottom soil compartment, calculated as a function of the groundwater level, or the boundary condition can be the free drainage of the soil profile.

SWAP contains simple and detailed crop growth modules, which should be selected by the user according to the available plant data. In the simple model the user provides the leaf area index (*LAI*), crop factor (K_c) and rooting depth as a function of the crop development stage (*DS*). These data are used to calculate the canopy interception P_i, potential transpiration T_p and potential evaporation E_p.

2.2.2 Experimental site and field experiment

An experimental test used to calibrate and compare the results of the SWAP model was performed between August 1st, 2008 and July 31st, 2009, at a private farm near the city of Barreiras (11°46'00'' S, 45°43'32'' W), in Bahia, northeast Brazil (Figure 2.1). The soil is classified as a Typic Hapludox according to the USDA Soil Taxonomy (Soil Survey Staff, 2010), with low natural fertility and is located in a Cerrado region. The precipitation is very variable, ranging from 800 to 1800 mm per year, with most events occurring from October to April. Meteorological data, acquired from the National Institute of Meteorology (INMET, Brazil), were collected at the meteorological station of the municipality of Barreiras, 90 km far from the experimental site. The input variables farmer irrigation depths and precipitation along the experimental year used for SWAP simulations are shown in Figure 2.2. Irrigation is not discontinued during the rainy season due to the fertilizer application carried out year round.

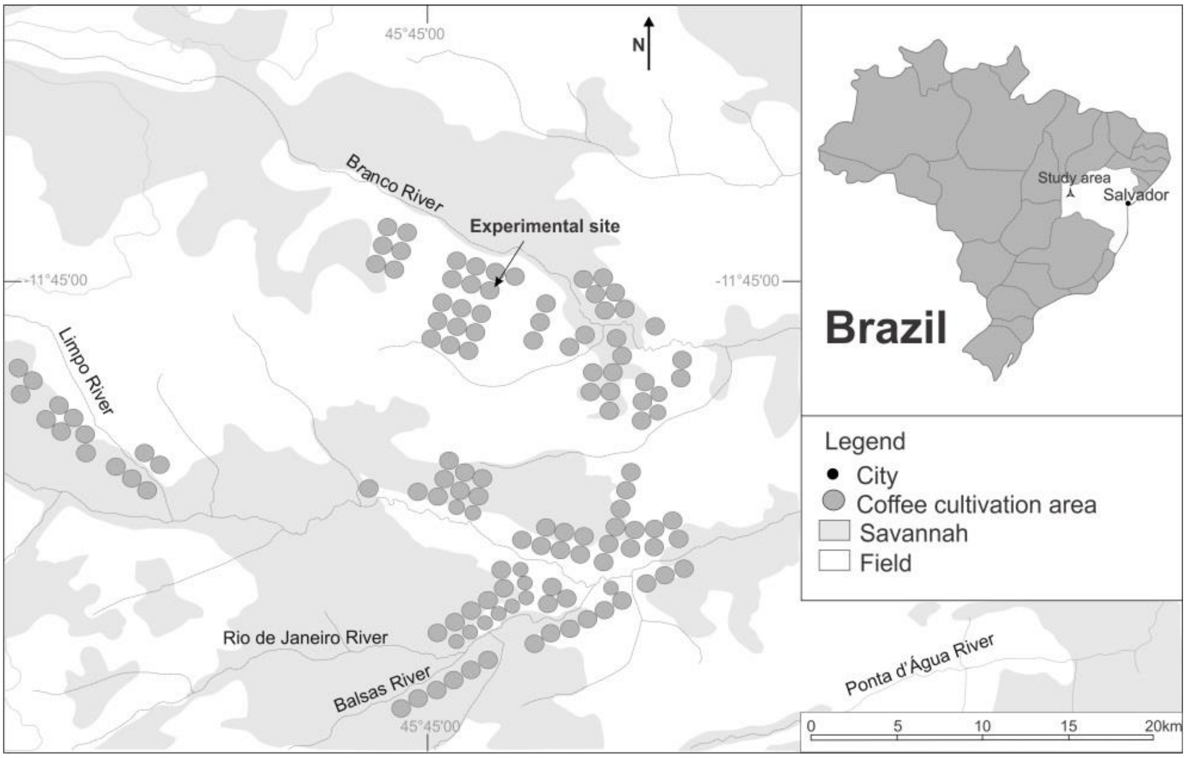

Figure 2.1 – Experimental site localization, showing central pivot circles in 2013

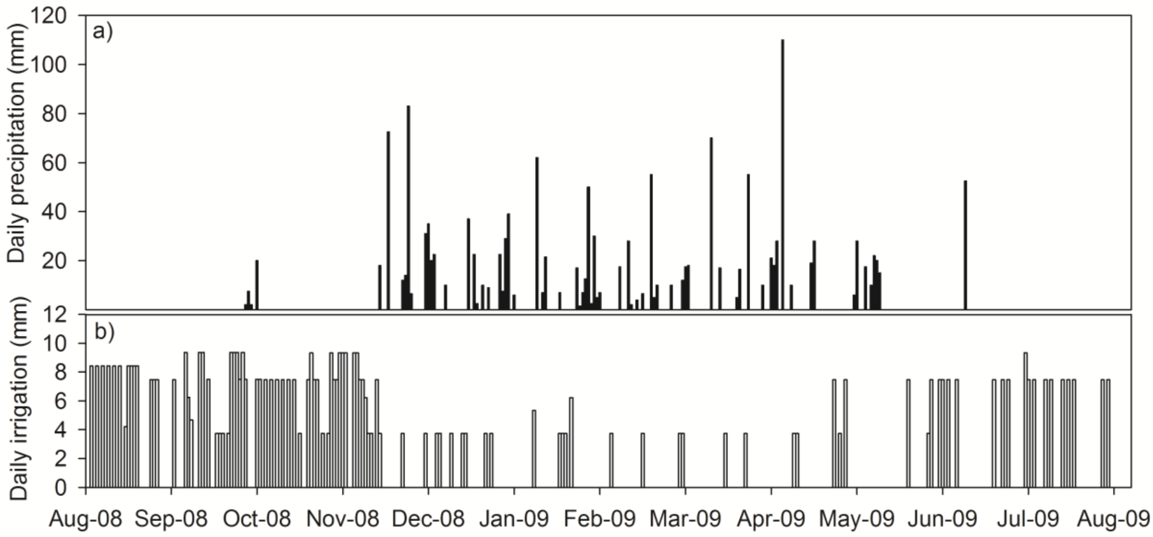

Figure 2.2 - Daily precipitation (a) and irrigation (b) during the experimental year (August 2008 to July 2009)

The coffee species was *Coffea Arabica L.*, variety *Catuaí Vermelho*. Plants were seven years old at the beginning of the experiment and were planted at a spacing of 3.8 m between lines and 0.5 m between plants in a circular arrangement for central pivot irrigation with a total area of 80 ha, adapted for fertigation. Irrigation was applied homogeneously over the planted area, and the experimental site consisted of the pivot circle number 4, starting from the center of the coffee plantation (BRUNO et al., 2011). Irrigation was performed by LEPA-type emitters, which distribute the water according to the circular coffee lines, avoiding the application of water in the interrow. The pivot operation was continuous during the year and stopped only during harvest (May-June), according to farmer´s practice.

For the saturated hydraulic conductivity K_s (cm d^{-1}), soil bulk density ρ_s (g cm^{-3}) and soil particle size analyzes, soil samples were extracted from soil layers 0-10, 10-20, 20-40, 40-60, 60-80, and 80-100 cm (Table 2.1) in the coffee field. In the laboratory, the constant head method (REYNOLDS et al., 2002) was employed for obtaining K_s. Soil water retention curves were constructed using sieved soil samples (2 mm sieve), assuming for sandy soils the structure of the samples is of little importance. Samples of each soil layer were submitted to the pressures of 100, 200, 330, 500, 1000, 3000, 5000, 10000, 15000 cm of water in the laboratory, using the Richards pressure plate extractors. A soil water retention curve was established by fitting the van Genuchten (VG) model to all water retention data (R^2 = 0.88) for the 1 m soil profile, using the RETC program (VAN GENUCHTEN; LEIJ; YATES, 1991).

The saturated and residual water contents (θ_s and θ_r, cm^3 cm^{-3}), the shape parameters n and α (cm^{-1}) needed for SWAP simulations were obtained together with their 5% upper and lower limits (Table 2.2). The upper limits of VG parameters were represented by θ_s^+, θ_r^+, n^+ and α^+, and the lower limits by θ_s^-, θ_r^-, n^- and α^-.

Table 2.1 - Physical characteristics of the experimental site soil as a function of depth

Soil depth (cm)	Number of samples for K_s test	K_s (cm d^{-1})	*S.D.* (cm d^{-1}).	ρ_s (g cm^{-3})	Sand[a] (%)	Clay[a] (%)	Silt[a] (%)
0-10	15	184	130	1.79	78	16	6
10-20	6	349	106	1.79	78	19	3
20-40	4	354	51	1.57	73	22	4
40-60	3	454	155	1.53	71	23	6
60-80	3	268	135	1.52	70	24	6
80-100	3	267	15	1.50	69	25	6

Note: K_s, saturated hydraulic conductivity; S.D., standard deviation of K_s; ρ_s, bulk density.
[a]Texture values are from three replicates.

Table 2.2 – Parameters of van Genuchten obtained for the 1m soil profile

van Genuchten parameters	5% lower	Mean	5% upper
θ_s (cm³cm^{-3})	0.367	0.387	0.407
θ_r (cm³cm^{-3})	0.076	0.097	0.117
n	1.379	1.636	1.893
α (cm^{-1})	0.009	0.016	0.025

Note: Upper and lower values for van Genuchten parameters represent upper and lower limits in the interval of 95% of confidence. Mean values of VG parameters were obtained with a determination coefficient R² = 0.88.

2.2.3 Climatologic Water Balance

Previous studies were performed in this coffee plantation as mentioned before, and the hydrological evaluation of this area was achieved by Bortolotto et al. (2012). In their study, the Climatologic Water Balances (CWB) were calculated for the pivot area with time intervals of 5 days, during the entire one-year coffee producing cycle, using a sequential method proposed by Rolim, Sentelhas and Barbieri (1998). Due to the characteristics of the plantation, flat and well drained with a deep water table located several meters below the soil surface, the *RO* was considered to be zero, as well as Q_{cr}. Bortolotto et al. (2012) estimated ET_p by the Thornthwaite (1948) and Penman-Monteith (1965) models. They considered the coffee crop factor (K_c) as equal to 1.0, based on studies that showed values in the range of 0.6

to 1.4 (PEREIRA; ANGELOCCI; SENTELHAS, 2002; PEREIRA; CAMARGO; CAMARGO, 2008; SANTINATO; FERNANDES; FERNANDES, 1996). The sequential CWB in Bortolotto et al. (2012) assumes P_i = 0 and calculates a component called water excess (*EXC*), which includes *RO* and *Q*. As *RO* and Q_{cr} are considered zero, $EXC = Q = Q_d$ is assumed, and *Q* is only the downward drainage which is lost from the crop below the 1 m depth.

2.2.4 Parameter estimation

Information about soil hydrology, plant, and meteorological data are the SWAP input requirements to run it. The model works with a collection of input files: main file, crop file, irrigation file and meteorological files for each year of the simulation. The irrigation file requires dates and amounts of water applied by irrigation and the meteorological file requires daily variables: air temperature T_{air} (ºC), solar radiation *RAD* (kJ m^{-2}), wind speed S_w (m s^{-1}), air vapor pressure H_a (kPa), and *P* (mm).

The water balance components were simulated for each month during the one-year period of study. The moment of crop emergence was set on August 1st, 2008 and the crop harvest was on July 31st, 2009, the period of the coffee cycle (BRUNO et al., 2011). The amount of water applied by irrigation was scheduled as shown in Figure 2.2.

The initial pressure head distribution in the soil was unknown and necessary for the water balance simulation, so the pressure head distribution in the soil profile at the end of one year of the first simulation with SWAP was used thereafter as the initial condition. The soil profile (0-1 m) was divided into three sub-layers with thicknesses of 10, 40 and 50 cm, each sub-layer containing 10, 8 and 5 layers with 1, 5 and 10 cm width, respectively. This possibility of soil profile discrimination in SWAP allows us to analyze in details the evolution of predicted θ and h in the time frame. The bottom-boundary condition of free drainage of the soil profile was selected in SWAP because the water table is located several meters below the soil surface. In this case, the bottom flux of the SWAP soil profile is equal to the hydraulic conductivity in the last soil compartment, as the gradient of water potential in soils under drainage can be assumed to be unity (KROES et al., 2008).

The empirical parameter of pore connectivity λ, proposed by Mualem (1976), is difficult to be evaluated directly. According to data compiled by De Jong van Lier, Dourado-Neto and Metselaar (2009), values of λ commonly vary between 6 and -6, whereas values of 0.5 or 0 are more often used. Therefore, several values of λ were used in the sensitivity analysis to show the influence of this parameter in our simulations. An average K_s-value (from Table 2.1) representative of the 1 m soil layer was used in the simulations.

The SWAP simple crop module requires information of the leaf area index, crop factor, maximum rooting depth as a function of the development stage, as well as the light extinction coefficient and the critical pressure head values of the Feddes distribution (FEDDES; KOWALIK; ZARADNY, 1978). The model is recommended for annual crops with short growing cycles, up to one-year maximum. Nonetheless, a small number of studies applied SWAP to perennial plants, including wine grapes (BEN-ASHER et al., 2006; RALLO et al., 2012) and citrus (MARTÍNEZ-FERRI; MURIEL-FÉRNANDEZ; RODRÍGUEZ DÍAZ, 2013). Because not all the data needed about the coffee plant was available in the database of Bruno et al. (2011) and Bortolotto et al. (2012), the simple crop module was our choice to represent the coffee plantation.

Coffee leaf area index (*LAI*) was estimated from leaf dry matter (available in BRUNO et al., 2011), the measured specific leaf area, *SLA* (18 m² kg^{-1}), per plant soil cover, *SCA* (1.9 m²). A variety of coffee leaf sizes was collected from the same experimental plants in 2013 to determine the average *SLA*. The obtained values of *LAI* for different stages (LAI_0, $LAI_{50\%}$, $LAI_{75\%}$ and $LAI_{100\%}$) along the experimental cycle are shown in Table 2.3.

For the characterization of the coffee crop in SWAP, we assumed a constant crop coefficient K_c for the entire year, equal to 1.1 (ALLEN et al., 1998). The coffee rooting depth R_d, as measured by Bortolotto et al. (2012) and Bruno et al. (2011) reaches the maximum depth of 1 m and was considered constant during the experimental year. Additional information about the root density (R_y) distribution along the soil profile was obtained for the crop based on visual observations of Bruno et al. (2011). Four times during the experimental year they collected an entire plant and measured the dry matter of leaves, branches, and roots, as well as root depth and distribution in the soil profile. According to these authors, the relative root density is abundant from the surface down to the 0.6 m depth, decreasing linearly from there until zero at 1 m.

The coefficient k_{gr} is the product of the extinction diffuse light coefficient for visible light (k_{dif}) and the extinction coefficient for direct visible light (k_{dir}). The parameter k_{gr} was analyzed using values between 0.2 and 2.2 (KROES et al., 2008) in the analysis of sensitivity. Measurements of the extinction coefficient of coffee are rare in the literature. Field measurements with a five-year-old coffee plantation of the São Paulo region showed an extinction coefficient of 0.53 for an average *LAI* equal to 3.8 (ANGELOCCI et al., 2008).

The interception coefficient of Von Hoyningen-Hune and Braden (i_c) was selected for the present study from Kroes et al. (2008), for ordinary crops.

The information regarding the limiting pressure head for soil water extraction by plant roots is described in the SWAP crop file. Between h_1 and h_2 water extraction by roots is assumed to increase linearly towards low values of h. The optimal root water uptake occurs between h_2 and h_{3h} (at high potential transpiration) or h_{3l} (at low potential transpiration). The wilting point was selected to be h_4 = -15000 cm. The values h_3 are those recommended for deciduous fruit plants shown in Taylor and Ashcroft (1972), which is the kind of plant that better adjusts to the characteristics of the coffee crops. The parameter values established in the soil and crop files for SWAP simulations in this study (Table 2.3) were called standard values.

Table 2.3 – Standard values used in SWAP simulations

Description	Parameter symbol	Value	Unit
Soil			
Saturated volumetric water content	θ_s	0.3874	$cm^3\ cm^{-3}$
Residual volumetric water content	θ_r	0.0969	$cm^3\ cm^{-3}$
Shape parameter of the retention curve	n	1.636	-[a]
Shape parameter of the retention curve	α	0.017	cm^{-1}
Shape parameter of hydraulic conductivity curve	λ	0.5	-
Saturated hydraulic conductivity	K_s	266	$cm\ d^{-1}$
Plant			
Light extinction coefficient for diffuse visible light	K_{dif}	0.9	-
Light extinction coefficient for direct visible light	K_{dir}	0.86	-
Leaf area index at the beginning of simulation	LAI_0	8.8	$ha\ ha^{-1}$
Leaf area index for 50% of the simulation period	$LAI_{50\%}$	10.3	$ha\ ha^{-1}$
Leaf area index for 75% of the simulation period	$LAI_{75\%}$	12.0	$ha\ ha^{-1}$
Leaf area index at the final of simulation	$LAI_{100\%}$	7.7	$ha\ ha^{-1}$
Crop coefficient	K_c	1.1	-
Interception coefficient of Von Hoyningen-Hune and Braden	i_c	0.025	-
Rooting depth during the experimental period	R_d	1.00	m
Relative root density in soil surface at RR_d = 0	R_{y0}	1.00	-
Relative root density at RR_d = 0.6	$R_{y0.6}$	1.00	-
Relative root density at RR_d = 1.0	$R_{y1.0}$	0	-
Critical pressure heads for root extraction	h_1	-1	cm
	h_2	-25	cm
	h_{3h}	-500	cm
	h_{3l}	-800	cm
	h_4	-15000	cm

Note: RR_d, relative root depth.
[a] "-" refers to non-dimensional parameters.

2.2.5 Model evaluation

In the analysis of sensitivity regarding the standard values of the parameters presented in Table 2.3, the Root Mean Square Error (*RMSE*) (SMITH et al., 1997) was used and calculated using Equation (2.4). SWAP Q_i simulations obtained with those standard values were compared with SWAP Q_i' simulations obtained when varying one of them and maintaining all other constant. The lower the value of *RMSE*, the smaller the sensitivity of the model to the varied parameter.

$$RMSE = \sqrt{\frac{1}{k}\sum_{i=1}^{k}(Q_i - Q'_i)^2} \qquad (2.4)$$

SWAP simulations were also compared to Bortolotto's CWBs, using equation (2.4), as follows:

$$RMSE = \sqrt{\frac{1}{k}\sum_{i=1}^{k}(F_i - B_i)^2} \qquad (2.4a)$$

where B_i are monthly values of Q or ET_a from Bortolotto et al. (2012), F_i the corresponding SWAP forecasted values, and k the number of observations. In this case, the lower the value of *RMSE,* the closer the proximity of the predicted F_i values to the B_i values.

To estimate Q errors for SWAP simulations, meteorological data were generated advancing and retarding the variables one and two days in relation to the real meteorological data presented in Figure 2.2. This approach resulted in five sets of monthly values of Q for which the averages and standards deviation were obtained, showed by bars in Figure 2.6.

2.2.6 Parameter sensitivity

The sensitivity of the SWAP model in relation to the crop (K_c, LAI, K_{dif}, K_{dir}, R_d, h_{3h} and h_{3l}) and hydrological soil parameters (θ_s, θ_r, n, α and λ) was performed before and after establishing the standard values (Table 2.3) of the parameters for the simulation. Before the establishment of standard values, a visual analysis was carried out by trial and error to detect the most sensitive plant and soil parameters. Afterward, a second analysis of sensitivity for soil parameters was made using several combinations of VG parameters. RMSE values were obtained replacing the standard combination of parameters by upper (θ_s^+, θ_r^+, n^+, α^+) and lower (θ_s^-, θ_r^-, n^-, α^-) values, according to Table 2.2. Each parameter was substituted once and the simulation with SWAP was performed. In the case of crop parameters, they were changed by 10% and 50% of the standard combination (Table 2.3), to obtain *RMSE* values.

2.2.7 Irrigation scenarios and water productivity

Different scenarios of irrigation were analyzed with the model, aiming to determine more efficient water managements in relation to deep drainage losses and water use efficiency at the farm under study. The irrigation scenarios were classified according to irrigation frequencies (*IF*), choosing intervals of 3 (IF_3), 5 (IF_5), 10 (IF_{10}) and 15 (IF_{15}) days between applications. For each IF_i, the amount of water applied was obtained based on the net irrigation depth (*ID*) between 1 and 50 mm (discounting *P* from *I* within each period), and when precipitation was higher than or equal to *ID*, irrigation was not applied. The scenarios with no irrigation and farmer irrigation management (IF_{Farmer}) were also evaluated, totalizing 34 setups (Table 2.4). The criterion for the irrigation scenarios was that *I* should not be too low (i.e. < 40mm) or too high (i.e. > 900mm) during the year, ensuring the comparison between the scenarios for the several *IF*.

Table 2.4 – Scenarios of irrigation generated for SWAP application

Irrigation depth	*I* (mm y^{-1})			
(mm)	IF_3	IF_5	IF_{10}	IF_{15}
1	83	46	-[a]	-
3	251	137	56	-
5	421	228	94	55
8	688	365	151	89
11	900	511	209	122
14	-	668	269	155
17	-	826	329	189
20	-	-	389	222
25	-	-	490	278
30	-	-	595	394
40	-	-	823	460
50	-	-	-	594

Note: IF_3, irrigation (*I*) applied each 3 days; IF_5, irrigation applied each 5 days; IF_{10}, irrigation applied each 10 days; IF_{15}, irrigation applied each 15 days.
[a] "-" represents not evaluated scenarios.

For each irrigation scenario, the water productivity WP_{I+P} (kg m^{-3}), which relates crop yield to water use, and the actual yield Y_a (t ha^{-1}), were calculated by Equations (2.5) and (2.6), respectively, for the interpretation of the effects of the scenarios during a year of coffee production.

$$WP_{I+P} = \frac{T_a}{T_p}\left(\frac{Y_p}{P+I}\right) \tag{2.5}$$

$$Y_a = \frac{T_a}{T_p} Y_p \tag{2.6}$$

where Y_p (t ha^{-1}) is the biological productivity of coffee, corresponding to the dry matter yield. Y_p was calculated based on the coffee fruit productivity for 2008/2009 (3060 kg ha^{-1} y^{-1}) and the coffee harvest index of 0.012 (NAIR, 1993).

As water is available in large quantities from rainfall and irrigation during the entire year, water stress conditions were not expected to take place. Coffee fruit productivity used here is the potential one. Calculated *WP* is a relative number because it was affected only by the irrigation scenarios and meteorological data. The *WP* relation is a new way to characterize water productivity, and it was described in details by Vazifedoust et al. (2008).

2.3 Results and discussion

An application of the SWAP model is presented for a perennial crop during one experimental year. SWAP input parameters and their influence on the simulations of the components of the water balance Q and ET_a were evaluated. For plant characterization, experimental data and information from studies found in the literature were used, and a simple coffee plant model was established for one year in 2008/2009. Water balances simulated by SWAP were then compared to a study developed in the same Cerrado area. After the model calibration, scenarios of irrigation were appraised looking for the best management that would benefit water and coffee productivity when compared to the farmer´s actual practices.

2.3.1 Sensitivity analysis and model calibration

Table 2.5 shows results of the *RMSE* for the estimations of *Q* for the several values of λ and combinations of VG parameters. Soil hydrological parameters assumed either the upper or lower value of a given VG parameter, delimiting the 95% confidence interval. When one parameter had its value changed from the standard value, the others remained in the standard combination. *RMSE* in relation to *Q* estimation was more sensitive to variations in λ. In this analysis, we varied λ between 6 and -6, but for values of λ equal to -6 and one value for -3 the simulations with SWAP resulted in the non-convergence of Richards' equation. Changes in VG parameters only affect the simulations of *RMSE* for *Q* slightly, and the shape parameter *n* had the greatest influence. *RMSE*-value equal to zero corresponds to the standard combination of VG and Mualem parameters.

Table 2.5 – Sensitivity of the SWAP model for deep drainage *Q* prediction evaluated trough the root mean square error (*Q*-RMSE), in relation to variations of the van Genuchten and Mualem parameters, for chosen values of pore connectivity

λ	*Q* –*RMSE* (mm)								
	STD[b]	n^-	n^+	α^-	α^+	θ_s^-	θ_s^+	θ_r^-	θ_r^+
6	13.1	15.9	12	13	13.1	14.7	11.9	11.9	14.9
5	11.6	14.6	10.5	11.4	11.7	13.3	10.3	10.3	13.5
3	7.5	11.1	6.9	7.1	7.9	9.6	6.1	6.1	9.9
1	1.6	6.5	3.8	1.6	2.3	4.6	2.5	2.5	4.8
0.5	0	5.3	4.2	1.1	1.2	3.3	3.7	3.8	3.5
0	1.5	2.7	5.3	1.9	1.9	2.7	4.2	4.2	2.9
-1	5.7	2.7	10.1	6.3	4.9	5.7	6.8	6.8	5.8
-3	29.5	10	-[a]	40.5	25	30.5	28.5	28.5	30.6
-6	-	-	-	-	-	-	-	-	-

Note: λ, pore connectivity parameter of Mualem (1976); n^- and α^-, shape parameter values of the lower limit of 5% interval; n^+ and α^+ shape parameter values of the upper limit of 5% interval; θ_s^- and θ_s^+, lower and upper values of saturated volumetric soil water content of the 5% interval; θ_r^- and θ_r^+, lower and upper values of residual volumetric soil water content of the 5% interval;
[a] Non-convergence of Richard's equation in SWAP.
[b] STD, Standard values of van Genuchten parameters.

We also studied the influence of K_s on model results of the water balance. For the component *Q*, the *RMSE* did not show great differences when K_s varies from 26 to 455 cm d^{-1}.

The component *Q* is highly affected by Mualem's λ (Table 2.5). The effect that the pore connectivity produces on the results of water balance components may be clarified by the behavior of the hydraulic conductivity function for different values of λ, shown in Figure 2.3

Almost all the h-values occurring during the experimental year remain in the range -60 to -15000 cm, where the K function can take several shapes depending on λ. An appropriate value of λ for the sandy soil should be determined, however, to obtain a more precise evaluation of the soil-plant system under study. Similar results of λ effects on the hydraulic conductivity function can be found in Sakai et al. (2009)

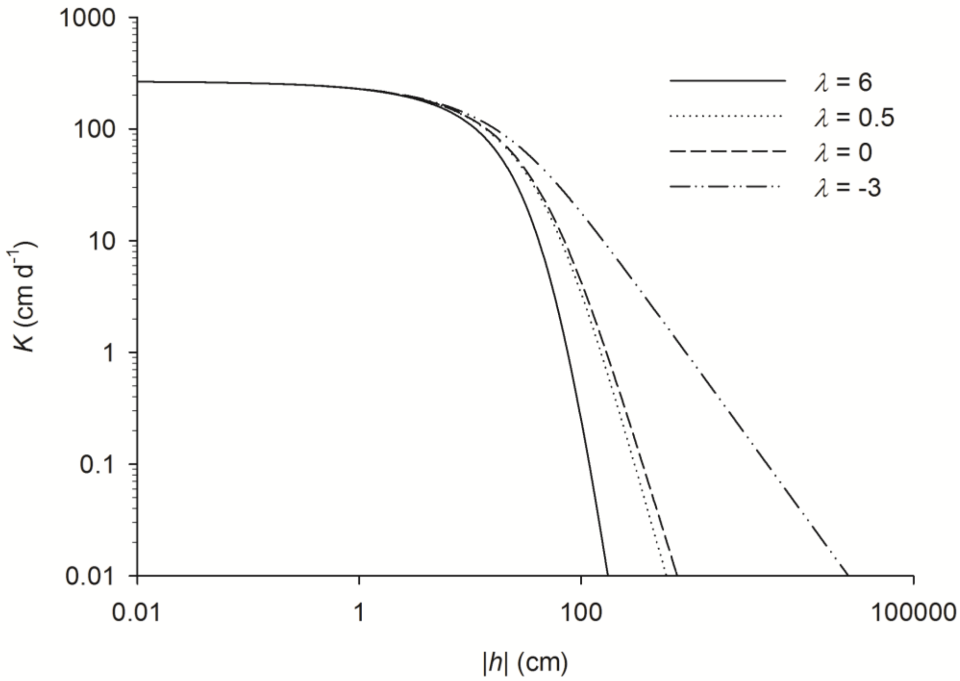

Figure 2.3 – Hydraulic conductivity K (cm d^{-1}) versus soil water pressure head h (cm) for different values of the pore connectivity parameter λ

SWAP results in Figure 2.4 showed the soil pressure head values between -1 and -25 cm was not reached in this study and, therefore, h_1 did not affect the simulated results. Pressure head h remains in the range of -100 and -15000 during the dry period and the range of -60 and -1000 cm during the rest of the year (wet period). In relation to soil evaporation, no difference was found in the annual result when applying the procedures of Black, Gardner and Thurtell (1969) or Boesten and Stroosnijder (1986). Soil evaporation simulated with SWAP is almost insignificant (lower than 1 mm y^{-1}) and consequently no effect would be expected to happen when changing the method of calculation.

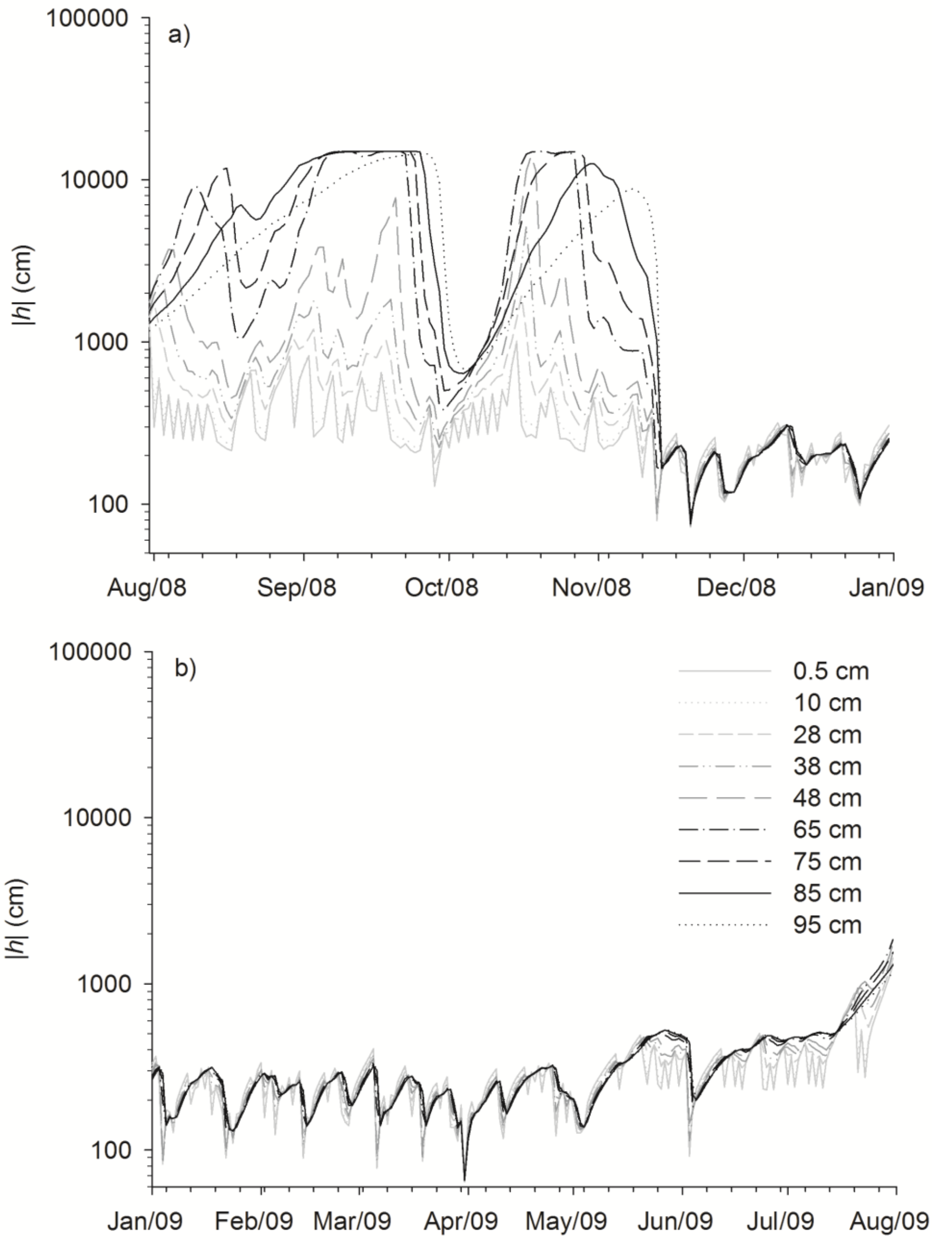

Figure 2.4 - Daily values of soil water pressure head *h* (cm) of the soil profile predicted by SWAP at depths 0.5 to 95 cm, a) from July 31st to December 31st, 2008 and b) from January 1st to July 31st, 2009

Table 2.6 shows the results of SWAP sensitivity analysis in relation to selected plant input parameters. As shown the results of *Q-RMSE* in this study, variations in the coffee light extinction coefficients (k_{dif} and k_{dir}), R_d, i_c and *LAI* in the SWAP crop file did not affect *Q*-values significantly. The parameters k_{dif} and k_{dir} are used in the calculation of soil evaporation, which in the conditions of the present study were very low, explaining the low influence of these parameters on the WB values. The *LAI* values estimated from leaf dry matter data were relatively high (Table 2.3) compared to literature values, however they can be acceptable when comparing to measurements performed in 2-4 years old coffee plants in the literature (GUTIÉRREZ; MEINZER, 1994). The analysis of sensitivity of *LAI* was not possible for +10% and +50% of the standard value because the results were higher than the maximum value allowable by SWAP. The critical soil water pressure head parameters were also evaluated in the sensitivity analysis and did almost not influence *Q* simulations with SWAP. The parameter K_c effected SWAP simulations for *Q* considerably, as *Q-RMSE* variations related to changes in this parameter were high.

Table 2.6 – Sensitivity of the SWAP model for deep drainage *Q* prediction evaluated trough the root mean square error (*Q-RMSE*), in relation to variations in 10% and 50% of plant standard parameters

Plant parameters	*Q-RMSE* (mm)			
	50%	10%	-10%	-50%
K_{dif}	0.003	0.000	0.004	0.08
K_{dir}	0.003	0.003	0.004	0.08
R_d	1.90	1.00	0.80	1.50
K_c	33.00	13.00	7.00	43.00
i_c	0.10	0.04	0.04	0.11
LAI	-[a]	-	0.027	0.135

Note: K_{dif}, extinction coefficient for diffuse light; K_{dir}, extinction coefficient for direct light; R_d, rooting length; K_c, crop factor; i_c, interception coefficient of Von Hoyningen-Hune and Braden; *LAI*, leaf area index;
[a] Not evaluated.

2.3.2 Model comparison

The comparison between SWAP predictions and Bortolotto's values of *Q* and ET_a is shown in Figure 2.5 and Figure 2.6. The monthly results of *Q* simulated with SWAP deviated from those of Bortolotto et al. (2012), presenting a linear relationship with $R^2 = 0.77$ (Figure 2.5a). Figure 2.5a shows specific months, those with the highest *Q* found during the year, responsible for the deviation of the tendency line. The resulted *RMSE* for *Q* is around 43 mm, a response to the predicted values in November and December of 2008, and March and April of 2009 (Figure 2.6). On these dates, a similar behavior for *Q* predictions by both models can be observed: in the months of November and March, *Q* simulated by SWAP resulted lower than the result of CWB, and in the respective next month of December and April, the inverse behavior occurred, Q obtained by CWB was lower than the simulated by SWAP. In the course of simulations, the water saved in one month is delivered to the next two months for both periods evaluated, the behavior of Q becoming closer to the 1:1 line in the third month of the sequence (Figures 2.5a and 2.6a).

This behavior of retaining and distributing water during the following months is confirmed when comparing the ET_a curves simulated in SWAP with those obtained by Bortolotto et al. (2012). These curves had similar results. Considering there are only two ways of losing water from this system (by evapotranspiration and drainage), the water transported by drainage Q in the simulations with SWAP is just distributed differently from Bortolotto's during the year.

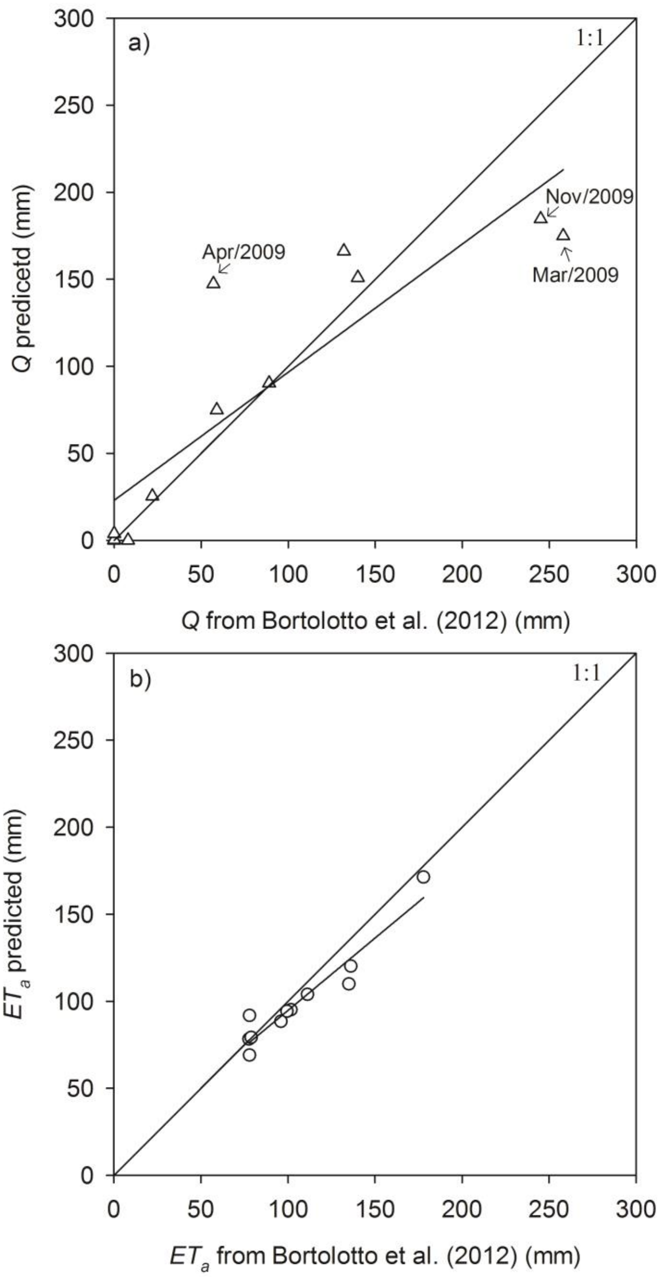

Figure 2.5 - Linear regression between Bortolotto et al. (2012) data and calculated (SWAP) monthly values of a) drainage Q (mm) and b) actual evapotranspiration ET_a (mm)

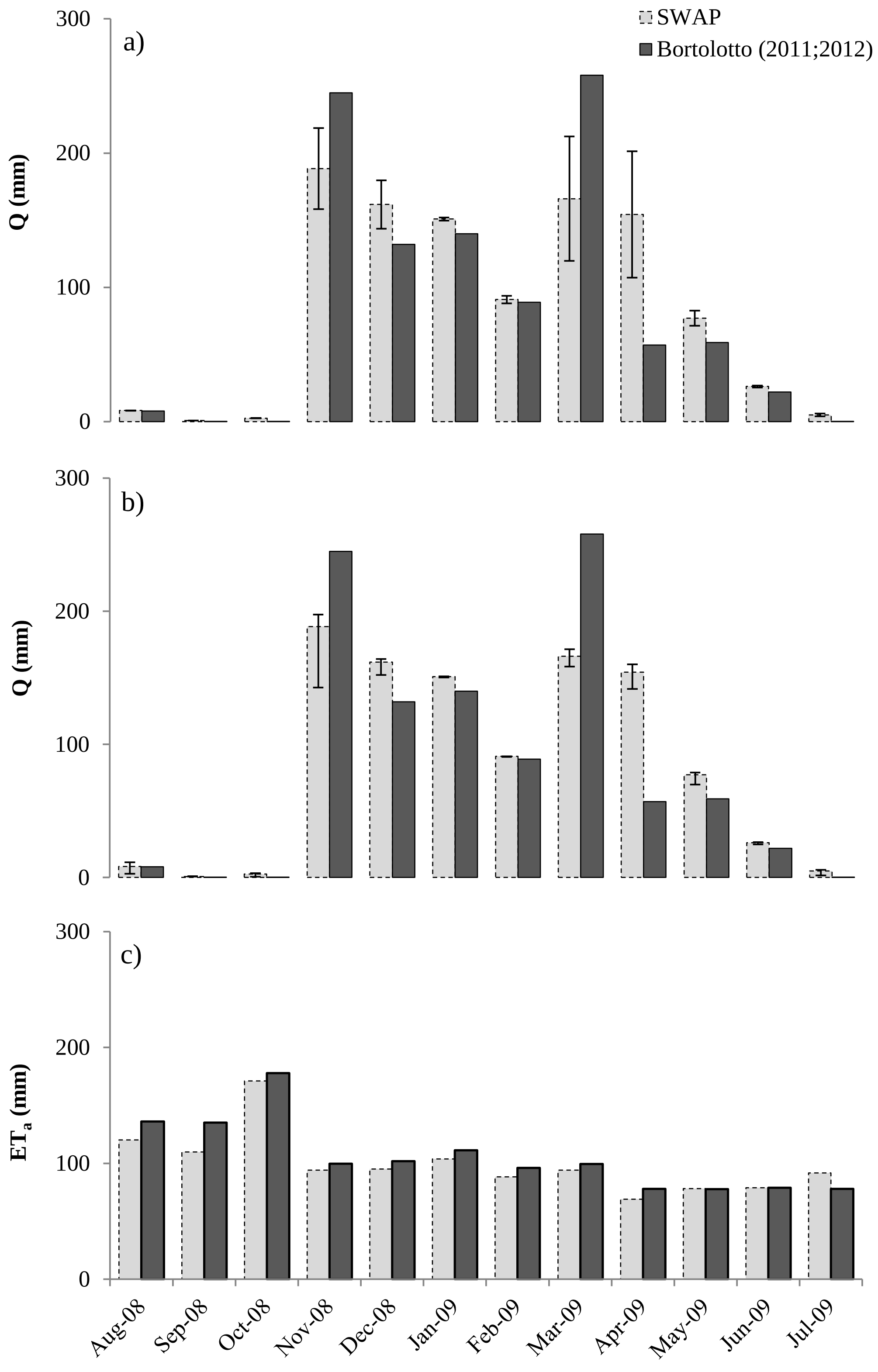

Figure 2.6 – Bortolotto et al. (2012) data and calculated (SWAP) monthly values of a) drainage *Q* (mm) with error bars representing the uncertainties due to temporal variations in the occurrence of precipitation events, b) drainage *Q* (mm) with error bars representing the uncertainties due K_s (m d^{-1}) variations in soil profile, and c) actual evapotranspiration ET_a (mm)

During the dry period of the experimental year, from July to November of 2008 (Figure 2.4a), soil pressure head at depths 65, 75, 85 and 95 cm assumed values equal to or very close to -15000 cm. However, *h* did not remain at these low values for a long time, a maximum of 23 days for the 85 cm depth in September and 12 days for the 65 cm depth in October. The behavior of *h* in the 65-95 cm soil layer during the dry period can initially (from August to September) be understood by the infiltration of water from irrigation and later due to the rain events of September (P = 31 mm in four days) and the beginning of November (P = 90.5 mm in two days). Irrigation water did not reach layers deeper than 95 cm during August and most of September, since *h* in this region decreases almost linearly and stabilizes at -15000 cm, increasing only due to the large rain event in late September. The rain events of November make the pressure head increase and become almost uniform along the soil profile. The simulated Q is, therefore, nearly zero from August to October of 2008 (Figure 2.6a), confirming there is no drainage due to irrigation during the dry period of the year. The water delivered by irrigation and rainfall during the dry period is retained in the 1 m of the soil profile and is kept available to plants or deep drainage in the wet period.

The simulated results of ET_a showed to be close to the observations of Bortolotto et al. (2012) since the linear regression between them was obtained with R^2 = 0.9. However, the model SWAP predicted ET_a values lower than those of CWB (Figure 2.5b). SWAP takes into consideration plant characteristics as already mentioned for the estimation of E_a and T_a. Since the ET_a calculation in Bortotlotto et al. (2012) is based only on soil water storage variations and the amount of precipitation, we should not expect an exact agreement between Bortolotto´s data and SWAP simulations.

The uncertainties of SWAP modeling for Q due to the meteorological input data and variations in K_s are shown in Figure 2.6a and 2.6b (see item 2.5). Based on the results of Figure 2.6a, we verified Q is highly influenced by the meteorological values and can vary more in the wet months. During the dry period of the year the uncertainties are smaller, which lead to the conclusion Q is mainly governed by the precipitation. Figure 2.6b shows the uncertainties of Q simulated with SWAP due to variations of K_s values from 26 m d^{-1} to 455 m d^{-1}, measured by laboratory tests.

In the CWB method, when the amount of precipitation of an event exceeds ET_p and at the same time soil available water capacity (AWC) is fulfilled due to antecedent rainfalls, there is an excess of water considered to be Q. Results of drainage Q obtained in Bortolotto et al. (2012) present uncertainties however due to specific considerations on the AWC calculations. In that study, the AWC was calculated as the difference in the soil water storage at field capacity (considered to be characterized by h = -33 kPa) and at wilting point (at h = -1,500 kPa). Nevertheless, the pressure head at field capacity can vary from -10 kPa to -33 kPa accordingly to the soil type and characteristics (RICHARDS; TIMM, 2004). Increasing field capacity to h=-10 kPa, for example, would increase directly the AWC and reduce Q amount obtained by CWB. This change in AWC could possibly approximate the Q results of CWB and SWAP model in Figure 2.6.

Table 2.7 presents the components of the annual water balance obtained by SWAP and the estimated results of Bortolotto et al. (2012). Although the monthly differences shown in Figure 2.6, the annual results of the components Q and ET_a ended up very close. As shown by the simulations of SWAP, only a small portion of the water entering the system during the year is converted into P_i. However, this component is much higher than the annual E_a that was 0.6 mm. These results could be consequences of the high density of leaves in the plantation since the coffee plants are at full maturity. Conclusively, all the water assigned as ET_a in Table 2.7 represents plant transpiration.

Table 2.7 – Components of the annual water balance simulated by SWAP and calculated by CWB of Bortolotto et al. (2012)

Water balance components (mm)	SWAP	CWB
P	1535	1535
I	697	697
P_i	18	-[a]
ET_a	1194	1270
RO	0	-
Q	1019	1010

Note: CWB, climatologic water balance; P, precipitation; I, irrigation; P_i, canopy interception; ET_a, actual evapotranspiration; RO, run-off; Q, bottom flux;
[a] Not available.

2.3.3 Scenarios of irrigation

In order to generate new information on water management for coffee cultivation in the west of the state of Bahia, several scenarios of irrigation were simulated with SWAP (Figures 2.7 and 2.8). With this information, we planned to demonstrate the influence of I on Q, and also to analyze different possibilities of management, in contraposition to the choice of the farmer. Usually, irrigation water is applied in several volumes distributed during the year by the farmers, and this routine is necessary because they fertigate the crop year round.

Alternatively, this information would also serve to lead farmers to adopt more sustainable practices of water management in this agricultural region.

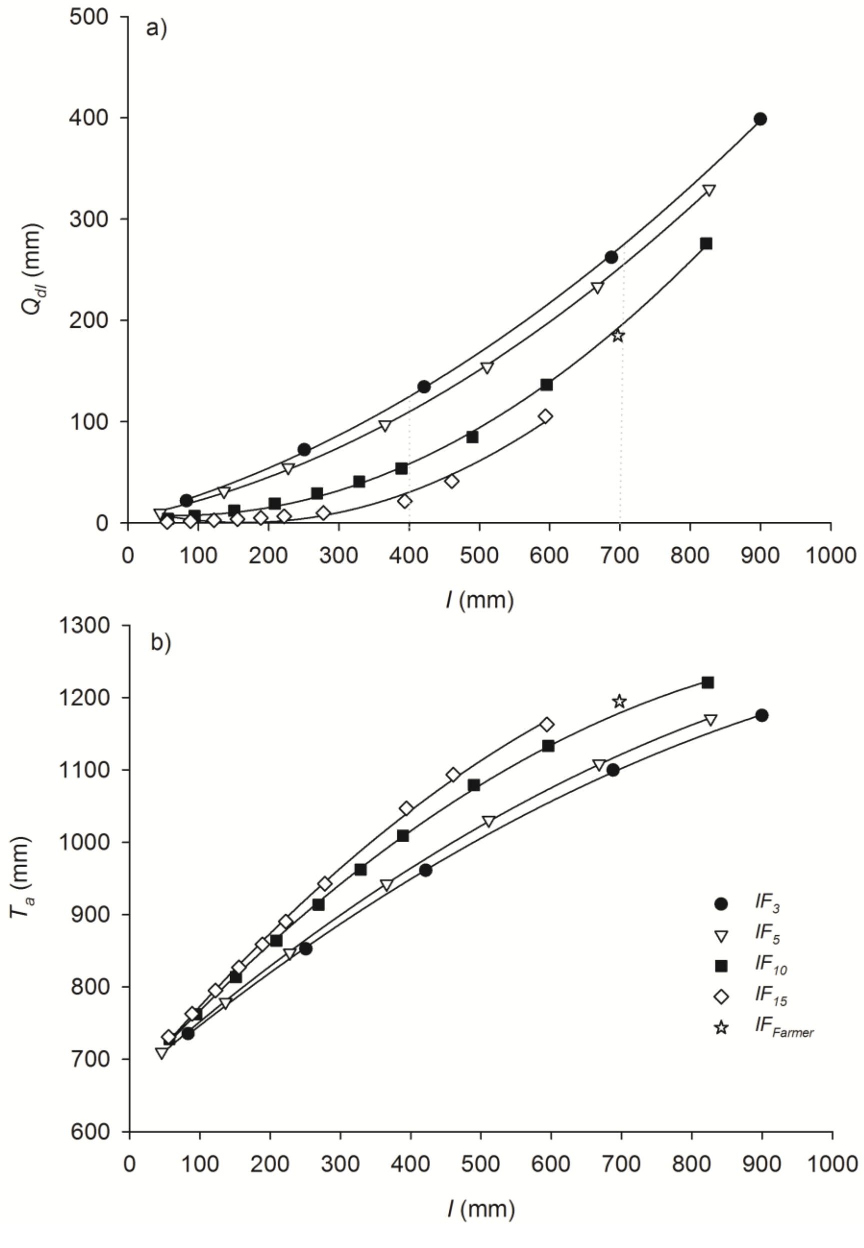

Figure 2.7 – a) Annual drainage due irrigation only Q_{dI} (mm) and b) annual plant transpiration T_a (mm) for different irrigation frequencies (*IF*) as a function of the amount of water applied *I* (mm) throughout the experimental year

SWAP simulation with no irrigation yielded the value of Q_{dP}, the drainage only due to rainfall (833.4 mm), which is very high, showing the rainfall is the main factor responsible for *Q* in the annual balance. This value was subtracted from the total *Q* to obtain Q_{dI}, the drainage due to irrigation only. For all simulations of Figure 2.7a, we present Q_{dI} maintaining the actual rainfall (2008/2009).

Each of the four curves in Figure 2.7a was fitted to a 2nd order polynomial model to appreciate their behavior better. Results indicate that Q_{dI} values tend to be lower when the frequency of irrigation is high (IF_3), which can be verified comparing the results for a fixed I. As an example, for 400 mm, the values of Q_{dI} from the respective regression curves are 24 mm for IF_{15}, 63 mm for IF_{10}, 109 mm for IF_5, and 129 mm for IF_3. In this case, Q_{dI} increases 39 mm from IF_{15} to IF_{10}, 46 mm from IF_{10} to IF_5, and 20 mm from IF_5 to IF_3, showing there is a considerable rise in Q_{dI} when reducing the irrigation frequency. Taking the amount of water applied by farmers (I = 697 mm), the correspondent Q_{dI} is 134 mm (IF_{15}), 205 mm (IF_{10}), 248 mm (IF_5), and 282 (IF_3). As it can be observed, farmer's irrigation management (IF_{Farmer}) practically encloses the IF_{10} curve. The IF_{10} and IF_{15} scenarios are characterized by having several days between applications of water and consequently in these scenarios there is no irrigation during the wet period of the year.

Plant response to irrigation scenarios is presented in Figure 2.7b. For fixed values of I, T_a increases as the frequency of irrigation (IF) decreases. Larger intervals of irrigation might induce a drier microclimate in the canopy, therefore, increasing T_a. Both results of T_a and Q showed there is less loss of water by drainage (more loss by transpiration) when the irrigation is applied with greater time intervals. For all the scenarios, there is a tendency of Q_{dI} and T_a to increase with the amount of water used yearly by the irrigation.

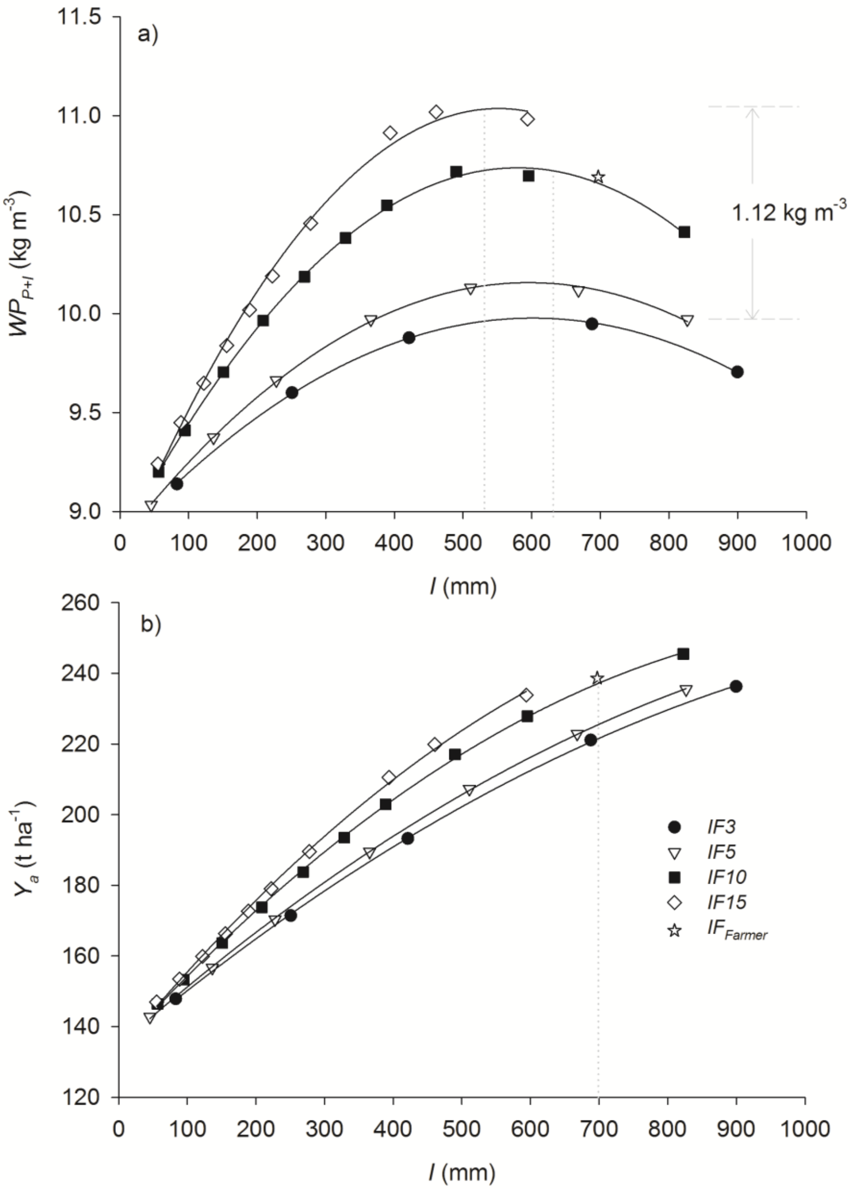

Figure 2.8 - a) Water productivity WP_{P+I} (kg m^{-3}) and b) actual yield Y_a for different irrigation frequencies (*IF*) and amount of water applied *I* (mm) throughout the experimental year

The effect of irrigation scenarios on the soil-plant system is interpreted in a different perspective when looking at water productivity (*WP*) outcomes. These results showed there is a limit for the amount of water used during the year, which is confirmed by the peak values in each curve of Figure 2.8a. For the same amount of irrigation, the difference between *WP* for the several *IF*-curves in Figure 2.8a does not pass 1.12 kg m^{-3} (1.12 kg of dry matter per ha, per mm of water). This relative low influence of *I* on the results of WP_{P+I} can be attributed to the dominant rainfall in this coffee cultivation region. In any case, when analyzing the efficiency of the irrigation scenarios, not only *WP* should be considered, but also the respective *Q*.

The maximum values of WP_{I+P} obtained from the regression curves in Figure 2.8a occurred when I was between 530 and 630 mm. When water was applied in intervals of 15 days (IF_{15}) during the year, the WP had the highest values. The best management practice, however, would bring benefits not just to water conservation, but also to coffee productivity. Figure 2.8b showed the actual coffee yield Y_a increased as a results of I increments. Any irrigation scenario with I between 650 and 750 mm and water application intervals of 15 days (IF_{15}) (Table 2.8), would result in higher Y_a values and also of WP in relation to the farmer´s management scenario (IF_{Farmer}). The scenario IF_{Farmer} resulted in Y_a equal to 238 t ha^{-1} and WP_{I+P} equal to 10.70 kg m^{-3} (10.70 kg ha^{-1} mm^{-1}), which is not so different from the most efficient irrigation management (WP_{I+P} that is around 11.06 kg m^{-3}, Figure 2.8a). In comparison, when I is extrapolated to 700 mm, with $IF_{15,}$ Y_a would result in 248 t ha^{-1}, WP_{I+P} in 10.90 kg m^{-3}, and the corresponding Q_I reduced by 49 mm in comparison to the farmer's irrigation scenario. Considering the time scale of coffee cultivation can reach up to 18 years, a yearly reduction of Q_{dI} and the increase of Y_a presented above, although relatively small, would greatly benefit water conservation and groundwater pollution, as well as coffee productivity.

Table 2.8 – Values of water productivity (*WP*), plant productivity (Y_a), and bottom flux due irrigation (Q_{dI}) for the scenarios of irrigation (*I*) and obtained from SWAP simulations

I	*WP* (kg m^{-3})		Y_a (t ha^{-1})		Q_{dI} (mm)		ΔQ_{dI}[a] (mm)	
(mm y^{-1})	IF_{15}	IF_{10}	IF_{15}	IF_{10}	IF_{15}	IF_{10}	IF_{Farmer} - IF_{15}	IF_{Farmer} - IF_{10}
600	11.05	10.72	238	228	88	149	96	36
650	10.99	10.69	243	233	111	176	74	8
700	10.90	10.64	248	237	136	207	49	-22
750	10.78	10.56	253	241	163	240	22	-55
800	10.61	10.45	257	244	193	275	-8	-90

Note: IF_{15} and IF_{10}, scenarios of irrigation with water application each 15 and 10 days, respectively; IF_{Farmer} farmers' scenario of irrigation; ΔQ_{dI}, difference between bottom flux due to irrigation only, using values obtained from IF_{Farmer} (Q_{dI} = 185 mm), IF_{15} and IF_{10} scenarios.

[a] Negative values means the bottom flux due to irrigation from IF_{Farmer} is higher than the amount in the considered scenario.

Low-frequency irrigation scenario could lead to a too dry soil condition in some periods of the year, considering the annual rainfall distribution in the area defines wet and dry periods. Evaluating the *h*-values in the soil profile for the scenario IF_{15} (I = 460.5 mm), as an example, it can be verified the soil water depletion occurs during the months of September and October from depths 48 to 95 cm (Figure 2.9). When analyzing monthly data, these low values of *h* apparently have a potential effect on plant transpiration. From SWAP simulation outcomes, plant transpiration in September isT_a = 107 mm (T_p = 145 mm) and in October is T_a = 85 mm (T_p = 197 mm). Daily *h*-values in this soil layer reveal the soil remains close to wilting conditions for about 45 days and T_a tends to decrease and reaches almost zero three times. An excessive depletion of the available water can convey irreversible consequences in coffee productivity and development, and this situation could occur for the scenarios with low amounts of water applied in the IF_{15} or IF_{10} choices. On the other hand, the coffee plant stress by a lack of water during a certain period of the year could bring benefits for production, as presented in the technical report of Guerra et al. (2005).

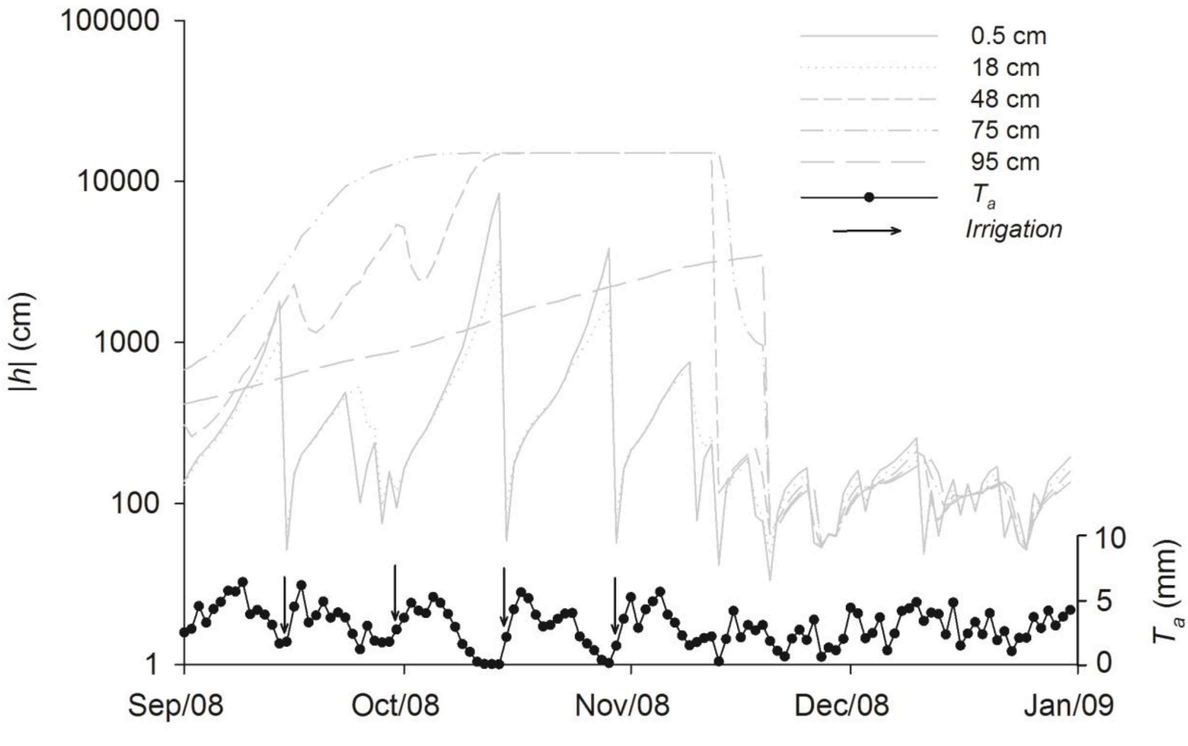

Figure 2.9 – Daily values of soil water pressure head *h* (cm) predicted by SWAP during the year at soil depths of 0.5, 18, 48, 75 and 95 cm, for the irrigation scenario *I* equal to 460.5 mm and *IF* of 15 days

We analyzed a year in which rainfall was considerably high (1535 mm), and this is an important detail to be considered for a complete search of the best management practice. As cited before, rainfall averages range from 800 to 1800 mm and, therefore, in a dry year, the results of the irrigation scenarios could be driven to distinct results of water use efficiency. The stochastic employment of meteorological data or exclusively of the rainfall applied in SWAP would be highly recommended for a complete evaluation of the behavior of the irrigation scenarios and also for the analysis of climate effects. Bennett, Bishop and Vervoot (2013) introduced a stochastic approach with SWAP to quantify time and space uncertainties in deep drainage due to rainfall, land management and soil hydraulic properties in Australia. Rainfall was the most important factor and a source of uncertainty to be considered for the drainage predictions in that study, and precise rainfall data is required in such kind of study. Another point to be concerned with is that the studied coffee plants were fully mature, and these predictions should be re-evaluated for young coffee crops.

This application of SWAP tried to find the best adjustment of the model to a perennial crop and showed ways of using it to evaluate the possibility for improvements in irrigation management. Some concerns exist nevertheless in respect to our evaluations, since the outcomes are restricted to the one-year of available experimental data, and a proper validation of model simulations was not possible. Our conclusions from the presented evaluations and scenarios with SWAP are subject to such limitations.

2.4 Conclusions

This study showed the potential of the SWAP model for studying a perennial crop in a Cerrado ecosystem in Brazil and for generating irrigation scenarios. SWAP's most sensitive input parameters were determined experimentally and other less sensitive were obtained from the literature to establish the calibration. Model simulations for monthly drainage when compared to the climatological water balance CWB data generated a determination coefficient R^2 of 0.77. Therefore, we assumed SWAP is already a validated model widely tested and proved to be efficient in different parts of the world. For that reason, we could predict scenarios of irrigation for our region of coffee cultivation.

Irrigation scenarios simulated with SWAP for the experimental year showed to be efficient in water use and coffee productivity when longer intervals of irrigation were used. According to this analysis, adopting an irrigation interval of 15 days and yearly water amount between 650 and 750 mm could be an option for better management compared to the farmer's scenario. The results of water productivity, plant productivity, and deep drainage indicated the farmer's management practices could be improved, minimizing loss of water by drainage and at the same time increasing coffee production. The information presented here should support farmers to improve their water irrigation management practices and alert them to environmental losses that might occur in these heavily fertilized coffee plantations in western Bahia, Brazil.

Some concerns still exist, however, with respect to the performed simulations: 1) there was limited experimental data for the simulations (a one-year period); this could be improved with a new study with information about the coffee plant and the SWAP plant module being structured year by year; 2) the absence of model validation with proper data; 3) the deterministic approach here used could be replaced by a new stochastic evaluation applied to meteorological and soil hydrological data, to solve spatial and temporal limitations of the simulations.

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3 Modeling nitrogen dynamics in a fertigated coffee plantation in the Brazilian Cerrado with ANIMO

Abstract

In agriculture, a focus merely on productivity leads to unsustainable use of inputs, which in turn can result in negative consequences to the environment and human health. An expected consequence of excessive fertilizers use is the degradation of groundwater and surface water in and around agricultural ecosystems. The Brazilian Cerrado has suffered transformations by the advance of intensive agriculture during the last decades, and information about current field nutrient management and its environmental impact is needed to establish sustainable practices for this modified biome. Process-based models are a useful tool for evaluating such aims under future scenarios. The coupled models SWAP/ANIMO were used in this study to simulate leaching and plant uptake of nitrate-nitrogen (NO_3-N) in a Cerrado soil of Bahia, Brazil, cultivated with coffee at an intensive mineral fertigation management. Main model parameters were measured under field conditions and ANIMO was calibrated for a scenario corresponding to an application with 400 kg N ha^{-1}y^{-1} mineral fertilizer. The model was tested with independent data of NO_3-N in soil solution measured in plots receiving 800 kg N ha^{-1} y^{-1}. Statistical analysis of the modeling with ANIMO showed the simulations were in agreement with experimental measurements during one year of study. The measured average annual N plant uptake was similar to ANIMO predictions. Sensitivity analysis showed pH and reference temperature are critical for predictions of NO_3-N leaching and concentration in soil solution. Model predictions of the organic cycling due to manure applications, plant roots, and leaf deposition were also obtained. Transformations and leaching of organic N were not measured experimentally and could not be considered in model validation. Besides the model evaluation for mineral fertilizer, we also present data needed for modeling decomposition of some organic fertilizers like poultry manure and coffee husks, which are widely used in similar agricultural systems. Obtained modeling results can give support for the implementation of better strategies for mineral and organic N fertilizer management for the Cerrado coffee production system of Bahia and alike production scenarios.

Keywords: Nitrogen cycle, leaching, ANIMO model, Cerrado

3.1 Introduction

The Cerrado zone in Bahia, one of Brazil´s northeastern states, presented the highest coffee productivity (average of 37.5 bags per hectare) of the country over the 2009-2014 period (CONAB, 2014). Its productivity was 22% higher than the second most productive region, the Cerrado of the southeastern state of Minas Gerais. Although Cerrado soils are notoriously infertile, the region in Bahia has several excellent qualities for modern agriculture. The flat land is accessible for planting, the sandy and sandy-loam soils are well drained, and surface and underground water sources are available for crop cultivation with irrigation (GASPAR; CAMPOS, 2007). Moreover, the well-defined rainy season (October-April) and an almost rainless season from May to September is a welcome climatic feature of this region with respect to coffee cropping. Coffee production in the Cerrado of Bahia is only possible due to the combination of irrigation and fertilizing practices, however.

Few studies evaluated the N processes occurring in the productive coffee cultivations of Bahia´s Cerrado and associated them to management practices. For this reason, it is questionable whether fertilizers have been managed efficiently and in a sustainable way in this region. Existing studies on the N management for coffee cultivation on Cerrado soils did not solve these questions. Bruno et al. (2014) studied the N efficiency uptake by mature coffee plants in western Bahia for different doses, concluding that a reduction from 600 to 200 kg N ha^{-1} y^{-1} was possible without reducing crop productivity and decreasing the leaching of N to groundwater. A study by the Brazilian Agricultural Research Corporation (Embrapa) resulted in the same dose (200 kg N ha^{-1} y^{-1}) for a maximum coffee yield on an Oxisol in the central Cerrado (SANZONOWICZ et al., 2003). Neto et al. (2011) found a dose of around 400 kg N ha^{-1} y^{-1} to yield maximum productivity of coffee plants of Bahia’s Cerrado. These are few achievements related to fertilization efficiency, and more studies need to be developed for the successful continuity of coffee cultivation in the Cerrado region and an efficient production system with sustainable and non-polluting farming practices.

The use of models is an important tool for understanding water and nutrient dynamics in agricultural systems, to evaluate sensitivities and to suggest strategies for reducing fertilizer input and propose scenarios for better management. The hydrological model SWAP (VAN DAM et al., 2008) and the nutritional model ANIMO (GROENENDIJK et al., 2005) are both widely used to simulate water and nutrient dynamics. SWAP simulates the physical mechanisms associated with water flow, heat flow and solute transport in the soil. ANIMO simulates the cycles of C, N, and P in the soil, as well as greenhouse gas emissions, emphasizing nutrient leaching together with decomposition, nitrification, denitrification, mineralization, immobilization, phosphorus (P) and nitrogen (N) soil sorption, and carbon (C) dynamics. Combined, SWAP and ANIMO are able to quantify nutrient losses and gains due to fertilization practices, water, soil and land management for various types of soils and different hydrological conditions, and can be applied to studies on climate change and agricultural management scenarios (SHEPHERD et al., 2011). Both simulation models were accepted by the research community on water and nutrient dynamic studies with applications in several places around the world and for different aims (DROOGERS et al., 2000; MARINOV et al., 2005; SINGH et al., 2006; RUIZ et al., 2008; GUSEV et al., 2010; NOORY et al., 2011; MA et al., 2011; VERMA; GUPTA; ISAAC, 2012; CRESCIMANNO; MORGA; VENTRELL, 2012; DE JONG VAN LIER et al., 2015).

In this study, we performed a parameterization of ANIMO for a fertilized Cerrado coffee cropping scenario assessing a recommendation for sustainable fertilizer use. The model was calibrated and validated using data on N uptake by plants and nitrate concentration in the soil solution. The model was used to predict the annual N balance for several fertilizer rate scenarios, and results were compared to observations obtained in field experiments with adult coffee plants.

3.2 Materials and methods

3.2.1 Field data

Field data used for calibration and testing are described in Bruno et al. (2011) and Bortolotto et al. (2011). These authors carried out an experiment from August 1, 2008, to July 24, 2009, on a private coffee farm in Barreiras (11°46 S, 45°43’ W) in the state of Bahia, Brazil. The area has virtually no slope (<1%) and was previously covered by Cerrado vegetation. The soil is classified as Typic Hapludox (SOIL SURVEY STAFF, 2010), has low natural fertility and is surrounded by remaining Cerrado ecosystem areas. Local precipitation ranges from 582 to 1687 mm per year according to historical data (1961-2013) of the National Institute of Meteorology (INMET). Wind speed, solar radiation, air temperature, and air humidity were used from the INMET weather station of Barreiras. Precipitation and irrigation were measured at the experimental field.

Coffee plants (*Coffea arabica* L., variety Catuaí Vermelho) were seven years old at the beginning of the experiment. The plant arrangement was circular, allowing irrigation and fertigation by a center pivot with a total irrigated area of 80 ha. Plants spacing was 3.8 m between lines (pivot circles) and 0.5 m between plants. In previous years, urea was applied as fertilizer by fertigation according to the expected crop productivity. The input of mineral N was of the order of 600 kg N ha^{-1} y^{-1}.

Irrigation was performed by Low Energy Precision Application (LEPA) emitters, which distribute the water according to the circular coffee lines, avoiding water application in the interrow. The operation of the pivot was continuous during the year and stopped only for harvest. An amount of 4 mm of water was applied every second day, and fertigation each fourteen days. The farmer´s practices for crop management included weed and pest control with pesticides, applications of phosphorus (P), potassium (K), micronutrients, lime and gypsum and several organic materials.

Experimental data from Bruno et al. (2011) were assembled to analyze the N distribution in coffee plant compartments and to obtain an annual N balance for applications of four fertilizer doses, with four replicates. Sixteen plots with three plants each received urea at rates of 200, 400, 600 and 800 kg N ha^{-1} y^{-1}. The annual amount of N fertilizer was partitioned for application each 14 days, over one full year, following farmer´s practice. The experiment was assembled in the fourth circle of the pivot (258 coffee trees grown as a hedge), counted from the center, which was disconnected from the farmer´s fertigation schedule. The experimental parcels were randomly distributed along the circle. A schematic representation of the experimental plots is available in Bruno et al. (2011).

Soil solution samples were taken using soil solution extractors, which were installed close to the middle plant trunk only in the parcels that received 400 and 800 kg N ha^{-1} y^{-1}. Soil solution was sampled at the 1.0 m depth, every two weeks during the second half of 2008 and once per month during the first half of 2009. Nitrate concentration in soil solution was measured by flow injection analysis.

3.2.2 Models and scenarios

ANIMO (GROENENDIJK et al., 2005) simulates carbon, nitrogen and phosphorus cycles in a one-dimensional layered soil-plant system and should be used in combination with a hydrological model. Commonly used in association with ANIMO, the SWAP model (KROES et al., 2008) simulates spatio-temporal variations of soil water content and temperature. Nutrient transport simulation by ANIMO is governed by the general formulation of the mass conservation and transport differential equation (GROENENDIJK et al., 2005; RENAUD et al., 2006). For additional information and details in relation to the ANIMO model and its operation, we refer to the studies of Berghuijs-van Dijk et al. (1985), Groenendijk et al. (2008), Roelsma and Hendriks (2014), Stolk et al. (2011) and De Willigen et al. (2008).

For simulation purposes, the growing season (year) was subdivided in two periods of six months: the first one from August to December 2008 and the second from January to July 2009. Simulations referred exclusively to coffee plants, i.e., no weeds or interrow crops were considered. The seven-year-old coffee plantation on a sandy soil was described in the input files of ANIMO using data directly collected in the experimental setups together with scientific database information available in other published materials related to agriculture in the Brazilian Cerrado area.

3.2.2.1 Hydrological module (SWAP)

The hydrological data used for ANIMO simulations were obtained using the SWAP model (KROES et al., 2008) with hydraulic parameters for the soil profile down to 1 m depth, and these outcomes can be found in Pinto et al. (2015). Soil hydraulic parameters were preserved during ANIMO simulations (Table 3.1). For the deeper soil layer (1.0-2.0 m) the hydrological parameters were obtained by fitting the Van Genuchten (1980) equation with Mualem parametric restriction to data obtained from disturbed soil samples ($R^2 = 0.92$) using the software RETC (VAN GENUCHTEN et al., 1991). The shape parameter λ for the deeper soil layer was obtained by inverse modeling.

Table 3.1 – Van Genuchten-Mualem soil hydraulic parameters used in SWAP simulations

Soil layer (m)	θ_r ($cm^3\ cm^{-3}$)	θ_s ($cm^3\ cm^{-3}$)	α (cm^{-1})	n	K_s ($m\ d^{-1}$)	λ
0-1.0	0.096	0.387	0.0169	1.636	0.266	0.5
1.0-2.0	0.115	0.525	0.0127	2.040	0.310	0.5[a]

Note: θ_r, residual volumetric soil water content; θ_s, saturated volumetric soil water content; n, α and λ the shape parameters of the retention curve; and K_s the saturated hydraulic conductivity. VG parameters were obtained with a determination coefficient $R^2 = 0.88$ (soil layer 0 – 1.0 m) and $R^2 = 0.92$ (soil layer 1.0 – 2.0 m).
[a] Initial value before calibration

3.2.2.2 Crop and soil parameters

Relevant crop (coffee) parameters are shown in Table 3.2. The relation C/N and pH for some Brazilian Cerrado soils and the estimations used in the present study are shown in Table 3.3. The estimated C/N ratio and pH of the soil in this study were comparable and close to values of other studies in the Cerrado. The depth of the root zone Z_r (1.0 m) was maintained constant during the experimental year. As observed in field tests, the majority of roots were found close to the soil surface. The soil layer with the relative highest root concentration (100%) was adjusted in SWAP from soil surface until 0.6 m, decreasing linearly down to 1% at the maximum root zone depth (1 m). The expected cumulative N uptake (U_p) values were obtained from data of N concentration and dry matter of the plant parts (leaves, branch, trunk, fruit, and litter) sampled during the year (BRUNO et al., 2011). The U_p was obtained for each plot of the study and a mean value was calculated at the end for the simulations. The difference between the N accumulated in the whole plant at onset and end of the experiments was the expected N uptake during the experimental period. Plant transpiration values were obtained from SWAP simulations. The parameter σ_N^{max} was established by calibration, to be discussed later.

Soil temperature was obtained by a numerical approach available in the SWAP model, making use of soil texture data, soil water and air volume fraction, and air temperature as the top boundary conditions. Initial amounts of NH_4-N and NO_3-N in the soil solution of compartments as required for ANIMO simulations were considered equal to zero for both inorganic N forms, since no soil solution analyzes for N concentrations were made in the beginning of the experiment (BORTOLOTTO et al., 2013) due to the occurrence of very low soil water contents.

Table 3.2 – Soil and plant input parameters used in ANIMO simulations for a Typic Hapludox (Soil Survey Staff, 2010) and *Coffea Arabica L.*, variety *Catuaí Vermelho*

Description	Parameter symbol	Value	Unit
Soil			
Thickness of Surface layer (0-0.1m)	Δz_1	0.1	m
Thickness of intermediary layer (0.1-1.0m)	Δz_2	0.9	m
Thickness of deep layer (1.0-2.0m)	Δz_3	1.0	m
Thickness of top soil compartment	Δz_{top}	0.02	m
Thickness of the reservoir for additions	Δz_{res}	0.05	m
Diffusion coefficient (Surface layer)	p_1	2.00[a]	-
Diffusion coefficient (Intermediate and deeper layers)	p_2	3.00[ab]	-
Saturated hydraulic conductivity of the root zone (Surface and intermediate layers)	K_{sr}	0.266	m d^{-1}
Saturated hydraulic conductivity of root zone (Deeper layer)	K_{sr}	0.310	m d^{-1}
Dry bulk density (Surface layer)	ρ_{d1}	1790	kg m^{-3}
Dry bulk density (Intermediate layer)	ρ_{d2}	1580	kg m^{-3}
Dry bulk density (Deeper layer)	ρ_{d3}	1480	kg m^{-3}
Soil carbon-nitrogen ratio (Soil profile)	C/N	10	-
Coefficient for organic matter transformations and nitrification	A_n	74826[a]	J mol^{-1}
Coefficient for dissolved organic matter transformations	A_d	74826[a]	J mol^{-2}
Soil pH (Surface layer)	pH_1	4.1[b]	-
Soil pH (Intermediate and deeper layers)	pH_2	3.8[b]	-
NH_4 sorption coefficient (Soil profile)	s_{NH4}	0.0003[b]	m^3 kg^{-1}
Reference temperature	T_{ref}	25.0[b]	ºC
Plant			
Depth of initial root zone	Z_r	1.00	m
Plant residues (roots)	P_r	1426	kg ha^{-1}
"Sowing" date (in the year of 2008)	t_p	213	Julian day
Harvesting date (in the year of 2009)	t_h	212	Julian day
Transitional data for uptake periods	t_c	365	Julian day
Cumulative transpiration in the first period	T_{a1}	0.59	m
Cumulative transpiration in the second period	T_{a2}	0.60	m
Maximum N transpiration stream concentration factor	σ_N^{max}	4.0[b]	-

[a] According to Groenendijk et al. (2005)
[b] Initial values considered before calibration

Table 3.3 – Carbon to nitrogen ratio (C/N) and pH for some Brazilian Cerrado soils

Soil	Soil pH	C/N	Reference
Sandy soils	-	12	Smaling et al. (2008)
Clay soils	-	12	Smaling et al. (2008)
Dystrophic soils	5	20	Pellegrini et al. (2014)
Dystrophic soils	5	19	Pellegrini et al. (2014)
Dystrophic soils	5	21	Pellegrini et al. (2014)
Dystrophic soils	5	21	Pellegrini et al. (2014)
Anionic Acrustox	4.9	14	Alcântara et al. (2004)
Oxisol	5.2	16	Lilienfein et al. (2003)
Oxisol	4.8	21	Nardoto and Bustamante (2003)
Oxisol	4.6	23	Nardoto and Bustamante (2003)
Oxisol	4	20	Jantalia et al. (2007)
Typic Hapludox	3.9	10	This study

3.2.2.3 N input characterization

The inputs of N in the simulated soil-plant system occur by dry and wet deposition, by rainfall, irrigation water, applications of fertilizers and manures, and by plant shoots (leaf litter) and decomposition of roots.

The average concentrations of NH_4^+ (c_{wNH_4}) and NO_3^- (c_{wNO_3}) in rainwater were obtained from studies of different parts of Brazil (Table 3.4) and used as input in the present simulations with ANIMO. The input of annual N dry deposition was assessed using the N wet deposition data predicted with ANIMO and the ratio values of the annual dry and wet deposition for NH_4-N (I_{dNH_4}/ I_{wNH_4}) and NO_3-N (I_{dNO_3}/ I_{wNO_3}) found in North and South America (Table 3.5). As water used for irrigation during the experiment was taken from the nearest by river, but concentrations of inorganic N were not measured in the irrigation water, we used the N concentration from streams and rivers of the Cerrado biome reported by Hunke et al. (2015). Although the rivers from the exact location of this research are not included in this dataset, an average value of these data was considered acceptable for our purpose, mainly because this input is low compared to fertilizer applications.

Fertilizing was done with urea, with the addition of poultry manure and dry coffee husks. After applied to the soil, urea molecules in solution are mostly transformed into NH_4, due to the action of the urease enzyme, or they percolate out of the root zone and are hydrolyzed afterward. Being converted exclusively to NH_4 in the soil, urea can be considered an ammoniacal fertilizer.

Table 3.4 – Mean concentration of ammonium (c_{wNH4}) and nitrate (c_{wNO3}) in rainwater in some locations of Brazil

Reference	Location	c_{wNH4} kg m^{-3}	c_{wNO3} kg m^{-3}
Fia et al. (2013)	Lavras (MG)	0.00026	0.00034
Rodrigues et al. (2007)	Teresópolis (RJ)	0.00054	0.00038
Coelho et al. (2011)	Ribeirão Preto (SP)	0.00079	0.00029
Flues et al. (2003)	Figueira (PR)	0.00081	0.00054
Migliavacca et al. (2005)	Porto Alegre/Charqueadas (RS)	0.00015	0.00051
Migliavacca et al. (2004)	Serra do Veleda (RS)	0.00096	0.00039
Migliavacca et al. (2004)	Aceguá (Brazil-Uruguay border)	0.00051	0.00016
This study (Average)	-	0.00058	0.00037

Table 3.5 – Ratio dry/wet deposition of N in the ammoniacal (I_{dNH4-N}/ I_{wNH4-N}) and nitric form (I_{dNO3-N}/ I_{wNO3-N})

Reference	I_{dNH4-N}/ I_{wNH4-N}	I_{dNO3-N}/ I_{wNO3-N}
Lawrance et al. (2000)	0.21	0.02
Trebs et al. (2006)	0.46	0.09
da Rocha et al. (2005)	0.09	0.49

Representative values for N, NH_4-N, NO_3-N and OM concentrations in poultry manure and coffee husks were obtained from reports from literature (Table 3.6). Characterization of input material is shown in Table 3.7. The decomposition rate constants (k_{fp} and $k_{sp)}$ for organic fractions of manures were estimated using data published in the literature. The experimental data of remaining material from Augusto (2007) or organic matter decomposition rates from Dias et al. (2010) were used to generate the decomposition curves for the fast and slow reaction parts of the poultry manure. Zoca et al. (2014) obtained curves of coffee husk decay and their data were used to estimate k_{fp} and k_{sp}. Data of decomposition rate constants for poultry manure or coffee husks came from a single source due to the lack of specific information. Coffee husks were considered as 100% organic, based on cited studies that found only negligible NH_4 and NO_3 concentrations in this material (Table 3.6).

Table 3.6 – Values of organic matter content (c_{OM}), carbon content (c_C), nitrogen content (c_N), C/N ratio, and contents of N in ammoniacal form (c_{NH4-N}) and nitrate form (c_{NO3-N}) in coffee husks and poultry manure and litter

Description	c_{OM} %	c_C g kg^{-1}	c_N g kg^{-1}	C/N	c_{NH4-N} %	c_{NO3-N} %	Reference
Poultry manure	37	-	-	-	0.95	0	Renaud et al. (2006)
	69	313	40	9	0.0259	0.0037	Vanegas Chacón (2006)
	45	192	46	-	0.0608	0.0058	Melo et al. (2008)
	53	326	29	11	-	-	Moral et al. (2005)
	-	175	53	2	-	-	Augusto (2007)
	55	288	28	10	-	-	Dias et al. (2010)
	15	-	14	6	-	-	Castro et al. (2006)
	-	342	28	-	-	-	Lehmann et al. (2003)
Poultry litter	82	411	44	-	0.0362	0.0082	Passos (2010)
	49	-	20	13	-	-	Teixeira et al. (2002)
	-	-	22-42	-	-	-	Miele and Milan (1983)
	-	371-399	42-45	-	-	-	Leal et al. (2012)
	65-90	-	24-40	-	-	-	Konzen and Alvarenga (2002)
	-	-	23-27	-	-	-	Avila et al. (2007)
Coffee husks	-	513	12	44	-	-	Dias et al. (2010)
	-	-	15[a]	-	-	-	Leitão et al. (2005)
	-	436	10	-	-	-	Zerbinatti et al. (2014)
	-	439	16	27	-	-	Saenger et al. (2001)
	96-93	450-400	18-15	30-23	-	-	Zoca et al. (2014)
	-	545-417	18-23	30-18	-	-	Shemekite et al. (2014)
	-	508-282	20-13	40-14	-	-	Dzung et al. (2013)

[a]Values of crude protein were transformed into c_N in coffee husks using a conversation factor 6.25 (Rodrigues et al. 2010).

Table 3.7 – Characterization of material added to the study site soil-plant system

Input parameter	Symbol	Unit	Parameter value				
			Mineral Fertilizer	Poultry manure	Coffee husks	Coffee roots	Coffee litter
Organic content per material	c_{OM}	%	0	60[a]	100[a]	100	100
NH_4-N content per material	$c_{NH_4\text{-}N}$	%	80	0.040[a]	0[a]	0	0
NO_3-N content per material	$c_{NO_3\text{-}N}$	%	20	0.006[a]	0[a]	0	0
N concentration in fast reaction part	c_{Nfp}	kg kg^{-1}	-	0.03[a*]	0.013[a]	0.016[f]	-
N concentration in slow reaction part	c_{Nsp}	kg kg^{-1}	-	0.03[a]	0.014[a]	0.016[f]	-
Decomposition rate of fast reaction part	k_{fp}	y^{-1}	-	15[bc*]	1.5[d]	2[g]	-
Decomposition rate of slow reaction part	k_{sp}	y^{-1}	-	0.5[b]	0.08[d]	0.2[g]	-
Percentage of fast reaction fraction	$\%F_{fp}$	%	-	50	30[e]	90[g]	-
Percentage of slow reaction fraction	$\%F_{sp}$	%	-	50	70[e]	10[g]	-
Coffee litter N concentration	c_{Nli}	kg kg^{-1}					0.026[f]
Coffee litter decomposition rate constant	k_{li}	y^{-1}					0.42[fh]

Note: Data values obtained from: [a] Table 3.5; [b] Augusto (2007); [c] Dias et al. (2010); [d] Zoca et al. (2014); [e] Barcelos et al. (2001); [f] Bruno et al. (2011); [g] Wu and McGechan (1998); and [h] Olson (1963).
* Initial values that were modified later during the calibration.

The residues of plant roots and the litter cover (leaves) were classified as materials which added N to the soil. Dead plant root material (P_r) was characterized using data of root dry matter (RDM) obtained on day 0, 181, 265, and 356 from plants of the experimental site. During the experimental year, RDM maximum occurred on day 265 (10131 kg ha^{-1}) and decreased to a lower value on day 356 (8705 kg ha^{-1}) (BRUNO et al., 2011). As RDM increased from the beginning of the experimental analysis until day 265 we could not estimate the amount of dead roots added to the soil during this period. However, from day 265 on, we assumed the reduction in RDM until day 356 was delivered to the soil. A general rate of decomposition value for roots was recommended by Wu and McCechan (1998) Litter was parameterized with available data of N concentration and dry matter. The litter decomposition rate constant was estimated as the ratio between the annual mass of deposited leaves and the remaining leaves on the ground (OLSON, 1963). We considered a mean value for k_{li} for all studied plant parcels, although the calculated values were different for the several parcels or N doses. Values of the decomposition rate constant for litter k_{li} obtained from other studies are shown in Table 3.8, and they can be compared to the mean value found in this study.

Table 3.8– Litter decomposition rate constant for some vegetation types

Soil Covering	Location	k_{li} (y^{-1})	Reference
Cerrado plant residues	Brazil	1.78	Jacobson et al. (2011)
Coffee plant and fruit-tree	Brazil	4.38	Lisboa (2013)
Coffee plant and fruit-tree	Brazil	1.17	Arato et al. (2003)
Shaded tree leaves	Venezuela	4.00	Cuenca et al. (1983)
Coffee leaves	Venezuela	10.00	Cuenca et al. (1983)
Agroforestry residues	Indonesia	0.37	Hairiah et al. (2006)
Agroforestry residues	Indonesia	0.40	Hairiah et al. (2006)
Agroforestry residues	Indonesia	0.54	Hairiah et al. (2006)
Agroforestry residues	Indonesia	0.55	Hairiah et al. (2006)

Note: k_{li}, decomposition rate constant for litter covering.

Table 3.9 presents data related to root exudates, dissolved organic matter (DOM), humus and biomass, nitrification and denitrification processes. The N concentration in root exudates (c_{Nex}) was considered to be the same as in coffee root dry matter, and the decomposition rate constant k_{ex} was the recommended by Wu and McGechan (1998). The decomposition rate constant of the dissolved organic matter (k_{DOM}) and of the humus and biomass (k_{hu}), as well as the reference nitrification rate constant (k_{nr}) and the denitrification rate constant (k_d), and the humus N concentration (c_{Nhu}) were obtained by calibration. To obtain the initial values of k_{DOM} and k_{hu} we considered that DOM is rapidly decomposed and humus is slowly decomposed in the soil. The interval of variation for k_{nr} and k_{dr} were those presented in Renaud et al. (2006), the maximum and minimum values acceptable in ANIMO for each parameter. For all the organic materials added to the system, we used a rate of assimilation *a* equal to 25% (WU; MCGECHAN, 1998) and mass fraction of material transformed directly into humus $\%F_{hu}$ of 75%.

Table 3.9 – Decomposition rate constant values and N concentration for some pools in the ANIMO model

Pool	Decomposition rate		Nitrogen concentration		Reference
	Symbol	Value (y^{-1})	Symbol	Value ($kg\ kg^{-1}$)	
Exudates	k_{ex}	365	c_{Nex}	0.016	Wu and McGechan (1998), Bruno et al. (2011)
Humus and biomass	k_{hu}	0.006[a]	c_{Nhu}	0.001[a]	Groenendijk et al. (2005)
Dissolved organic material	k_{DOM}	30[a]			
Nitrification	k_{nr}	300[a]			
Denitrification	k_d	365[a]			

Note: k_{ex}, decomposition rate constant for root exudates; k_{hu}, decomposition rate constant for humus and biomass; k_{DOM} decomposition rate constant of dissolved organic matter; k_{nr} nitrification rate of reference; k_d denitrification rate; c_{Nex} concentration of N in root exudates; c_{Nhu} humus N concentration.
[a] Initial values accounted for calibration

3.2.2.4 Fertilizer management

3.2.2.4.1 Scenarios of N doses (part 1)

Scenarios characterized in this section refer to the experimental doses in the study of Bruno et al. (2011). Four levels of N doses were used with ANIMO: 200, 400, 600 and 800 kg N ha^{-1} y^{-1}, identified by M_{200}, M_{400}, M_{600}, and M_{800} respectively. Each N-management scenario consisted of 27 mineral N applications during one year (one application each 14 days).

3.2.2.4.2 Scenarios of N dose partition (part 2)

To evaluate the effects of annual N doses and fertilizer partition during the year on N plant uptake efficiency (NUpE) (Equation 3.1) and on NO_3-N leaching accumulated during one year, scenarios of N management were generated as described forward. The doses of 200, 300, 400, 500, 600, 700, and 800 kg N ha^{-1} y^{-1} were evaluated for the following frequencies of applications (dose partition): i) N application every second day ($NA_{1/2d}$) ; ii) once a week ($NA_{1/1w}$); iii) each 14 days ($NA_{1/2w}$); iv) once a month ($NA_{1/1m}$); v) seven times during the year ($NA_{7/12m}$); and vi) three times during one year ($NA_{3/12m}$). The models SWAP/ANIMO generated a total of 48 scenarios from the combinations of different N amounts and dose partitions during the year.

3.2.2.4.3 Scenarios of precipitation amount (part 3)

To evaluate the effects of annual precipitation amounts on simulations of plant N uptake efficiency (NUpE) (Equation 3.1) and on NO_3-N leaching accumulated during one year, different scenarios of precipitation amounts (table 3.10) were generated and evaluated. The scenarios of precipitation were generated based on daily precipitation events occurred during the experimental period in 2008/2009. According to the wanted scenarios, we increased (MaP_{30}) or reduced ($AP_{03\text{-}13}$, AP_{r10}, AP_{r20}, MiP_{30}) the amount of precipitation of default events of the yearly precipitation regime used for SWAP/ANIMO calibration and validation. For the scenarios with reduced precipitation, supplementary irrigation was scheduled in the SWAP module for maintaining the average soil water storage at field capacity (-10 kPa). For this scheme of scenarios the yearly doses of 200, 300, 400, 500, 600, 700, and 800 kg N ha^{-1} y^{-1} were evaluated with N applications each 14 days.

Table 3.10 – Yearly amount of precipitation selected for simulations of scenarios

Description	Identification	Precipitation amount (mm)
Annual precipitation used in SWAP/ANIMO validation	P_{Defaut}	1535
Average annual precipitation in Barreiras (2003-2013)	$AP_{03\text{-}13}$	957
Average annual precipitation in Barreiras reduced 10%	AP_{r10}	861
Average annual precipitation in Barreiras reduced 20%	AP_{r20}	766
Historical annual maximum precipitation in Barreiras (30 years)	MaP_{30}	1687
Historical annual minimum precipitation in Barreiras (30 years)	MiP_{30}	582

3.2.2.4.4 Organic inputs and volatilization

The following managements were equally used for all the scenarios of simulation described above in part 1, part 2 and part 3 sections.

Coffee leaf fall was simulated scheduling the addition of the litter material to the soil surface each 14 days, with a cumulative yearly mass of 8031.5 kg ha^{-1} y^{-1}. Poultry manure (2.5 Mg ha^{-1}) and coffee husks (3.0 Mg ha^{-1}) were applied on the soil surface once on DAB = 71 (NETO et al., 2011). The events of material inputs were scheduled in the management module of ANIMO accordingly to the experimental sequence. The model applications of mineral fertilizer were made in the artificial reservoir of the soil existing in ANIMO and the organic parts of the plant in the first compartment, as recommended by Renaud et al. (2006). The percentage of N volatilized from mineral fertilizer was estimated according to soil water content on the day and day after fertilizer application and adjusted in the model (Table 3.11).

Table 3.11 – Percentages of NH_3 volatilization from mineral fertilization according to the soil moisture status on several days after the beginning of the simulations (DAB)

Rain or irrigation	NH_3 volatilization (%)	DAB (Julian day)
On day and next	0.0	15, 85, 99, 155, 323, 337, 351, 141
On day	0.5	1, 43, 127, 169, 183, 295
On next day	5.0	29, 57, 71
No rain or irrigation	10.0	113, 197, 211, 225, 239, 253, 267, 281, 309, 365

3.2.3 Nitrogen uptake efficiency (NUpE)

The efficiency of N uptake (NUpE) was calculated by the Equation 3.1, which is an adaptation of the relation proposed by Moll, Kamprath and Jackson (1982).

$$NUpE = \frac{\text{(N plant uptake).(\% of N taken from fertilizer)}}{\text{N fertilizer dose}} \tag{3.1}$$

The yearly N plant uptake was obtained by simulations with ANIMO for each dose of N fertilizer applied in the scenarios of management. The percentage of N taken from fertilizer is an average value equal to 39%, which was obtained using the ^{15}N tracer in the study of Bruno et al. (2011).

3.2.4 Model sensitivity analysis

The sensitivity of ANIMO simulations to parameter variations was calculated using the relative partial sensitive index η (Equation 3.2). For this analysis, a selected parameter was changed by 1% (Δp/p=0.01) while others were maintained at default. The effect on annual results of each N cycle process (ΔV/V) were obtained and analyzed:

$$\eta = \frac{\Delta V / V}{\Delta p / p} = \frac{p \Delta V}{V \Delta p} \tag{3.2}$$

In this study a value of |η|≤0.5 was interpreted as a low sensitivity of the output (the N process under evaluation) to the chosen parameter. Two scenarios of N management (M_{400} and M_{800}) were evaluated for parameter sensitivity analysis. The parameters analyzed by the index η were chosen after a screening of sensitivity to find the most important parameters to be evaluated. Soil parameters (pH, K_{sr}, ρ_d, s_{NH4} and T_{ref}), plant parameters (σ_N^{max}, U_p, and T_a), and materials and transformation process parameters (c_{Nfr}, c_{Nsr}, k_{fr}, k_{sr}, k_{nr}, N dose, and volatilization percentage) were selected for the sensitivity evaluation. The most sensitive parameters were in this way selected for model calibration.

3.2.5 Model calibration and validation

The experimental outcomes from 200, 400, 600 and 800 kg N ha^{-1} y^{-1} doses of mineral N fertilizer were used for model calibration and validation. As four independent groups of data were available, the calibration was performed using the experimental data of NO_3-N concentration in soil solution measured in four parcels of three plants that received 400 kg N ha^{-1} y^{-1} during 2008/2009. The model simulations were validated using two different output variables, which were measured experimentally: 1) the NO_3-N concentration in soil solution for plant plots receiving 800 kg N ha^{-1} y^{-1}; 2) the plant uptake after one year obtained in plots receiving 200, 400, 600 and 800 kg N ha^{-1} y^{-1}. To generate results, each fertilizer management (M_{200}, M_{400}, M_{600}, M_{800}) simulated with ANIMO used the same group of parameters established by calibration.

Soil parameters pH, s_{NH4}, k_{fr} and c_{Nfr} of poultry manure, k_{nr}, k_d, σ_N^{max}, k_{hu}, k_{DOM}, c_{Nhu}, (ANIMO), the shape parameter λ_{dsl} and the root density (SWAP) were adjusted during model calibration. Several combinations of parameters were tested according to ranges between maximum and minimum values for each parameter available in Renaud et al. (2006). The best combination of parameters was found to be λ_{dsl} = 6.0, soil pH_1 = 4.3 (surface layer) and pH_2 = 3.8 (middle and deep layer), s_{NH4} = 0.0003 m^3 kg^{-1} (soil profile), k_{fr} = 10.2 and c_{Nfr} = 0.07 kg kg^{-1} (Poultry manure), k_{nr} = 400 y^{-1}, k_d = 365 y^{-1}, σ_N^{max} = 3.5, k_{hu} = 0.008 y^{-1}, k_{DOM} = 30 y^{-1}, and c_{Nhu} = 0.001 kg kg^{-1}.

3.2.6 Model evaluation

Statistical analysis of the model simulations and consistency with experimental data was performed using the root mean square error RMSE, the index of agreement *d* (WILLMOTT, 1981) and the Nash-Sutcliffe model efficiency NSE (NASH; SUTCLIFFE, 1970).

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(J_i - O_i)^2} \tag{3.3}$$

$$d = 1 - \frac{\sum_{i=1}^{N}(O_i - J_i)^2}{\sum_{i=1}^{N}\left(\left|O_i - J\right| + \left|O_i - \bar{O}\right|\right)^2} \tag{3.4}$$

$$NSE = 1 - \frac{\sum_{i=1}^{N}(O_i - J_i)^2}{\sum_{i=1}^{N}(O_i - \bar{O})^2} \tag{3.5}$$

where O_i represents the experimentally observed value with a mean of $\bar{O}$, J_i is the model predicted value, and *N* the number of observations. The lower the value of *RMSE,* the closer is the proximity of predicted and observed values. The index d equal to 0 indicates no agreement and 1 perfect agreement. *NSE*-values closer to 1 indicate a more efficient model. *NSE*-values below 0 indicate the average of observed values is a better predictor than the model. A full explicative description of these statistical functions and their use for model validation and calibration can also be found in Groenendijk et al. (2014).

3.3 Results and discussion

3.3.1 Sensitivity analysis

The most influential parameters for model simulations were established by sensitivity analysis. The proportional effect of parameter variation on the simulations of leaching below 1.0 m depth, plant uptake, and N transformations (nitrification, volatilization, mineralization, and denitrification) was evaluated using the η index. The sensitivity analysis of ANIMO simulations was performed for two scenarios of N management (400 and 800 kg N ha^{-1} y^{-1}), and results obtained independently are shown in Tables 3.12 and 3.13.

Table 3.12 – Parameter sensitivity and effects of their increase on N processes simulated by ANIMO when N dose was 400kg ha^{-1}

Parameter	Default value	Relative partial sensitivity η*						
		Crop uptake	NO_3-N leaching	NH_4-N leaching	NH_4-N nitrified	N_{org} mineralized	N_{org} Leaching	NO_3-N denitrification
pH_1	4.3	**0.82**	**2.92**	**1.00**	**4.70**	**4.79**	**2.01**	**8.22**
pH_2	3.8	0.31	**5.15**	**-3.00**	**3.26**	**3.04**	-0.50	0.00
ρ_{d1}	1790	0.02	0.00	0.00	-0.13	0.00	0.00	0.00
ρ_{d2}	1580	0.04	-0.17	0.00	-0.17	0.00	-0.25	0.00
s_{1NH4}	0.0003	0.02	0.00	0.00	-0.13	0.00	0.00	0.00
s_{2NH4}	0.0003	0.04	-0.17	0.00	-0.17	0.00	0.00	0.00
T_{ref}	25	-0.29	**-2.23**	**1.00**	**-2.20**	**-2.13**	**-0.75**	**-1.37**
σ_N^{max}	3.5	0.09	**-0.52**	0.00	-0.17	0.00	0.00	0.00
U_{p1}	147.192	0.18	**-0.69**	0.00	**-0.51**	0.00	0.00	0.00
U_{p2}	343.447	0.00	0.00	0.00	-0.08	0.00	0.00	0.00
T_{a1}	0.59	-0.16	**0.86**	**1.00**	0.38	0.00	0.00	0.00
T_{a2}	0.6	0.04	0.00	0.00	0.00	0.00	0.00	0.00
c_{Nfr} (Poultry manure)	0.07	0.02	0.17	0.00	0.13	0.38	0.25	0.00
k_{fr} (Poultry manure)	10.2	0.02	0.17	0.00	0.04	0.23	0.00	0.00
k_{nr}	400	-0.02	**0.52**	**-1.00**	**0.55**	0.00	0.00	0.00
N dose	400	**0.62**	**1.37**	**1.00**	**0.93**	0.00	0.00	0.00
% of volatilization	-[a]	-0.02	0.00	0.00	-0.04	0.00	0.00	0.00

Note: pH_1, soil pH of surface layer (0-0.1m); pH_2, soil pH of intermediary (0.1-1.0m) and deep layers (1.0-2.0m); ρ_{d1}, dry bulk density of surface layer; ρ_{d2}, dry bulk density of intermediary and deep layers; s_{1NH4}, sorption coefficient of surface layer; s_{2NH4}, sorption coefficient of intermediary and deep layers; T_{ref}, temperature of reference; σ_N^{max} , maximum N transpiration stream concentration factor; U_{p1} and U_{p2}, expected cumulative uptake in the first and second period, respectively; T_{a1} and T_{a2}, transpiration in the first and second period, respectively; c_{Nfr} , nitrogen concentration in fast reaction part of organic materials; $k_{fr,}$ decomposition rate constant of fast reaction part organic materials; k_{nr}, nitrification rate of reference.

[a] Table 3.11

*Positive/negative value means an increase/decrease in the N process simulated in relation to its value when simulated with the standard combinations of parameters; "Zero" means insignificant or none changes in N process simulated with the modified parameter. Highlighted values indicate high sensitivity (|η|>0.5) of N process simulated in relation to the parameter.

Table 3.13 – Parameter sensitivity and effects of their increase on N processes simulated by ANIMO when N dose was 800kg ha^{-1}

Parameter	Default value	Relative partial sensitivity η*						
		Crop uptake	NO_3-N leaching	NH_4-N leaching	NH_4-N nitrified	N_{org} mineralized	N_{org} Leaching	NO_3-N denitrification
pH_1	4.3	0.00	**2.87**	**-1.41**	**2.17**	**4.71**	**2.01**	**6.25**
pH_2	3.8	0.02	**3.87**	**-10.92**	**2.10**	**3.04**	-0.50	0.00
K_{sr1}	0.266	0.00	0.05	0.00	0.00	0.00	0.00	**-2.50**
ρ_{d2}	1580	0.00	-0.10	-0.35	-0.02	0.00	-0.25	0.00
s_{2NH4}	0.0003	0.00	-0.10	**-0.70**	-0.02	0.00	0.00	0.00
T_{ref}	25	0.02	**-1.72**	**3.17**	**-1.31**	**-2.21**	**-0.75**	**-2.50**
U_{p1}	147.2	0.27	**-0.62**	-0.35	-0.07	0.00	0.00	0.00
U_{p2}	343.5	**0.73**	**-0.96**	**-1.06**	-0.47	0.00	0.00	0.00
T_{a1}	0.59	-0.23	**0.62**	0.00	0.03	0.00	0.00	0.00
T_{a2}	0.6	**-0.73**	**0.91**	**0.70**	0.41	0.00	0.00	0.00
c_{Nfr} (Poultry manure)	0.07	0.00	0.14	0.00	0.08	0.30	0.25	0.00
k_{fr} (Poultry manure)	10.2	0.02	0.10	0.00	0.03	0.15	0.00	0.00
k_{nr}	400	0.04	0.43	**-1.76**	0.29	0.00	0.00	0.00
N dose	800	0.00	**2.10**	**1.06**	**1.14**	0.00	0.00	0.00
% of volatilization	-[a]	-0.02	0.00	-0.35	-0.05	0.00	0.00	0.00

Note: pH_1, soil pH of surface layer (0-0.1m); pH_2, soil pH of intermediary (0.1-1.0m) and deep layers (1.0-2.0m); K_{sr1}, saturated hydraulic conductivity of the root zone (0-0.1m); ρ_{d2}, dry bulk density (0.1-1.0m); s_{2NH4}, sorption coefficient (0.1-1.0); T_{ref}, temperature of reference; σ_N^{max} , Maximum N transpiration stream concentration factor; U_{p1} and U_{p2}, expected cumulative uptake in the first and second period, respectively; T_{a1} and T_{a2}, transpiration in the first and second period, respectively; c_{Nfr} , nitrogen concentration in fast reaction part of organic materials; $k_{fr,}$ decomposition rate constant of fast reaction part organic materials; k_{nr}, nitrification rate of reference.

[a] Table 3.11

[*] Positive/negative value means an increase/decrease in the N process simulated in relation to its value when simulated with the standard combinations of parameters; "Zero" means insignificant or none changes in N process simulated with the modified parameter. Highlighted values indicate high sensitivity (|η|>0.5) of N process simulated in relation to the parameter.

Soil pH, T_{ref}, U_p, T_a, and k_{nr} were the most important parameters for the simulations with ANIMO in this study.

The simulated N processes showed high sensitivity to specific parameters, depending on the N dose. Denitrification was sensitive to K_{sr}, and NH_4-N leaching was sensitive to the sorption coefficient only for the N dose of 800 kg N ha^{-1} y^{-1}. An increase on K_{sr} diminished the availability of NO_3-N for denitrification since plant roots absorb preferentially nitrate from the soil surface in M_{800} (these results are discussed ahead). In spite of increasing K_{sr}, plant N uptake was not affected in our simulations. The increase in parameter σ_N^{max} produced a decrease in NO_3-N leaching but did not significantly change plant uptake for a dose of 400 kg N ha^{-1} y^{-1}. ANIMO has distinct calculation schemes for plant uptake depending on N soil availability. The maximum concentration factor σ_N^{max} is important only when NO_3-N is not highly available in the system and its amount is lower than plant requirements (without luxurious uptake). When the dose of N was 800 kg N ha^{-1} y^{-1}, a large amount of NO_3-N was presented in the system due to ammonium nitrification and σ_N^{max} did not regulate plant uptake or even influenced N leaching. In fact, the maximum transpiration concentration factor σ_N^{max} was not critical for our simulations with high doses of N. The expected uptake U_{p2} and transpiration T_{a2} of the second period were sensitive for crop uptake, NO_3-N and NH_4-N leaching simulations when a dose of 800 kg N ha^{-1} y^{-1} was applied. However, no influence of these parameters on the tested N processes was found when the N dose was 400 kg N ha^{-1} y^{-1}. The cumulative T_{a1} was sensitive for the simulated leaching of NO_3-N (M_{400} and M_{800}) and NH_4-N (M_{400}). The input U_{p1} was sensitive for NO_3-N leaching in both managements. When the expected uptake U_p was increased we could predict less nutrient would be available for leaching. However, we could not explain why plant uptake decreased at the same time transpiration T_{a1} increased when the inverse behavior would be expected. The reason why the U_{p2} and T_{a2} sensitivity behaviors were different for the management scenarios M_{400} and M_{800} is as well unclear.

Plant uptake was significantly influenced by soil pH and by the small increases in the N dose for M_{400}. The most important parameters for plant uptake in the management scenario M_{800} were U_{p2} and $T_{a2,}$ and for leaching of NO_3-N and NH_4-N independently, and NH_4-N nitrification, were soil pH, T_{ref}, and k_{nr} for both management scenarios in the sensitivity analysis. The leaching of NO_3-N and NH_4-N were highly affected when the N dose was increased by 1% in both managements M_{400} and M_{800} as well. Comparing the sensitivity indexes of NH_4-N leaching in the table 3.12 with the results in table 3.13, different values of η were found when the annual dose was 400 or 800 kg N ha^{-1} y^{-}1.The leaching of NH_4-N was affected by several parameters when the N dose was the higher. The processes of N_{org} mineralization, N_{org} leaching, and NO_3-N denitrification were largely influenced by soil pH and T_{ref}, and their sensitivities to the tested parameters were similar for both doses.

Soil pH strongly affected the N processes simulated in this study. Simulated results of NH_4-N nitrification, NO_3-N leaching, and N_{org} mineralization increased around 5% for a soil surface pH increase of 1% (Table 3.12). Leaching of NH_4-N was highly affected (-11%) by soil pH increase as shown by the sensitivity analysis of the scenario with N dose 800 kg N ha^{-1} y^{-1} (Table 3.13). The observed high influence of soil pH on the simulations is strongly related to the high amounts of fertilizer and rate of nitrification occurring in this system. The NH_4-N nitrification is regulated by environmental factors and depends on soil moisture, temperature, aeration and soil pH. An exponential effect of soil pH on nitrification is adopted in ANIMO (RENAUD et al., 2006). The fact that soil pH was characterized for only three soil layers (Table 3.2) and an average value was accounted for each layer could also be determinant for the analysis of the presented results. Time variation of soil pH was desirable for the simulations, but this is still a missing behavior in the model. For fertilized agricultural systems, soil pH variations during time are expected to exist. Results in the literature showed soil pH can vary on long-term (SCHRODER et al., 2011) and short-term (TONG; XU, 2012) due to fertilizer reactions on soil and induced nitrification, or due to additions of agricultural products for improvement of soil quality. For a more realistic modeling of highly fertilized agricultural systems and a best estimative of N processes, we suggest ANIMO to have soil pH revised as being variable in time and influenced by processes, plants, and input materials.

The simulated N losses by volatilization were not affected by the parameters evaluated in table 3.12 and 3.13, but only by the small variations of the N dose (resulting in η=2.16, for M_{400}, and η=0.71, for M_{800}). The soil and material parameters (p_1, p_2, ρ_{d1}, K_{sr}, C/N, c_{Nex}, c_{Nhu}, c_{DOM}, c_{Nsr} of poultry manure and coffee husks, and k_{sr} and k_{fr} of coffee husks, and k_{sr} of poultry manure, k_{ex}, k_{DOM}, k_{hu} and k_d) had very low or almost no influence on N simulations. The N concentration in manures did not influence the N balance. These weak effects of manures on simulation results can be explained by the low amount of poultry manure and coffee husks used in the agricultural management system and by the slow rate of decomposition of these materials, and consequently low amount of N input due to organic fertilizers in this system. A similar low sensitivity occurred for irrigation, natural wet, and dry N input since corresponding amounts of nutrients were very low compared to the mineral fertilizers.

3.3.2 Aboveground N inputs

Table 3.14 shows the several N inputs in this coffee cropping system resulting from simulations under the established scenarios.

Table 3.14 – Nitrogen inputs to the soil-plant system during the experimental year from several sources

Source	N fertilizer management	NH_4-N (kg ha^{-1} y^{-1})	NO_3-N (kg ha^{-1} y^{-1})	N_{org} (kg ha^{-1} y^{-1})
Urea (80% NH_4-N, 20% NO_3-N)	M_{200}	160	40	-
	M_{400}	320	80	-
	M_{600}	480	120	-
	M_{800}	640	160	-
Dry deposition	-	0.30	0.50	-
Wet deposition	-	4.50	2.00	-
Irrigation water	-	0.30	0.10	0
Coffee litter	-	0	0	209
Coffee husks	-	0	0	41
Poultry manure	-	1.00	0.10	74

Note: M_{200}, M_{400}, M_{600}, and M_{800} are the simulated managements that differed only in relation to the amount of mineral fertilization added.
*The same for all the managements

ANIMO requires initial values for the inorganic fractions NH_4^+, NO_3^- and organic fractions of the materials added, including mineral fertilizers. The amount of N available as urea was around 80% converted into NH_4. Uncertainties like whether the urea fertilizer should be either understood as a totally ammoniacal fertilizer or adjusted with nitrate/ammonium percentages as a result of the calibration may exist in such modeling. Although urea-N converts rapidly to NH_4 in soil, to consider a total conversion of urea-N into ammonium prior to application in the soil of simulations with ANIMO may be a gross approximation of reality. Other processes in the field might affect this fertilizer before its conversion into ammonium, for instance, leaching and runoff, and a distinct scenario of the N cycle in the simulations might happen compared to the real field system. Besides dividing them into forms of N, an option for characterizing the mineral N fertilizers would improve the simulation of chemical reactions of mineral fertilizers in the soil by ANIMO. The adopted features of urea in this study were obtained based on a slow reaction of the fertilizer in the soil and as a result of model calibration. Kaufmann et al. (2014), for instance, described urea as mostly being converted to NO_3 in ANIMO simulations but did not give a specific reason for this consideration.

No differences in added organic N, like amounts of poultry manure, coffee husk, discarded coffee roots and plant litter were introduced in the simulated scenarios. Poultry manure was the only organic material containing NH_4-N and NO_3-N. Due to its dependence on animal management and added litter (for poultry litter), variations in contents and composition of organic N in poultry manure are common. For that reason, this study presented scientific data related to poultry manure analyzed by some studies from different locations in Brazil (Table 3.6). Organic compounds and plant parts together showed to be great sources of organic N for the system. As presented ahead, the organic N inputs due to manures and plant litter were an important source of NH_4 since they were linked to the mineralization process.

The estimated N wet deposition was of the same order of magnitude as reported by Araujo (2015) for southeast Bahia, 2.7 kg ha^{-1} y^{-1} (NH_4-N and NO_3-N). The average inorganic N concentration assumed for irrigation water was comparable to values found by Lucio (2010), who obtained concentrations of NO_3-N between $2.0 \cdot 10^{-4}$ kg m^{-3} and $1.5 \cdot 10^{-3}$ kg m^{-3}, and NH_4-N between $4.7 \cdot 10^{-5}$ kg m^{-3} and $1.5 \cdot 10^{-3}$ kg m^{-3} in samples of the Cachoeira River, Bahia. Higher concentrations of NO_3-N, between $3.4 \cdot 10^{-1}$ kg m^{-3} and $7.0 \cdot 10^{-1}$ kg m^{-3}, were found by Santos et al. (2013) in the Catolé River, in the southeast region of Bahia.

3.3.3 Calibration and validation

The temporal evolutions of the NO_3-N concentration at 1 m depth for calibration (M_{400}) and validation (M_{800}) are shown in Figure 3.1. The calibration curve (Figure 3.1a) showed less variability than the experimental observations but represented the cumulative behavior of soil NO_3-N until the end of the period. During the first 100 days of simulation, the concentration of NO_3-N increased very slowly, in agreement to the dry season (Figure 2.2). During this period, the NO_3-N concentration in the soil could not be measured experimentally due to the very dry soil condition. A visual examination of the validation curve (Figure 3.1b) show it to represent well the experimental data, although the simulated curve underestimates some observed values and did not reach the high levels observed on days 190 and 263, in the wet period. The concentration of NO_3-N in the soil decreased during the period between days 291 and 321 for both the calibration and the validation scenario, but this did not show up in the simulation results. This decline of nitrate concentration in the soil solution may be associated to higher plant absorption. According to Bruno et al. (2011), coffee fruit N recovery started on day 181 and continued until day 356, this period being the most recommended for N application. However, these peak demands for N by plants were not simulated in ANIMO and might be associated to the period in which both calibration and validation curves did not follow exactly the experimental results. The choice for zero initial concentrations of NO_3-N and NH_4-N in soil solution lead to acceptable results since the first measurements agreed very well with simulations (Figure 3.1).

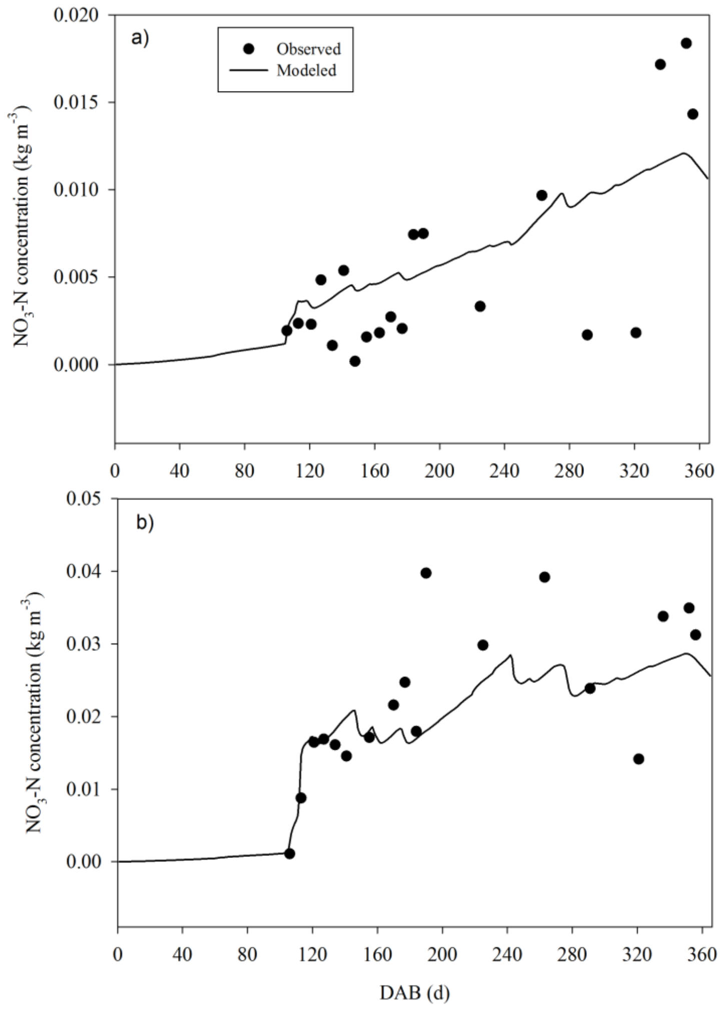

Figure 3.1 – Simulated and experimental daily concentrations of NO_3-N at the 1 m soil depth as a function of days after the beginning of experiments (DAB), during the experimental year in the (a) calibration with scenario M_{400} and (b) validation with scenario M_{800}

To quantitatively evaluate the model outcomes, simulated concentrations of NO_3-N between 0.1 m and 1.4 m depths were statistically compared to the experimental values at 1.0 m (Table 3.15). RMSE and d index for the calibration simulations did not vary considerably in the soil region between 0.8 m and 1.0 m, and statistical results for 1.0 m indicated an accurate simulation and calibration (GROENENDIJK et al., 2014). The simulations of NO_3-N at 1.0 m depth for validation were of medium quality as revealed by NSE values but of good quality according to RMSE and d index. In relation to RMSE, both the calibration and the validation showed relatively low values at 1.0 m depth. Deviations on the validation curve were mainly caused by NO_3-N concentrations measured on days 190, 263 and 321. When these outliers were eliminated from validation, results were NSE = 0.90 and index d = 0.93 at 1.0 m depth. Different scenarios for the initial NO_3-N and NH_4-N concentration in soil solution were evaluated also accounting for the output values of these inorganic forms simulated in soil solution after one year of M_{200}, M_{400}, and M_{600}. After evaluating the statistical parameters, we found the accordance between experimental and simulated amounts of NO_3-N in the soil at 1.0 m depth would be lower than the original (zero concentrations) for each of those tested scenarios.

An important point to be taken into consideration is that the available experimental data are average of several plots. The experimental values of NO_3-N concentrations shown in Figure 3.1 were obtained from composite soil water samples taken from four replicates of experimental parcels of M_{400} (calibration) and of M_{800} (validation). The calibration and validation of ANIMO simulations relied on a few NO_3-N concentration measurements for the statistical analysis here presented.

Table 3.15 – Values of the statistical relations root mean square error (RMSE), Nash-Sutcliffe model efficiency (NSE) and index of agreement (d) resulted from the calibration and validation

Soil depth	RMSE (10^{-3} kg m^{-3})		NSE		d	
(m)	Calibration	Validation	Calibration	Validation	Calibration	Validation
0.1	4.0	11.4	0.43	-0.34	0.79	0.67
0.2	4.9	12.3	0.16	-0.58	0.77	0.66
0.3	5.9	14.3	-0.24	-1.13	0.71	0.62
0.4	6.4	15.7	-0.44	-1.56	0.69	0.59
0.5	5.8	14.1	-0.24	-1.06	0.71	0.63
0.6	4.4	10.5	-0.44	-0.14	0.69	0.72
0.7	5.8	9.2	0.46	0.13	0.81	0.76
0.8	3.7	8.3	0.51	0.29	0.82	0.78
0.9	3.8	7.7	0.50	0.39	0.81	0.79
1.0	**3.9**	**7.3**	**0.46**	**0.45**	**0.80**	**0.80**
1.1	6.0	17.7	-0.25	-2.22	0.70	0.54
1.2	7.2	22.4	-0.83	-4.19	0.65	0.47
1.3	7.6	23.3	-1.02	-4.64	0.64	0.46
1.4	7.6	23.4	-1.02	-4.64	0.64	0.46

3.3.4 Scenarios of N doses (Part 1)

Simulated annual N plant uptake was compared with experimental N amount in the whole plant from Bruno et al. (2014) (Figure 3.2). For N applications of 400, 600, and 800 kg N ha^{-1} y^{-1}, simulated results of annual N uptake were within the experimental error intervals (Figure 3.2). ANIMO formulations used for N uptake modeling performed well for the highly N available scenarios in this study, similar to conclusions by Wolf et al. (2005). For the 200 kg N ha^{-1} y^{-1} scenario, however, simulated average N uptake was lower than observed values and without the error interval. This discrepancy between model prediction and observation for M_{200} is possibly explained by other mechanisms for nutrient absorption not accounted for by ANIMO. Before the experiment, the coffee plants used for this study were grown for seven years under a high N management (600 kg N ha^{-1} y^{-1}). Plants were therefore used to high amounts of fertilizer and one year receiving lower doses would not be enough to change their habit. Thus, plants should stimulate mechanisms for continuing at high uptake rates.

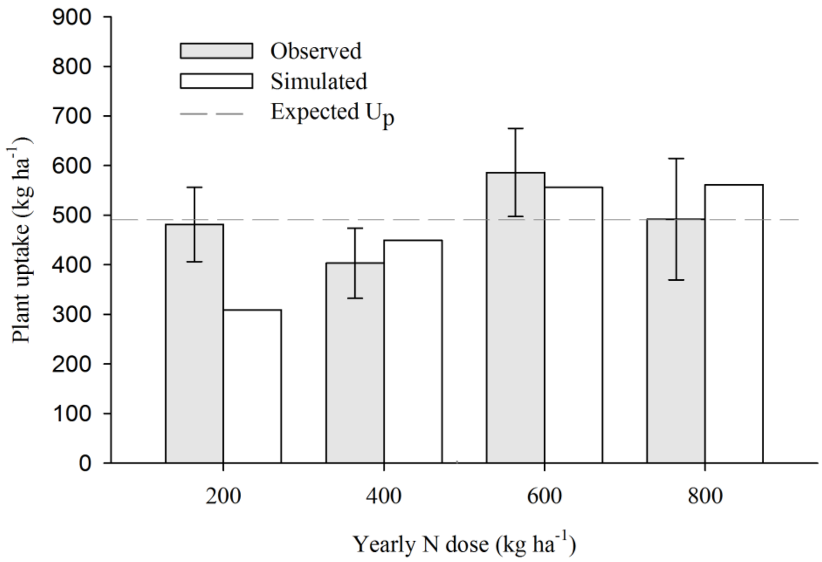

Figure 3.2 – Simulated and observed cumulative N plant uptake for scenarios M_{200}, M_{400}, M_{600} and M_{800} during 2008/2009. The dotted line represents the expected N uptake by plants (U_p) used for simulations with all scenarios

The total N taken up by plants in ANIMO simulations can be divided into NO_3-N or NH_4-N preferences, and also in relation to the main region of nutrient absorption in the soil. For the M_{200} scenario, uptake was 41% NO_3-N and 59% NH_4-N. For the M_{400}, M_{600} and M_{800} scenarios, NO_3-N uptake was predominant (52, 63 and 86% respectively). The highest plant preference for NO_3-N occurred precisely for the highest dose of N (800 kg N ha^{-1} y^{-1}). The high amount of N expected to be taken up by plants (U_p) caused the plant to take up both forms of N when the nutrient was available in relatively low doses, but preferentially NO_3 when supply was ample. In relation to distribution over depth, the first 0.1 m of soil provided 39% (M_{200}), 36% (M_{400}), 32% (M_{600}) and 28% (M_{800}) of the total NO_3-N, and 49% (M_{200}), 46 % (M_{400}), 42% (M_{600}) and 29% (M_{800}) of the total NH_4-N. The surface layer was the main pool of N for plants in this system when the fertilizer doses were less than 600 kg N ha^{-1} y^{-1}. For the N dose of 800 kg N ha^{-1} y^{-1}, the N uptake was mostly of NO_3-N and absorbed from the depths between 0.1 and 1.0 m.

Table 3.16 presents the annual inputs of inorganic N, conversions of NH_4-N by nitrification, and losses by leaching, volatilization, and denitrification down to 1.0 m depth.

The annual NH_4-N input due to the mineralization of organic substances in the system was 130 kg ha^{-1} y^{-1} was accounted in total inorganic input. The leaching of organic N was around 40 kg ha^{-1} y^{-1}. The poultry manure application (2500 kg ha^{-1} y^{-1}) improved the NH_4-N formation by 29 kg ha^{-1} y^{-1} and coffee husks (3000 kg ha^{-1} y^{-1}) were responsible only for 1.9 kg ha^{-1} y^{-1} of NH_4-N added to the system.

Table 3.16 – Predictions of nitrogen processes below a coffee plantation for different fertilizer managements

Input (kg ha^{-1})		NH_4-N → NO_3-N (kg ha^{-1})	NH_4-N and NO_3-N losses (kg ha^{-1})			
Mineral fertilizer	Total inorganic N	Nitrification	NO_3-N leaching	NH_4-N leaching	NH_4-N volatilization	NO_3-N denitrification
200	340	131	29	8	7	7
400	540	235	57	11	14	7
600	740	360	110	18	21	7
800	940	571	206	33	28	8

The amounts of NO_3-N lost by leaching (Table 3.16) represented 8.6% (M_{200}), 10.6% (M_{400}), 15.0% (M_{600}) and 22.0% (M_{800}) of the total inorganic N input. In increasing order of N-dose, the fractions of NH_4-N leached in relation to N input were 2.4%, 2.0%, 2.4%, and 2.2%. Simulated NO_3-N leaching was compared to experimental results obtained by Bortolotto et al. (2013) for the same experimental coffee growing area. Their results for NO_3-N leaching were 24.2 kg N ha^{-1} y^{-1} (at 400 kg N ha^{-1} y^{-1}) and 153 kg N ha^{-1} y^{-1} (at 800 kg N ha^{-1} y^{-1}), corresponding to 42% (M_{400}) and 74% (M_{800}) of the ANIMO simulated values. An exact agreement between the results of both models, however, was not expected, due to the differences in the hydrological cycle simulated by SWAP (PINTO et al., 2015) and using a sequential water balance as in Bortolotto et al. (2013). In addition, we used ANIMO to simulate the cumulative N leaching amount for a one year period, differently from the cited study with results obtained during a nine-month period.

The ANIMO prediction of annual NO_3-N leaching expressed per millimeter of rainfall and irrigation was 26 g ha^{-1} mm^{-1} for M_{400}, which is comparable to values found in other studies. Cannavo et al. (2013) obtained a NO_3-N leaching of 59 g ha^{-1} per millimeter of rainfall at the 1.2 m depth in a study with unshaded coffee plants fertilized with 250 kg N ha^{-1} y^{-1}. Harmand et al. (2007) determined a NO_3-N leaching of 43 g ha^{-1} per millimeter of rainfall in coffee plants fertilized with 180 kg N ha^{-1} y^{-1}. Considering NO_3-N leaching depends on soil properties, plant, and nutrient management, values will vary from one location to another.

However, the simulated amounts of NO_3-N leaching in the studied coffee plantation of western Bahia were compatible to the other cultivation areas.

The temporal variation of NO_3-N in the soil profile, coupled to precipitation, irrigation, fertigation (M_{400}) and manure events, is presented in Figure 3.3. In the dry period of the year, due to the fertilizer applications and low soil moisture, the NO_3-N was highly concentrated in soil layer between surface and 0.3m depth. Water from isolated rain events increased the leaching amount during the dry period and NO_3-N concentration decreased in the soil surface layer. During the wet period NO_3-N concentration in soil solution of deeper layers increased. At the end of the simulated period, with fewer rain events, the NO_3-N concentration in the soil surface increased, as well as in the soil profile below 0.6 m. The N leaching due to fertigation can be identified in the contour graph of Figure 3.3 (M_{400}) and Figure 3.4 (M_{800}). Due to the characteristics of the sandy soil, irrigation and peak rain events, the NO_3-N accumulated below the layer with the highest root concentration from 0-0.6 m depth at the end of the year. A large difference exists in NO_3-N soil concentration of Figure 3.3 compared to Figure 3.4 due to the amount of N applied in the managements.

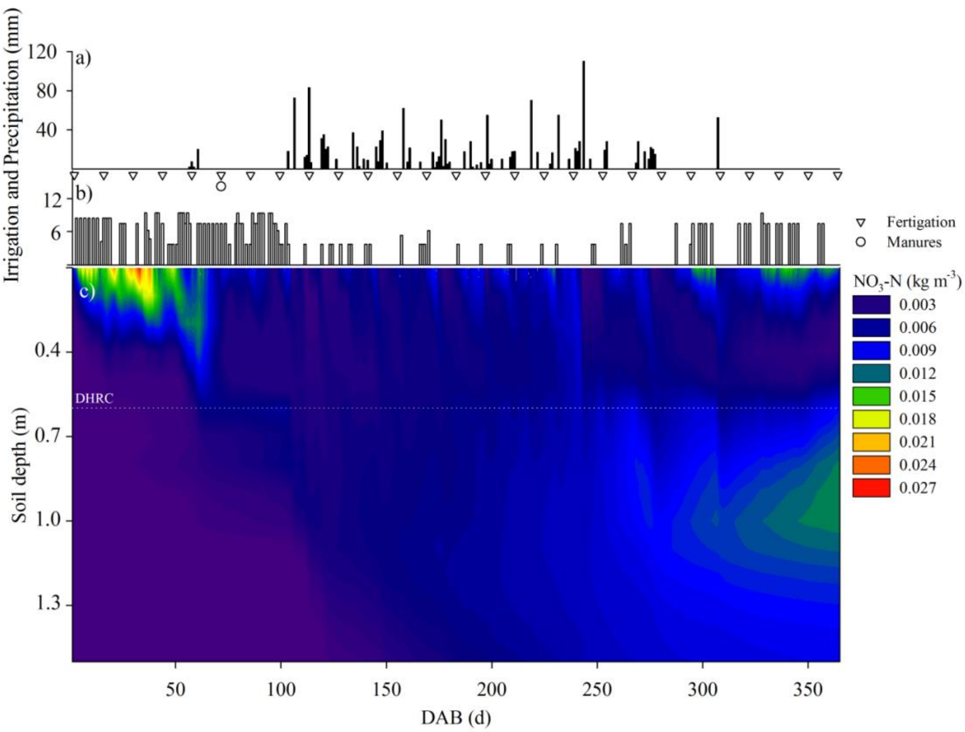

Figure 3.3 – Timeline of rainfall (a), irrigation, and farm input events (b), and NO_3-N concentration in the soil profile (c) as a function of time for the scenario M_{400}. The lower boundary of the layer with highest root concentration (DHRC) is indicated by the dotted line

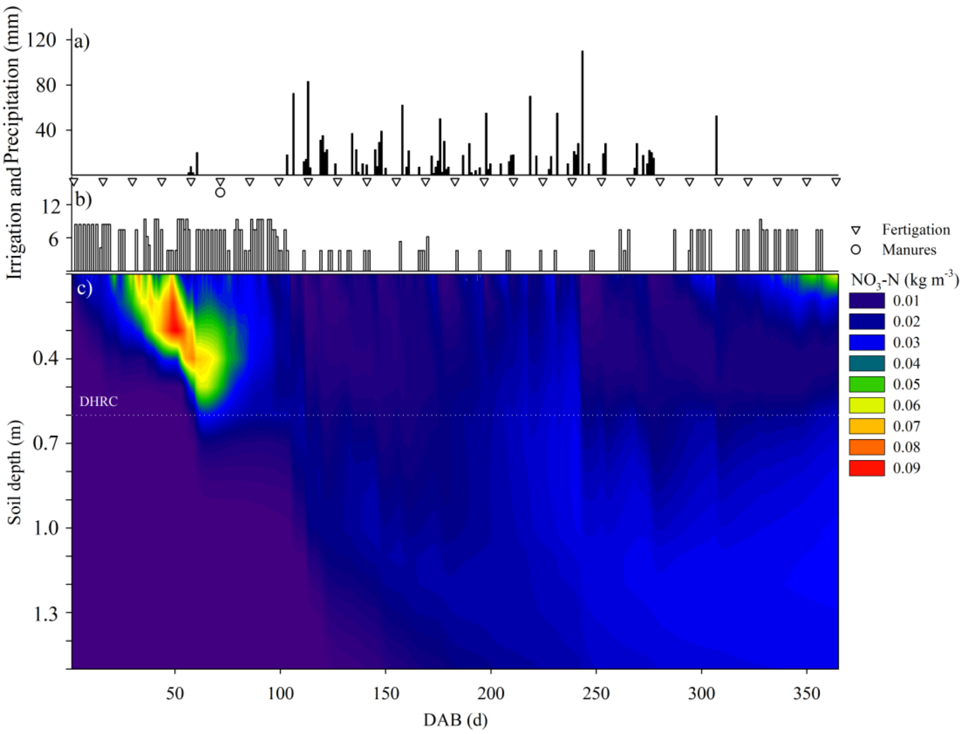

Figure 3.4 – Timeline of rainfall (a), irrigation, and farm input events (b), and NO_3-N concentration in the soil profile (c) as a function of time for the scenario M_{800}. The lower boundary of the layer with highest root concentration (DHRC) is indicated by the dotted line

The existence of NH_4-N leaching in this coffee plantation is an important fact associated with the modeling/validation. Bortolotto et al. (2013) considered the NO_3-N leaching in this same area as being the total N leaching since they did not detect NH_4-N concentrations in their soil solution samples. However, for all studied scenarios, NH_4-N was predicted to be present in detectable concentrations (> 25 µg L^{-1}) in the soil solution and to be transported by drainage (Table 3.16). Therefore, we simulated the effect of increased rates of nitrification and volatilization on NH_4 present in the soil. When the nitrification rate k_{nr} was increased to the highest value allowed by ANIMO (500 y^{-1}), the NH_4-N leaching was still present (8.6 kg ha^{-1} y^{-1} for M_{400}). At the same time, increasing the nitrification rate affected modeling accuracy at 1.0 m depth (d = 0.79 and NSE = 0.41). In a next scenario, the volatilization of NH_3 was increased to 50% of applications during dry periods, resulting in a NH_4-N leaching of 9.8 kg ha^{-1} y^{-1} in M_{400} (d = 0.80 and NSE = 0.35 for NO_3-N concentration prediction at 1.0 m depth). These results showed NH_4-N leaching is predicted even under very high levels of nitrification and volatilization. The undetected traces of NH_4-N in soil samples can be a result of nitrification along the period of time between field sampling and laboratory analysis, since there was a considerable distance between both locations.

We suggest NH_4-N can be found in the soil solution or leachate in the experimental site as shown by simulations.

Emissions of N_2O simulated by ANIMO resulted to be relatively high (table 3.16) when compared to results on cultivated or native Cerrado (METAY et al., 2007; CRUVINEL et al., 2007; CARVALHO et al., 2006). Denitrification is present generally in flooded terrains or due to the presence of anoxic microsites, common in well-drained soils under high-intensity irrigation like in the present study. Moreover, when the litter cover is predominant, soil moisture is conserved and the provision of C increased, contributing to the intensification of denitrification. Soils under irrigated coffee cultivation are prone to denitrification, although this may not be the main N loss process in this system.

For all scenarios, prediction of volatilization was low compared to the N inputs (Table 3.16). During the simulations, only 37% of the fertilizer application events had the highest losses of NH_4-N considered by volatilization (10% of N in each application). The low rates of volatilization during the year are partly justified since coffee plants received the urea in solution by fertigation and most of these events (63%) were followed by irrigation or rainfall, processes which minimize losses of N by volatilization (JANTALIA et al., 2012; HOLCOMB et al., 2011). Nevertheless, as the volatilization simulations could not be validated experimentally, the obtained values of NH_4-N losses by this process are uncertain and results could diverge from experimental measurements. For that reason, we simulated the N balance with ANIMO considering 1% of N input was volatilized from fertilizer when rain/irrigation happened on the same day of application, 10% when the rain/irrigation happened on the next day of fertilizer application, and 30% when fertilizer application was not followed by rain/irrigation events, or during the dry period of the year. When the cited volatilization percentages were considered, the simulated annual losses of N by volatilization resulted 20.0 kg ha^{-1} y^{-1} (200 kg^{-1} N ha^{-1} y^{-1}), 50.0 kg ha^{-1} y^{-1} (400 kg^{-1} N ha^{-1} y^{-1}), 60.0 kg ha^{-1} y^{-1} (600 kg^{-1} N ha^{-1} y^{-1}), and 80.0 kg ha^{-1} y^{-1} (800 kg^{-1} N ha^{-1} y^{-1}). When the volatilization percentages were increased the values of N balance components did not chance significantly and NO_3-N concentrations in soil solution 1m depth simulated with ANIMO could be validated, although statistical indexes values (d = 0.78, NSE = 0.33) decreased in relation to those in table 3.15. We consider the results of annual volatilization obtained from the cited volatilization percentages 1%, 10% and 30% of N doses are the upper limits for our study area, since the statistical indexes values d and NSE indicated a low quality of simulations when these percentages were higher. We conclude that, for the conditions described in this study, the amounts of volatilization between 7.0 and 20.0 kg ha^{-1} y^{-1} (200 kg^{-1} N ha^{-1} y^{-1}), 15.0 and 50.0

kg ha^{-1} y^{-1} (400 kg^{-1} N ha^{-1} y^{-1}), 21.0 and 60.0 kg ha^{-1} y^{-1} (600 kg^{-1} N ha^{-1} y^{-1}), and 28.0 and 80.0 kg ha^{-1} y^{-1} (800 kg^{-1} N ha^{-1} y^{-1}) are representative of the studied coffee cultivation area.

As volatilization, denitrification and NH_4-N leaching were not measured experimentally, the validation of model predictions for these processes, unfortunately, could not be performed. Steenvoorden et al. (1997) stated this is a problem for model performance evaluation, since nitrate leaching or NO_3-N concentration can be calculated precisely and confirmed by validation for different values or combinations of amounts of volatilization, denitrification, and mineralization. Field measurements are highly recommended then to confirm the rates of the simulated processes (Table 3.16) with ANIMO for this coffee cultivation system.

As presented here, the model ANIMO was calibrated and validated with the experimental results obtained in a coffee plantation during one year. With these previous results and data assembled, the scenarios of fertilizer and crop management, as well as climate change predictions, can be generated with the association SWAP/ANIMO. The obtained results of simulated N processes can serve as support for other studies and perhaps be useful in guiding research towards the most important topics on this N cycle that is still waiting to be better evaluated and estimated experimentally.

3.3.5 Scenarios of N dose partition (Part 2)

Figures 3.4 and 3.5 show the results of N efficiency uptake (NUpE) and NO_3-N leaching, respectively, obtained from simulations of scenarios with different N application frequencies and N doses.

The NUpE descreased approximately in the same proportion that the N dose increased for all the scenarios of N application frequency (Figures 3.4). For each of the selected scenarios of N application frequency, the reduced proportion in NUpE when dose increased from 200 to 300 kg N ha^{-1} y^{-1} was higher than NUpE decrease when dose increased from 300 to 400 kg N ha^{-1} y^{-1} or in any other case. For a selected N dose, differences in NUpE values were not significant between fertilizer application frequency scenarios simulated with ANIMO (Figure 3.4).

For each scenario of N application frequency, increases in N dose significantly increased NO_3-N leaching (Figures 3.5). Reducing the frequency of N application to less than once each 14 days ($NA_{1/2w}$) to seven or three times during the year showed to increase the NO_3-N leaching when comparing results of the same N dose. For each evaluated N dose, there were almost no differences in the results of NO_3-N leaching obtained from the scenarios of N application $NA_{1/2d}$, $NA_{1/1w}$, and $NA_{1/2w}$ (Figure 3.5). The lowest value of NO_3-N leaching resulted from the simulation of the scenario with 200 kg ha^{-1} y^{-1} applied every second day ($NA_{1/2d}$).

We consider an efficient N management should provide at least 50% of NUpE and NO_3-N leaching less than 15% of the total N dose. Evaluations of NUpE and NO_3-N leaching values resulted from the scenarios of N application frequency and N doses simulated with ANIMO suggested the efficient managements are those with dose partition at least once every 14 days and N doses equal or less than 300 kg ha^{-1} y^{-1}.

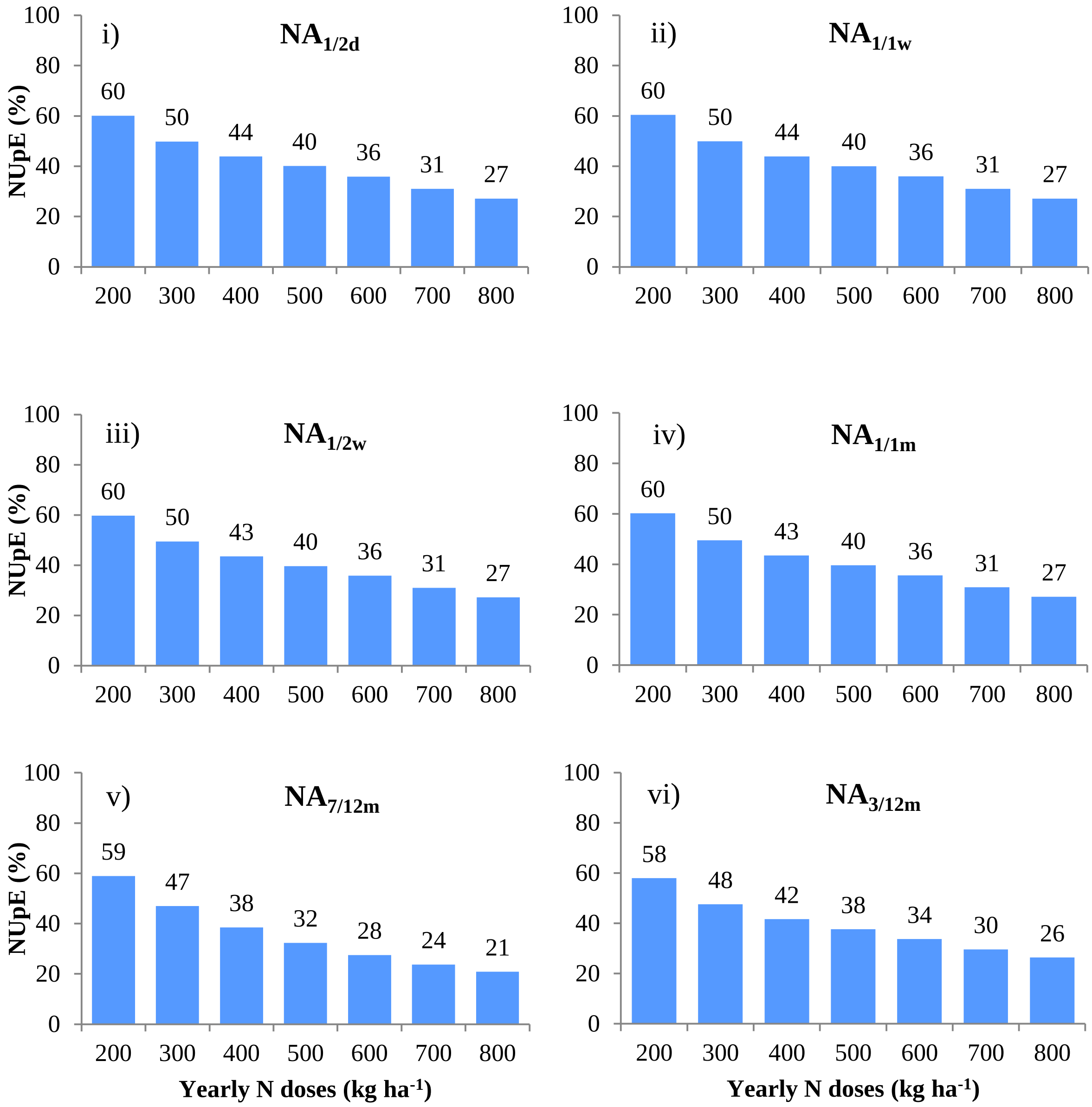

Figure 3.4 – Nitrogen efficiency uptake (NUpE) values for different N application frequencies and yearly N doses. i) every second day ($NA_{1/2d}$) ; ii) once a week ($NA_{1/1w}$); iii) each 14 days ($NA_{1/2w}$); iv) once a month ($NA_{1/1m}$); v) seven times during the year ($NA_{7/12m}$); and vi) three times during one year ($NA_{3/12m}$)

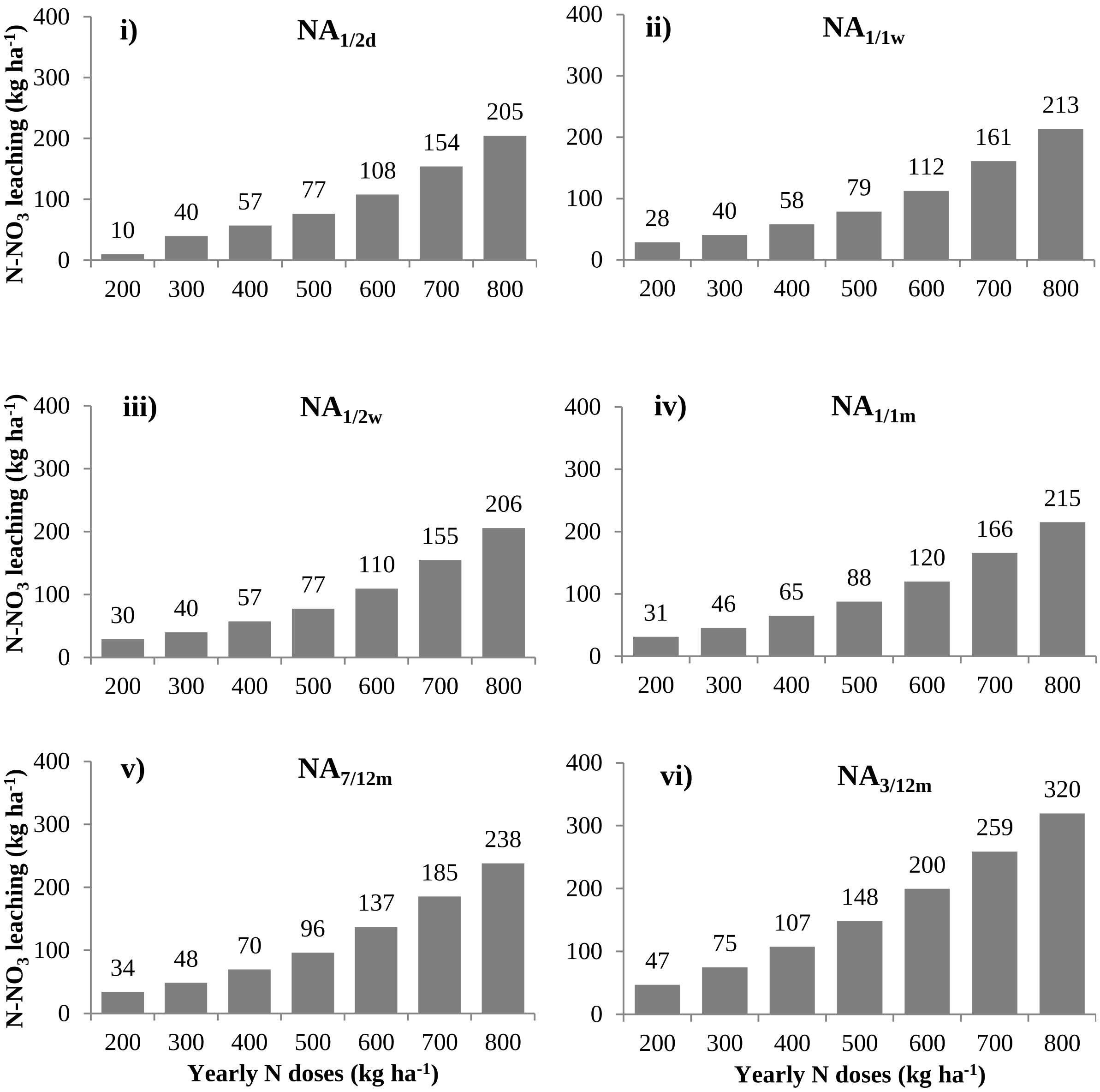

Figure 3.5 – Leaching of NO_3-N values for different N application frequencies and yearly N doses. i) every second day ($NA_{1/2d}$) ; ii) once a week ($NA_{1/1w}$); iii) each 14 days ($NA_{1/2w}$); iv) once a month ($NA_{1/1m}$); v) seven times during the year ($NA_{7/12m}$); and vi) three times during one year ($NA_{3/12m}$)

3.3.6 Scenarios of precipitation amount (Part 3)

Figures 3.6 and 3.7, respectively, show the results of N efficiency uptake (NUpE) and NO_3-N leaching obtained from the simulations of scenarios with different amounts of precipitation and N doses applied in the same frequency during the year (each 14 days).

Variations in annual precipitation did not influence plant NUpE obtained from the simulations of scenarios with ANIMO (Figure 3.6). For the same N dose, results of NUpE obtained from the scenario P_{defaut} compared to other scenarios with increased or reduced precipitation amount did not differ significantly.

Leaching of NO_3-N was very influenced by the variations in the cumulative amount of precipitation (Figure 3.7). Results of NO_3-N leaching obtained from simulations of scenarios AP_{03-13}, AP_{r10}, and AP_{r20} with N doses of 200, 300 and 400 kg ha^{-1} y^{-1} were very close accordingly to ANIMO simulations. Comparing values of NO_3-N leaching resulted from the scenario with the average annual precipitation of Barreiras (AP_{03-13}) with the scenario of the historical annual maximum precipitation (MaP_{30}), the precipitation increase between these scenarios were responsible for 63% and 67% of NO_3-N leaching increase for the N doses 300 and 600 kg ha^{-1} y^{-1}, respectively. These results showed the increase in N dose did not affect substantially the NO_3-N leaching when the annual precipitation amount was increased. When the extreme event historical annual minimum precipitation was evaluated with ANIMO, the values of NO_3-N leaching did not vary significantly between N doses of 200, 300, 400 and 500 kg ha^{-1} y^{-1}.

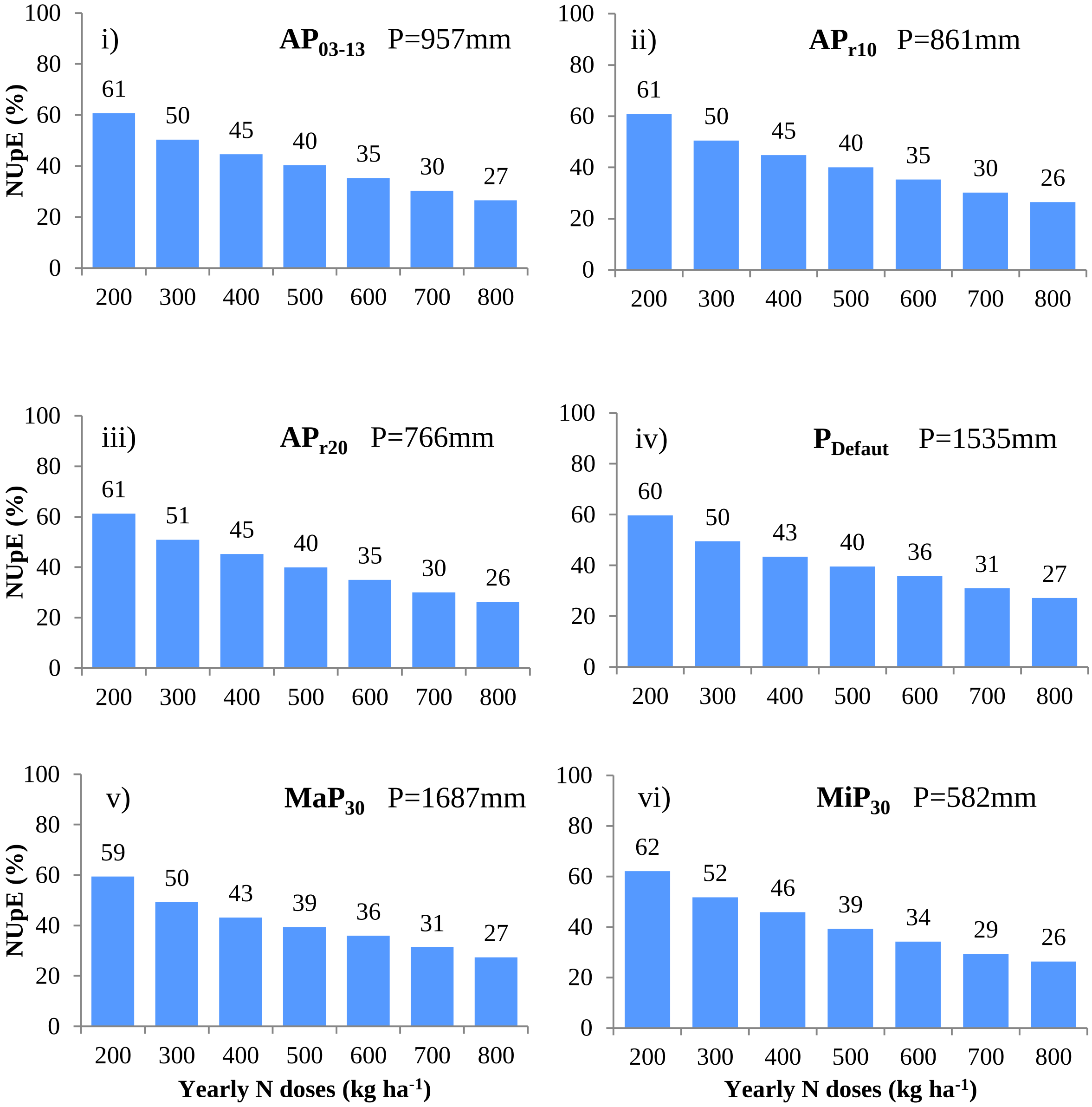

Figure 3.6 - Nitrogen efficiency uptake (NUpE) values for different yearly precipitation amount and N doses. i) Average precipitation in Barreiras during 2003-2013 (AP_{03-13}); ii) Average precipitation in Barreiras reduced in 10% (AP_{r10}); iii) Average precipitation in Barreiras reduced 20% (AP_{r20}); iv) Precipitation amount used in SWAP/ANIMO validation ($P_{Default}$); Maximum historical precipitation in Barreiras during the last 30 years (MaP_{30}); Minimum historical precipitation in Barreiras during the last 30 years (MiP_{30})

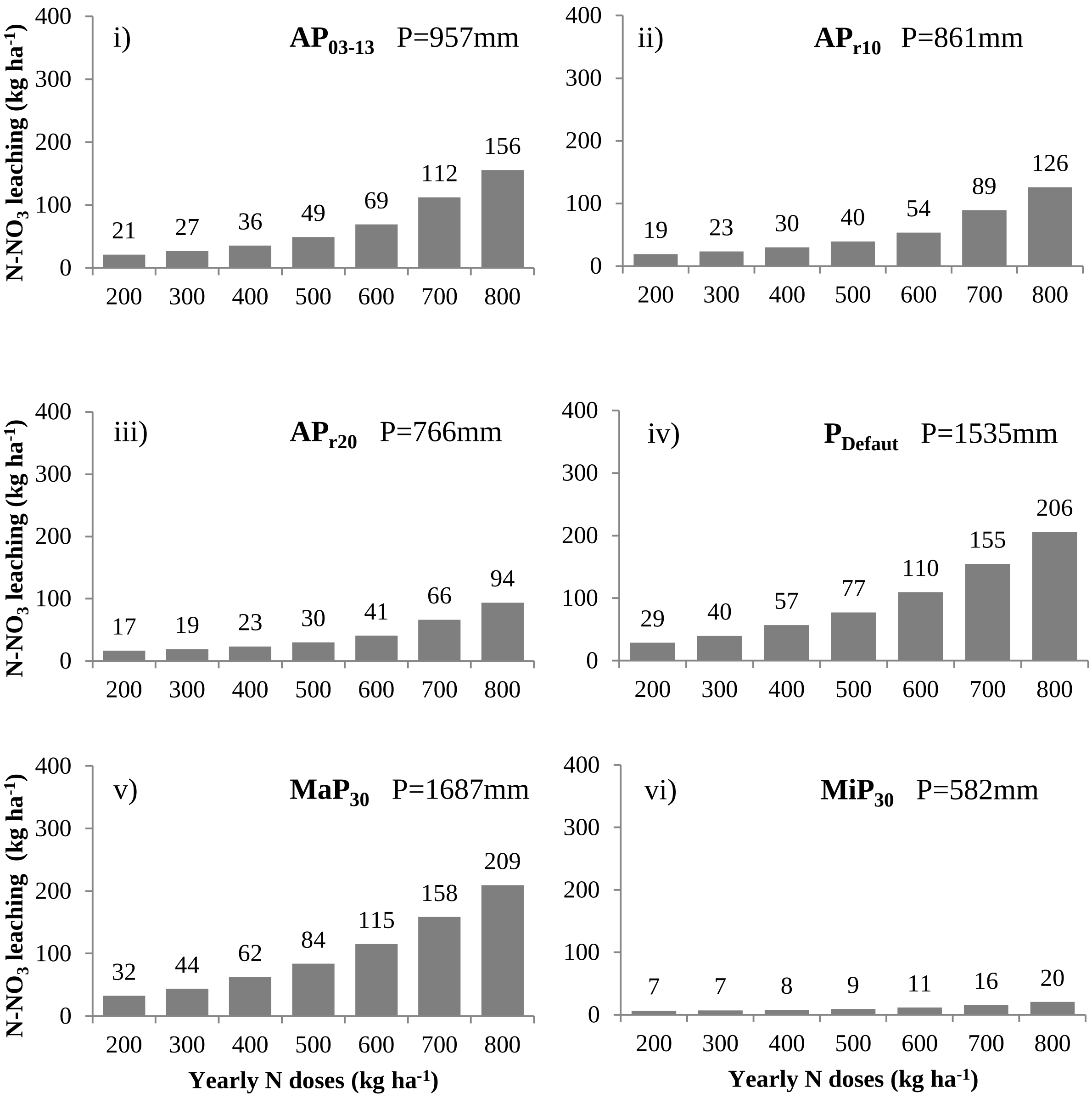

Figure 3.7 - Leaching of NO_3-N values for different yearly precipitation amount and N doses. i) Average precipitation in Barreiras during 2003-2013 (AP_{03-13}); ii) Average precipitation in Barreiras reduced in 10% (AP_{r10}); iii) Average precipitation in Barreiras reduced 20% (AP_{r20}); iv) Precipitation amount used in SWAP/ANIMO validation ($P_{Default}$); Maximum historical precipitation in Barreiras during the last 30 years (MaP_{30}); Minimum historical precipitation in Barreiras during the last 30 years (MiP_{30})

3.3.7 Evaluation of N use and expenses

Nitrogen leaching, volatilization, and denitrification resulted from applications of doses 200, 300, and 400 kg ha^{-1} y^{-1} with frequency $NA_{1/2W}$ and precipitation P_{Defaut} were calculated in kilograms of N for a pivot circle area of 100 ha during one experimental year (Figure 3.8). The relation between the total N losses (leaching, volatilization, and denitrification added up) with N dose amounts was significant for one pivot circle unit, since increasing N dose from 200 to 300 kg N ha^{-1} y^{-1} increased total N losses by 1550 kg y^{-1}, and from 300 to 400 kg N ha^{-1} y^{-1}, raised the total N losses by 2240 kg y^{-1}. Reducing N doses from 600 kg ha^{-1} y^{-1} to 300 kg ha-1 y-1 (as proposed in section 3.3.5), would reduce the N total losses by 8860 kg y^{-1}.

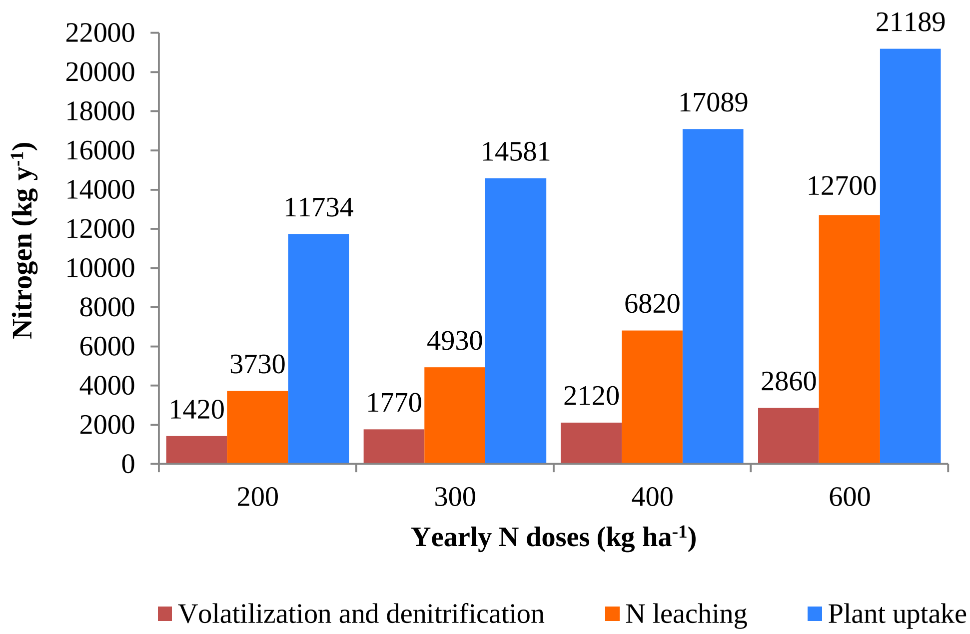

Figure 3.8 – Nitrogen losses to the environment by leaching (NO_3-N), volatilization (NH_4-N) and denitrification (NO_3-N) for simulated fertilizer doses of 200, 300, 400 and 600 kg N ha^{-1} y^{-1} applied with frequency $NA_{1/2W}$ in a planted area of 100 ha during one experimental year

We simulated the fertilizer costs for application doses of 200, 300, 400 and 600 kg N ha^{-1} y^{-1}, the fractions associated to coffee plants uptake and the wasted fractions by leaching, volatilization and denitrification, in one pivot circle (100 ha) during one year (Figure 3.9). Since fertilizer prices in Brazil diverge between regions, can also vary accordingly to the U$/R$ rate, we used the urea prices obtained by different studies in the period of 2014/2015. The urea (raw material, 45% N) prices were the following: i) average of R$ 1,537.00/t from Jully to September 2015, according to "Federação de Agricultura e Pecuária de Goiás – FAEG" (FAEG, 2015); ii) between R$ 1,042.52/t and R$ 1,404.29/t in September 2015, according to ARGUS (ARGUS, 2015); iii) average of R$ 1,353.50/t in April/March 2015, according to "Centro de Estudos Avançados em Economia Aplicada" (CEPEA, 2015); iv) and average of R$ 800.00/t in the period of 2014-2015, according to World Bank data (WORLD BANK, 2015). The average price of urea obtained from cited data was R$ 1,227.00/t (or R$ 1.23/kg), which was converted to kilograms of N resulting in R$ 2.73/kg N. Figure 3.9 presents the scenarios of average costs by employing the N doses of 200, 300, 400 kg ha^{-1} y^{-1} and farmers dose of 600 kg ha^{-1} y^{-1} (in 2008/2009) with urea prices of 2014/2015. A pivot circle managed with high doses of N fertilizer demands high investments, by which a large quantity is wasted due to the N losses. Based on simulations of fertilizer plant uptake (39% of total plant uptake), total N leaching and losses by volatilization and denitrification with ANIMO model, the costs with fertilizer for the coffee cultivation in Cerrado would be significantly reduced by employing N doses between 200 and 300 kg $ha^{-1}y^{-1}$. These outcomes showed the average economic savings that farmers would have reducing the amounts of fertilizer applications.

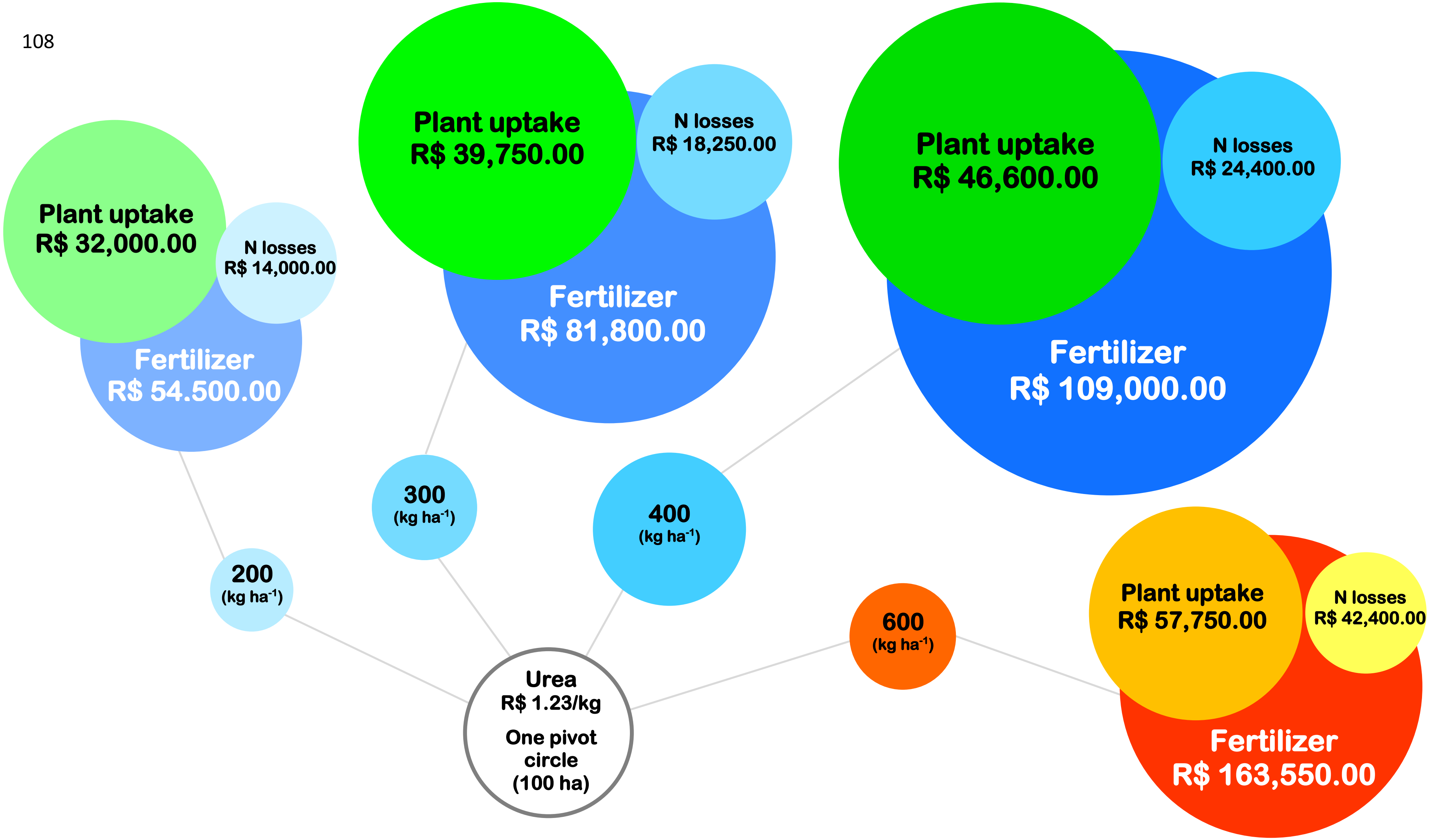

Figure 3.9 - Average annual expenses (R$) with fertilizers, coffee plant uptake and N losses in a pivot circle (100 ha) associated to the fertilizer doses (200, 300, 400 and 600 kg ha^{-1} y^{-1}). For each dose of fertilizer, the plant uptake, and N losses expenses are fractions of fertilizer total cost. Plant uptake expenses were calculated using N fertilizer plant uptake values, and N losses expenses were calculated using annual values of leaching, volatilization and denitrification added up. Expenses were calculated based on urea prices in 2014-2015 (FAEG, 2015; ARGUS, 2015; CEPEA, 2015, WORLD BANK, 2015)

3.4 Final considerations

A field-scale application of the SWAP/ANIMO model to a coffee plantation scenario for the Brazilian Cerrado has been developed and the results of modeling were presented. The model ANIMO was evaluated by a sensitivity analysis and the most important parameters for the intensively fertilized system were obtained. For a soil-plant system like this, in which no other source of N besides urea is significant, emphasis should be given to soil pH and soil temperature of reference (T_{ref}). These parameters were especially sensitive for the simulations of the annual N balances when mineral fertilizer was applied at the rate of 400 kg N ha^{-1} y^{-1} and 800 kg N ha^{-1} y^{-1}. The soil pH was the most sensitive modeling parameter. A 1% increase of pH made NO_3-N leaching increase almost 3% for both M_{400} and M_{800}. Although the detailed processes simulated by ANIMO require several input parameters, in the evaluated scenarios not all of them were sensitive for modeling. The modeling with ANIMO can be simpler and more objective when the most sensitive parameters are established. For instance, for an agricultural system managed only with organic manures, the N concentration in the organic fractions of materials (c_{Nfp} and c_{Nsp}) and the decomposition rate constants (k_{fp} and k_{sp}) become the most important parameters to be characterized for use in ANIMO. The cited parameters soil pH and T_{ref} should be taken into account anyway and be well adjusted independently of the study conditions.

Some ANIMO parameters were taken from literature and can be seen as potential sources for new investigations. Future studies should consider, for instance, the maximum transpiration stream concentration factor σ_N^{max} that is frequently adopted as a unique value independently of the soil-plant system. A description of σ_N^{max} behavior for ordinary crops would be welcome for ANIMO applications in systems with limited soil nitrogen availability. Some parameters of material characterization like the decomposition rate constant (k) are difficult to find, and for that reason we summarize important information related to poultry manure and coffee husks. With this information, we expect to benefit other investigations related to coffee cultivation.

This study also showed the N processes simulated by ANIMO have a distinct sensitivity behavior to the input parameters of soil, plant, and materials depending on the annual N dose. Plant uptake, leaching of NO_3-N and NH_4-N, and nitrification were affected differently by the same parameters in M_{400} and M_{800} and sometimes were sensitive to a certain parameter only for a specific N dose. These results challenged our purposes of using ANIMO for studying the N cycle processes establishing a unique set of parameters representative of the system under several N dose scenarios.

The model ANIMO was calibrated and validated for the coffee plantation of Cerrado and simulations were evaluated employing the statistical parameters RMSE, NSE and d index. The model accurately predicted the majority of daily NO_3-N concentrations in soil solution at 1.0 m depth during validation, resulting RMSE = $7.3 \cdot 10^{-3}$ kg m^{-3}, NSE = 0.45 and index d = 0.80. The simulated annual N plant uptake values for doses of 400 kg N ha^{-1} y^{-1} (calibration) and 800 kg N ha^{-1} y^{-1} (validation) were similar to the average values obtained by field experiments. We conclude that the one-dimensional process-based model ANIMO was able to describe satisfactorily the average N cycle of the evaluated soil-plant system.

From the presented outcomes, we are encouraged to propose improvements for the model ANIMO that could make simulations more realistic or better describing fertigated agricultural systems. Firstly, the inorganic fertilizer characterization should be better described to simulate the soil chemical reactions of nitrogen fertilizers. The upper boundary conditions could be enhanced as well, considering the detailed input of mineral nitrogen by irrigation (fertigation) as an option in the management file of ANIMO. The inclusion of other process occurring in the above ground system, e.g. N leaf interception, would be desirable in this case. Secondly, ANIMO's simple consideration of the soil pH as time independent can be determinant under such conditions. Because soil pH can be affected by fertilizer input and subsequently influence another process like nitrification, we consider including the soil pH time variability as a model parameter would benefit model performance.

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4. CONCLUDING REMARKS

The hypotheses and objectives of this work were presented in section 1. In section 2 the study "Deep drainage modeling for a fertigated coffee plantation in the Brazilian Cerrado" showed the results of SWAP calibration and comparison of water balance outcomes with a conventional model, the Climatologic Water Balance. The sensitivity of water balance components to input parameters of soil and plant were obtained, and the potential of SWAP for generating scenarios of irrigation was evaluated.

Drainage simulated by SWAP showed to be highly sensitive to the van Genuchten equation parameter n and Mualem equation parameter λ, and by plant crop factor Kc.

Results of annual water balance simulated by SWAP and calculated by CWB were equal, but these models showed to predict differently monthly drainage. SWAP is a robust model, which was also validated in several studies and conditions. We expect the drainage results obtained from this process-based model to be more realistic than the CWB, which is simpler in its formulation.

Irrigation scenarios simulated with SWAP for the experimental year showed to be efficient in water use and coffee productivity when longer intervals of irrigation were used. According to this analysis, adopting an irrigation interval of 15 days and yearly water amount between 650 and 750 mm could be an option for better management compared to the farmer's scenario. Results of water productivity, plant productivity, and deep drainage indicated the farmer's management practices could be improved, minimizing loss of water by drainage and at the same time increasing coffee production.

In section 3 the study "Modeling nitrogen dynamics in a fertigated coffee plantation in the Brazilian cerrado with ANIMO" showed the simulations results of N dynamics due to natural entries and fertigation management in the studied coffee cultivation of Cerrado. The combinations of models SWAP/ANIMO was calibrated and validated with data of NO_3-N concentrations in soil solution obtained experimentally. The sensitivity of N processes simulated with ANIMO to the input parameters was evaluated. The potential of SWAP/ANIMO for generating scenarios of N fertilizer application were evaluated in this section.

ANIMO was calibrated and validated for the coffee plantation of Cerrado and simulations were evaluated employing the statistical parameters RMSE, NSE and d index. The model accurately predicted the majority of daily NO_3-N concentrations in soil solution at the 1.0 m depth during validation, which was confirmed by the obtained ranking of statistical index values. The simulated annual N plant uptake was close and within the uncertainty interval of the experimental value available in the validation scenario. Evaluations of NUpE and NO_3-N leaching results from the scenarios of N application frequency and N doses simulated with ANIMO suggested the most efficient managements are those with dose partition at least once every 14 days and N doses equal or less than 300 kg ha^{-1} y^{-1}.

We conclude that the combination of one-dimensional process-based models SWAP/ANIMO was able to describe satisfactorily the average N cycle of the evaluated soil-plant system of Cerrado in Bahia, Brazil.

ANNEX

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Deep drainage modeling for a fertigated coffee plantation in the Brazilian savanna

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ABSTRACT

Modeling in agriculture represents an important tool to understand processes as water and nutrient losses by drainage, or to test different conditions and scenarios of soil and crop management. Among the existing computational models to describe hydrological processes, SWAP (Soil, Water, Atmosphere and Plant model) has been successfully used under several conditions. This model was originally developed to simulate short cycle crops and its use also to cover longer cycles, e.g. perennial crops, is a new application. This report shows a SWAP application to a mature coffee crop over one-production cycle, focusing on deep drainage losses in a typical soil–plant–atmosphere system of the Brazilian savanna (Cerrado). The estimated annual deep drainage Q = 1019 mm obtained by SWAP was within 99% of the value determined by the climatologic water balance of 1010 mm. Monthly results of SWAP for Q compared to the estimative using the climatological method presented a determination coefficient of 0.77. A variety of coffee fertigation scenarios were simulated using SWAP and compared to farmer's management scenario, leading to the conclusion that larger irrigation intervals result in lower Q losses, better water productivity and higher crop yield.

1. Introduction

The savanna ecoregion (Cerrado) prevails in central Brazil, also reaching the northeast part of the country and including part of the state of Bahia. The savanna domain in Bahia is highly suitable for irrigated agriculture due to the great availability of surface and underground water resources. According to Brazil's National Grain Supply Company (CONAB), western Bahia is an important food (grain) provider and holds, for example, the highest coffee yield under savanna conditions in the country. However, there are some concerns in respect to the modern agriculture practiced in this producer region. Due to the ineffective land management during the last decades, the irrigated farms concentrated at specific areas and, therefore, conflicts over water use already took place in western Bahia (Lima, 2011). At the same time, management practices applied by farmers are not sustainable in terms of fertilizer and water usage, especially due to the lack of scientific studies that support their decisions (Bruno et al., 2011).

Numerical modeling applied to agriculture is a useful tool to simulate biophysical processes and can be used to obtain short-term results and future predictions under defined scenarios. The information generated is helpful for establishing a more sustainable agriculture as well as supporting strategies for the mitigation of pollution, named by Strauch et al. (2013) as the "Best Management Practices". The hydrological model SWAP (Soil, Water, Atmosphere and Plant) is one of the existing algorithms used worldwide for a variety of soils, crops and climatic conditions (Chirico et al., 2013; Crescimanno et al., 2012; Eitzinger et al., 2004; Kamble et al., 2013; Ma et al., 2011; Noory et al., 2011). The model has shown consistent results when applied to maize crops in sub-tropical climates (Pinheiro et al., 2013) and to soybeans and common beans in tropical climates (Scorza Junior et al., 2010; Durigon et al., 2012). SWAP was successfully validated already under several climatic and environmental conditions as cited Ines et al. (2006). More recent studies

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