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QUANTITATIVE STUDIES ALONG THE SOIL – VEGETATION – ATMOSPHERE INTERFACE OF WATER – LIMITED ENVIRONMENTS: PRACTICE-ORIENTED APPROACHES BASED ON STABLE WATER ISOTOPES, MODELING AND MULTIVARIATE ANALYSIS

VON DER FAKULTÄT FÜR BAUINGENIEURWESEN UND GEODÄSIE
DER
GOTTFRIED WILHELM LEIBNIZ UNIVERSITÄT HANNOVER

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The first principle of spirituality states: *"Whoever you meet in your life, you're supposed to meet and there's a purpose in meeting that person"*. And the second: *"What happens is the only thing that could have happened"*. I trust in these and would like to express my deepest appreciation to every person crossing my way during the last five years. I met many people on this way and I'm thankful for the lessons I learnt, even in sometimes difficult and conflicting situations. Some people particularly influenced me in my scientific as well as personal development and I owe special thanks to them.

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DEDICATION

FÜR MEINEN VERSTORBENEN OPA UND BESTEN FREUND WALTER GÜNDEL, DER VERBUNDENHEIT MIT DER NATUR WIE KEIN ANDERER VORZULEBEN UND ZU VERMITTELN WUSSTE. DANKE, LIEBER OPI, DASS DU DIES AN MICH WEITER GABST!

„ZUM ZIELE STREBTE DER FLUSS, SIDDHARTHA SAH IHN EILEN, DEN FLUSS, DER AUS IHM UND DEN SEINEN UND AUS ALLEN MENSCHEN BESTAND, DIE ER JE GESEHEN HATTE, ALLE DIE WELLEN UND WASSER EILTEN, LEIDEND, ZIELEN ZU, VIELEN ZIELEN, DEM WASSERFALL, DEM SEE, DER STROMSCHNELLE, DEM MEERE, UND ALLE ZIELE WURDEN ERREICHT, UND JEDEM FOLGTE EIN NEUES, UND AUS DEM WASSER WARD DAMPF UND STIEG IN DEN HIMMEL, WARD REGEN UND STÜRZTE AUS DEM HIMMEL HERAB, WARD QUELLE, WARD BACH, WARD FLUSS, STREBTE AUFS NEUE, FLOSS AUFS NEUE.“

HERMANN HESSE, SIDDHARTHA

KURZFASSUNG

Wasserknappheit ist ein weltweites Problem, besonders in ariden und semi-ariden Gebieten (oder: wasserlimitierte Gebiete – WLG), die nahezu die Hälfte der globalen Landoberfläche einnehmen. Über neunzig Prozent der Bevölkerung in diesen Gebieten ist auf Grundwasser angewiesen, um den häuslichen Wasserbedarf zu decken und Viehzucht betreiben zu können. Die vorrangig betriebene landwirtschaftliche Praxis in WLG ist Regenfeldbau. Trotz dieser Abhängigkeiten sind grundlegende hydrologische Prozesse entlang der Schnittstellen Boden-Vegetation-Atmosphäre in WLG nicht vollständig untersucht und verstanden, was eine nachhaltige Bewirtschaftung von Grundwasserressourcen sowie die landwirtschaftliche Planung zu einer großen Herausforderung macht. Um diese Situation langfristig zu verbessern sind interdisziplinäre Forschungsansätze notwendig.

Das **Hauptziel** dieser Doktorarbeit ist es zu der Entwicklung von praxisorientierten Methoden zur Untersuchung von ökohydrologischen Prozessen entlang der Schnittstellen zwischen Boden, Vegetation und Atmosphäre in WLG beizutragen. Angesichts der Komplexität und Vielfältigkeit des Systems Boden-Vegetation-Atmosphäre wurden spezifische Forschungsaspekte ausgewählt: i) Niederschlagscharakteristiken und deren Einfluss auf den Regenfeldbau; ii) die Bestimmung von Grundwasserneubildungsraten; und iii) die Quantifizierung von Wurzeltiefen und Transport von Wasserdampf an Standorten mit tiefen ungesättigten Bodenzonen. Ein primäres Ziel dieser Arbeit ist es, wissenschaftlich fundierte aber dennoch unkomplizierte Methoden zu erarbeiten, die sich nicht ausschließlich auf qualitative Aspekte beschränken, sondern quantitative Abschätzungen ermöglichen. Weiterhin zielen die entwickelten Methoden auf eine Anwendbarkeit in datenarmen Regionen ab und sollen dazu beitragen die Parametrisierung von Modellansätzen für die ungesättigte Zone zu unterstützen. Ein weiteres Anliegen dieser Arbeit ist es zu einem verbesserten Verständnis des komplexen Systems Boden-Pflanze-Atmosphäre in WLG beizutragen.

Die angewandten **Methoden** dieser Arbeit sind vielfältig und wurden nach Datenlage sowie der räumlich-zeitlichen Skala des betrachteten Problems ausgewählt. Für die Untersuchung von Niederschlagscharakteristiken und deren Einfluss auf Regenfeldbau (Studie i) wurde eine Methodenkombination entwickelt, die aus mehreren Einzelansätzen besteht: Einer multi-kriteriellen Auswertung von Niederschlagscharakteristiken, der Anpassung des Boden-Pflanze-Atmosphären Modells (SVAT) DAISY an beobachtete Daten und einer uni- und multivariaten Auswertung von Niederschlagscharakteristiken und landwirtschaftlichen Erträgen. Für diesen

letzten Schritt wurden selbstorganisierende Karten (self-organizing maps; SOM) gewählt, ein Ansatz der auf künstlichen neuronalen Netzen basiert. Studie i) basiert ausschließlich auf Fernerkundungsdaten und konnte daher auf einer großen Raum-Zeit Skala durchgeführt werden. Im Gegensatz dazu sind die Studien ii) und iii) auf der Punktskala angesiedelt und sämtliche Daten selbst aufgezeichnet, was den zeitlichen Horizont der Untersuchungen auf kurze Zeiträume beschränkt. Die Hauptmethode in diesen Untersuchungen sind spezifisch konzipierte Feldexperimente mit dem stabilen Wasserisotop Deuterium (^2H oder deuteriertes Wasser, ^2H_2O) als künstlicher Tracer. In Studie ii) wurde die Anwendbarkeit von ^2H_2O untersucht, um die etablierte peak-Versatz Methode zur Abschätzung der Grundwasserneubildung weiter zu entwickeln und für WLG zu optimieren. Studie iii) nutzt eine tiefenkontrollierte Markierstrategie für ^2H_2O zur Untersuchung von Wurzeltiefen und der Wurzelwasseraufnahme durch Pflanzen sowie um die Bewegung des Tracers über den Zeitraum einer Trockenzeit zu beobachten. Nach der Boden- und Pflanzenprobenahme wurde im Labor mittels kryogenischer Vakuumextraktion das Wasser aus den Proben extrahiert und anschließend die Konzentration der Isotope im cavity ring-down Spektrometer (CRDS) bestimmt. Für die Interpretation der Daten wurden duale (^{18}O und ^2H) Isotopenplots und Tiefenprofile der stabilen Isotope verwendet.

Die **Erkenntnisse** dieser Doktorarbeit können als Beiträge zu einem verbesserten Verständnis von Wassertransportprozessen entlang des Systems Boden-Pflanz-Atmosphäre in WLG zusammengefasst werden. Im Besonderen zeigen die Ergebnisse der präsentierten Studien die enorme Bedeutung der inner-saisonalen Verteilung von Niederschlag in der Regenzeit für die Erträge des Regenfeldbaus auf (Studie i), liefern neuartige Methoden um Wassertransportprozesse in Böden und Pflanzen zu untersuchen und offenbaren die Notwendigkeit, Transportprozesse in tiefen ungesättigten Zonen (z.B. in Form von Wasserdampftransport oder durch Wasseraufnahme von Tiefwurzlern) in WLG zu berücksichtigen (Studien ii und iii). Die in dieser Arbeit entwickelten Methoden ermöglichen wissenschaftlich fundierte und praxisorientierte Ansätze die mit minimalen Vorkenntnissen auch in datenarmen Regionen angewandt werden können.

Studie i) zeigt die Bedeutung der inner-saisonalen Verteilung von Niederschlag auf. Die Verwendung von Gesamtniederschlagsmengen, der Anzahl von Trocken- und Nasstagen oder Nassperioden als alleinige Indikatoren für den Erfolg des Regenfeldbaus sind nicht geeignet. Stattdessen eignen sich Indikatoren die sich auf Dauern beziehen (Dauer der Regenzeit und maximale Dauer von Nass- und Trockenperioden) in Kombination als geeigneter. Inkonsistente

Regenzeiten, d.h. viele Wechsel zwischen Trocken- und Nassperioden, wirken sich am negativsten auf Maiserträge aus. Die multivariate Analyse mit SOM zeigt darüber hinaus, dass die Verwendung der Charakteristik Regenzeitdauer in Kombination mit Gesamtniederschlagsmengen, der Dauer von Trocken- und Nassperioden und der Anzahl von Trockenperioden den Erfolg von Regenfeldbau im Untersuchungsgebiet am besten beschreiben. Diese Ergebnisse können für die zukünftige landwirtschaftliche Planung bedeutsam sein. Erträge könnten beispielsweise drastisch steigen, wenn die maximale Trockenperiode innerhalb der Regenzeit durch kleinskalige Bewässerung überbrückt werden könnte. Die entwickelte methodische Verknüpfung kann für nachhaltige Management-Analysen oder die Untersuchung des Einflusses des Klimawandels verwendet werden und ist leicht adaptierbar.

Die Anwendung von stabilen Wasserisotopen als künstlicher Tracer (Studien ii und iii) erlaubt quantitative Abschätzungen von Grundwasserneubildungsraten und liefert zusätzliche Informationen für das Verständnis von ökohydrologischen- und Wasserdampf-Transportprozessen. Darüber hinaus wird die Parametrisierung von SVAT-Modellen unterstützt. Eine Haupterkenntnis von Studie ii) ist, dass $^{2}H_2O$ ein geeigneter Tracer ist, um die Wasserbewegung in Trockengebieten über einen längeren Zeitraum (> 3 Monate) zu verfolgen. Die Studie und nachfolgende Verbesserungen der peak-Versatz Methode erweitern das Portfolio der Methoden zur Neubildungsabschätzung in WLG. Die tiefenkontrollierte Applikation von $^{2}H_2O$ (Studie iii) resultierte in einer neuartigen Methode zur Untersuchung von Wurzeltiefen und Wurzelwasseraufnahmetiefen. Darüber hinaus konnte in dieser Untersuchung Wasserdampftransport aus der tieferen ungesättigten Zone nachgewiesen werden. Dieser Transport könnte eine wichtige Komponente in der Wasserbilanz von WLG darstellen.

Schlagworte: wasserlimitierte Gebiete; Ökohydrologie; Regenfeldbau; stabile Wasserisotope, Grundwasserneubildung; Wurzeltiefe; Wasserdampftransport

ABSTRACT

Water scarcity has become an issue world-wide, especially in arid and semi-arid environments (or, water-limited environments – WLE) which occupy almost half of the global land area. More than ninety percent of the people living in these environments depend on groundwater for domestic and livestock water supply whereas the omnipresent farming practice is rain-fed agriculture. Despite this, the underlying water flow processes along the soil-vegetation-atmosphere interface in WLE are scientifically not yet well understood complicating a proper management of groundwater resources and agricultural planning. In order to remedy this situation, interdisciplinary approaches are required.

The **main objective** of this PhD is to contribute to the development of practice-oriented approaches for the investigation of ecohydrological processes along the soil-vegetation-atmosphere interface with a focus on WLE. In view of the complexity of the system soil-vegetation-atmosphere, specific research aspects were selected: i) rainfall characteristics and their impact on rain-fed agriculture; ii) the determination of groundwater recharge; and iii) the quantification of rooting depths and water vapor transport processes in thick unsaturated zones. First and foremost, this PhD thesis aims at developing straightforward, yet scientifically accurate methods which enable quantitative estimates rather than purely qualitative descriptions. Secondly, the proposed approaches are meant to be appropriate for their application in data scarce environments and support the parameterization of unsaturated zone models. Finally, this thesis aims to contribute to the improvement of the current understanding of the complex system soil-vegetation-atmosphere in WLE.

The **methods** used were manifold and chosen according to the availability of data as well as the spatiotemporal scale of the particular research aspect. For the investigation of rainfall characteristics and their impact on rain-fed agriculture (study i), a research framework composed of several methods was developed. These methods constitute a multi-criteria analysis of rainfall characteristics, fitting of the soil-vegetation-atmosphere transfer (SVAT) model DAISY and subsequent uni- and multivariate analyses between rainfall characteristics and agricultural yields using the artificial neural network approach of self-organizing maps (SOM). Study i) is solely based on remote sensing data and thus could be applied on a large spatial scale and multiple (12) years. In contrast, studies ii) and iii) are field investigations at the point scale and the data used was completely self-collected. Hence, these studies were rather short-term. The main methodologies used in these studies were specifically designed on-site experiments

utilizing stable water isotopes as artificial tracer. In study ii), the well-established peak displacement method for the estimation of groundwater recharge was adapted and improved for dry environments using deuterated water (^2H_2O) as tracer. In the last investigation (study iii) it is made use of the same tracer but with a depth-controlled labeling strategy in order to investigate rooting depths, trace water uptake by plants and monitor the distribution of ^2H_2O (i.e. water vapor transport) over one dry season. After sample collection and cryogenic vacuum-extraction of soil and plant samples the resulting water samples were subsequently analyzed for their isotopic concentrations using cavity ring-down spectroscopy (CRDS). For the interpretation of this data dual-isotope plots as well as isotopic depth-profiles were evaluated (studies ii and iii).

The main **outcome** of this thesis is a contribution to an improved understanding of processes governing water transport at the soil-vegetation-atmosphere interface in WLE. In particular, the results from the presented studies highlight the importance of the intra-seasonal distribution of rainfall for agricultural success (study i), provide methodologies to illuminate water transport processes in soils and plants and reveal the need to consider transport processes (i.e. through water vapor and deep tapping roots) in thick unsaturated zones (studies ii and iii). The methodologies developed provide scientifically precise, yet straightforward, practice-oriented approaches that can be applied with minimum prior knowledge even in data-scarce regions.

Study i) reveals the importance of the intra-seasonal distribution of rainfall. Using total rainfall amounts, total counts of dry/wet or wet spells days as single indicators for evaluating or predicting yields from rain-fed agriculture is not sufficient. Rather than that results show that indicators related to durations (rainy season duration, maximum dry/wet spell duration) are more suitable proxies for agricultural success. Inconsistent rainy seasons, i.e. many shifts of wet and dry spells, were found to affect yields most negative. The multivariate analysis using SOM further reveals that total duration of the rainy season as indicator conjunctively with total rainfall, maximum wet and dry spell durations and the number of dry spells are main determinants for current success of rain-fed agriculture. These findings have implications for future agricultural planning. For instance, yields could improve drastically, if the maximum dry spell could be bridged by a small-scale irrigation. The developed modeling framework can be applied for management analyses or studies on the impact of future climatic changes and easily be adapted if better data becomes available.

The use of water stable isotopes as artificial tracer (studies ii and iii) was proven to yield quantitative estimates of groundwater recharge and valuable additional information for understanding water vapor transport mechanisms and the parameterization of SVAT models. One major outcome of study ii) is that using $^{2}H_2O$ as artificial tracer is appropriate for monitoring water transport in dry environments over longer (> 3 months) time scales. Hence, this study and subsequent improvements of the peak-displacement method provide an additional method for the portfolio of techniques to estimate groundwater recharge in WLE. The depth-controlled application of $^{2}H_2O$ (study iii) resulted in a novel method for investigating rooting and root water uptake depths. An additional outcome of this study is the potential to illuminate water vapor movement, which might have a major impact on the sub-surface water balance of WLE.

Keywords: water-limited environments; ecohydrology; rain-fed agriculture; water stable isotopes; groundwater recharge; rooting depth; water vapor transport

Acronyms

BGR	Federal Institute for Geosciences and Natural Resources
CAMS	Climate Anomaly Monitoring System
CEB	Cuvelai-Etosha Basin
CMB	Chloride Mass Balance
CMORPH	CPC Morphing Technique
CPC	Climate Prediction Center
CRD	Cavity Ring-Down
DAISY	Daisy Mechanistic Simulation of Agricultural Fields Model
DNA	Deoxyribonucleic Acid
ECMWF	European Center for Medium-range Weather Forecasts
ERA-Interim	ECMWF Interim Analysis
FAO	Food and Agricultural Organization of the United Nations
GCM	Global Circulation Model
GMWL	Global Meteoric Water Line
GPCP	Global Precipitation Climatology Project
GPROF 6.0	Goddard Profiling Algorithm, version 6
GSMap MVK	Global Satellite Mapping of Precipitation moving vector with Kalman filter
IPCC	Intergovernmental Panel on Climate Change
IR	Infra-red
ISIRIC	International Soil Reference and Information Center
ISIRIC-WISE	ISIRIC World Inventory of Soil Emission Potentials
KED	Kriging with External Drift
LMWL	Local Meteoric Water Line
OA-ICOS	Off-Axis Integrated Cavity Output Spectroscopy
PERSIANN	Precipitation Estimation from Remotely Sensed Information using Artificial Neural Networks
PEST	Parameter Estimation
RFE	Rainfall Estimation Algorithm
ROSETTA	Rosetta Computer Program for Estimating Soil Hydraulic Parameters with Hierarchical Pedotransfer Functions
SADC	Southern African Development Community
SASSCAL	Southern African Science Service Centre for Climate Change and Adaptive Land Management
SOM	Self-organizing Map
SRFE	Satellite-based Rainfall Estimates
SSA	Sub-Saharan Africa
SVA	Soil-Vegetation-Atmosphere
SVAT	Soil-Vegetation-Atmosphere-Transfer
TRMM	Tropical Rainfall Measuring Mission
UZRB	Upper Zambezi River Basin
WLE	Water Limited Environments
WMO	World Meteorological Organization

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1 INTRODUCTION

1.1 BACKGROUND

1.1.1 MOTIVATION FOR THIS THESIS

I'm somewhere in the middle of nowhere, northern central Namibia, approximately 300 kilometers from the famous Etosha Pan. My throat is completely dried out and I can feel the dust covering my mouth. I'm dizzy and my feet and legs are hurting. It is 5 PM but still 25 °C and after a day of field work I joined the local adolescents for a soccer session. The game takes place on a dried out pan which has not received enough water during the rainy season. Two large wooden sticks connected by old cans threaded on a rope represent the goals. I'm the only one wearing shoes. And, even though some of the kids are playing here since more than three hours, none of them brought drinking water. My one liter bottle is empty after only 20 minutes. I almost feel ashamed. But we have a good time; the locals because they probably never played soccer with a white person and me because I get to know these people and got a slight idea of how life is here. After the game we sit and talk. The question I hear most often is 'When do you bring us water?' or when we open the recently established monitoring borehole nearby for the people.

Water scarcity has become an issue worldwide. We see images of droughts or people not having sufficient water on TV every day and hear politicians saying things like *'future wars will be for water, not for oil'*. But do we really *understand* and *feel* what this means? We, those growing up and living in the wealthy western world? How do people live in places not so blessed with as much water as we have in Europe? How is it to have to walk miles to fetch water from a dirty old hand-dug well? What do you do, if this well is dry? If all the wells are dry? How is it to be completely dependent on the rainy season? Such questions always kept my mind busy, and I found out that the most important question for me is this one: *How can we help to improve and remedy this situation?*

It is this question that motivated me to pursue a degree in hydrology and conduct practice-oriented research in water scarce environments.

The Intergovernmental Panel on Climate Change (IPCC) stated that for Africa *'By 2020, between 75 and 250 million of people are projected to be exposed to increased water stress due to climate change'* (IPCC, 2007). In regard to agriculture, the summary paper includes the following statement: *'By 2020, in some countries, yields from rain-fed agriculture could be reduced by up to 50%. Agricultural production, including access to food, in many African countries is projected to be severely compromised. This would further adversely affect food security and exacerbate malnutrition'* (IPCC, 2007). Of the total cropland in Sub-Saharan Africa (SSA), 97% is and will be dominated by rain-fed, subsistence agriculture (Calzadilla et al. 2013) until the foreseeable future, i.e. farmers completely depend on rainfall. Agricultural planning is based on a trial-and-error principle and thus, completely dependent on the experience of the farmer and to a certain degree, luck: Seeds are usually planted after the first stronger rains. If these are followed by a dry spell, the risk of losing the whole sowing is high. Where weather forecasts exist, they are usually not accessible by most rural farmers (Reason et al., 2004). In order to predict the effects of future changes in precipitation it is necessary to assess the determining factors for the success or non-success of rain-fed agriculture. But what are suitable research methods to assess this?

For domestic water supply, on the other hand, groundwater represents the main source. More than half of the world's population relies on this resource. In SSA alone, 100 million people depend on sub-surface water resources for domestic supplies and livestock (Adelana and MacDonald, 2008). In order to manage these resources sustainably, not only the spatial extent of an aquifer, its depth below ground and its quality are important, but also the rate by which it is naturally replenished. Groundwater recharge therefore is often regarded the most important parameter for the sound management of aquifers (Kinzelbach et al., 2002). At the same time, it is the most difficult to be measured (Beekman and Xu, 2003) which is even more true in environments with low recharge rates (Walker, 1998).

For scientific investigations on water resources, adequate data from several sources is required (e.g. climatic data, groundwater levels, soil moisture, data on agricultural yields). The collection and maintenance of such datasets is a major issue throughout Africa. The continent, despite covering one fifth of the world's total land area, has *'the worst climate observation system and one that is in a deteriorating state'* (Washington et al., 2006). The density of climate stations is one per 26.000 km², which is eight times lower than the recommendations proposed by the WMO (Kaspar et al., 2015; SciDevNet, 2016). Where data exists, time-series are often too short the quality is questionable (Kaspar et al., 2015; Taylor et al., 2012; Thiemig et al., 2013). The reasons behind these issues are manifold, but a generally low degree of development, education and other societal challenges are amongst the key determinants in regard to this.

Nevertheless, water resources need to be investigated and quantified in addition to strengthening the monitoring network. In order to do so, remotely sensed products currently emerging are applied extensively. Such investigations are often limited to a large spatial scale and provide estimates with high uncertainties. On the other hand, site-specific studies can be carried out in order to obtain more precise results, but on a smaller (point-) scale. Both approaches are equally important and ultimately have the same goal: To provide quantitative estimates of available water resources now and in the future. This can only be achieved by applying models that are accurately representing the natural system and account for all the relevant processes of the water balance in a particular environment. In semi-arid environments, these processes are yet not fully understood.

The intention of this PhD work is to develop methodologies based on remotely sensed products and site-specific field applications to increase the understanding of (eco-) hydrological processes at the soil-vegetation-atmosphere interface and in the unsaturated zone. The first study, which is combining remotely sensed products, modeling and the application of an artificial neuronal network aims at a large scale investigation of the interplay between rainfall dynamics and agricultural yields from rain-fed farming. In the second and third studies the stable isotope deuterium is used as applied tracer to investigate groundwater recharge and rooting depths on a site scale. A main motivation of all studies was to provide a framework that is easily applicable and adaptable. Another main intention is to provide methods that enable a more precise parameterization of SVAT (Soil-Vegetation-Atmosphere Transfer) models, which is mainly referring to the latter two investigations. The processes studied here (groundwater recharge, rooting depths and water vapor movement) have been difficult to investigate in the past but potentially have a great impact on the water balance of the unsaturated zone. Therefore, this PhD thesis aims to contribute in understanding relevant processes in the unsaturated zone of water-limited environments (WLE) better than previously.

1.1.2. Ecohydrological Processes along the Soil-Vegetation-Atmosphere Interface in semi-arid environments

Despite covering approximately one third of the global land surface (Svoray et al., 2015), water flow processes along the soil-vegetation-atmosphere (from here on referred to as SVA) interface in arid and semi-arid (‘water limited environments’; WLE) are not yet well understood (Hendrickx et al., 2005; Newman et al., 2006; Svoray et al., 2015). Thus, quantitative estimates of fluxes in the unsaturated zone are difficult to determine (Pfletschinger et al., 2014). An understanding of the system SVA requires an interdisciplinary approach because the influence of vegetation on the creation of deep drainage and the soil water balance in general is believed to be significant (Phillips, 1994; Seyfried et al., 2005). Therefore, an integration of hydrological and ecological, but also hydrogeological research is required to understand water movement in WLE (Newman et al., 2006; Seyfried et al., 2005; Svoray et al., 2015).

This introductory chapter discusses the interaction of the atmosphere, soil and vegetation and processes involved in WLE. As a starting point, a brief conceptual description of ecohydrological processes typically present in WLE is illustrated in Figure 1.1.

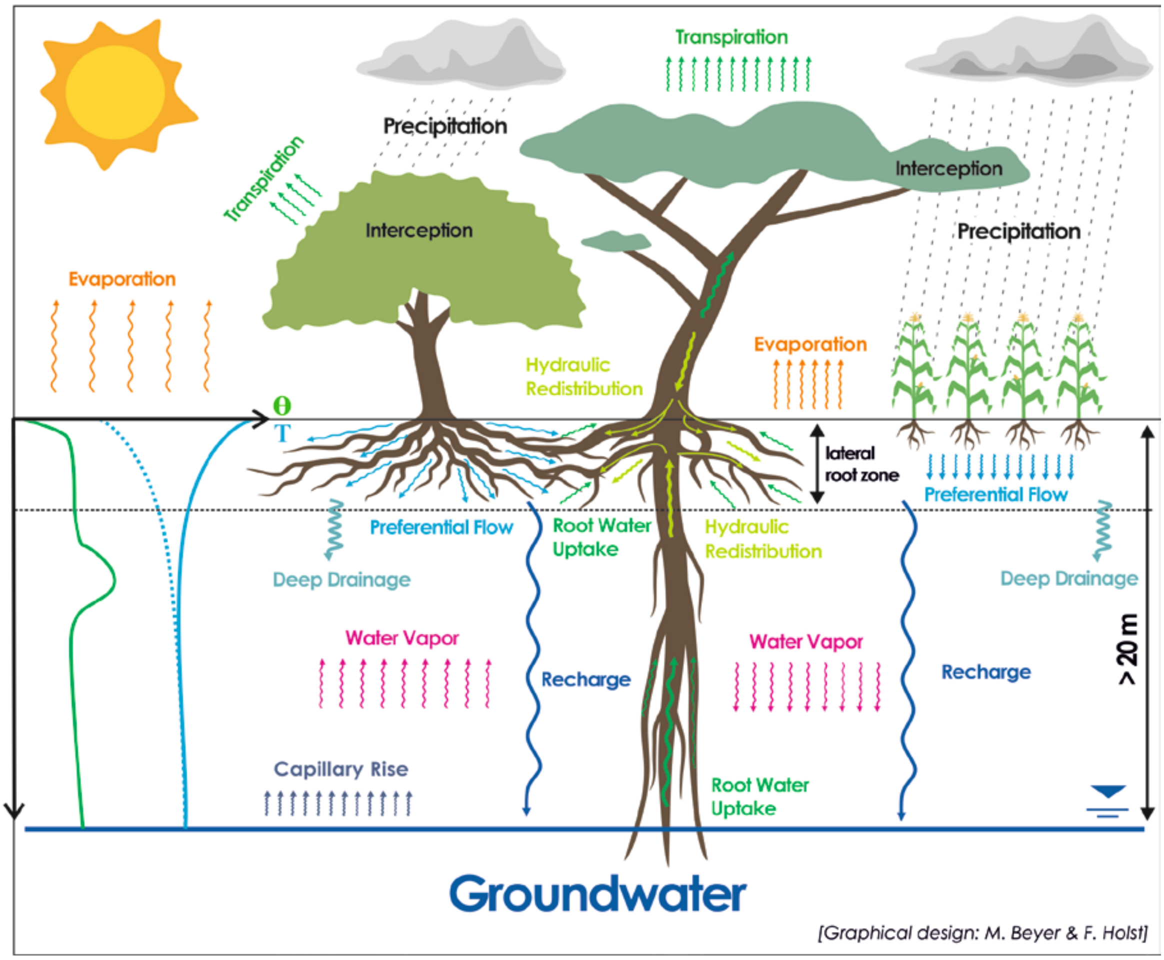


Figure 1.1: Conceptual illustration of water transport processes in the unsaturated zone and plants of WLE. On the left side, typical profiles for the dry season (or after-rainy-season) for soil moisture (Θ - green line) and temperature (T – solid blue line – day; dashed blue line – night) are shown.

The figure summarizes the most relevant mechanisms for water movement in WLE. In addition, typical depth-profiles for an after-rainy-season situation for soil moisture (green line) and soil temperature (solid blue line – day; dashed blue line – night) are depicted. The soil moisture profile shows the extremely low water contents near the surface due to a high temperature and a large water vapor deficit in the atmosphere. Underneath the direct effect of evaporation, water contents increase but remain low until the end of the lateral root zone. The subsequent bulk water represents water that infiltrated during the rainy season and surpassed the lateral root zone (deep drainage). Water contents generally homogenize to a certain degree in the deep unsaturated zone due to diffusion (in both the liquid and vapor phase). The temperature profiles show the characteristic shift between day and night caused by large differences of the atmospheric temperature during the dry season. Thus, the gradients for thermal vapor flux change on a diurnal basis (refer sub chapter '*Water vapor movement'* down below).

The most dominant processes for water movement in the unsaturated zone of WLE (other than the main driver, precipitation) are evaporation, root water uptake and water vapor transport. Subsequently, these are discussed briefly and major current research issues pointed out. A more thorough description can be found in Lubczynski (2009) or Newman et al. (2006).

Precipitation

In humid regions precipitation often occur as stratiform rainfall due to moderate temperatures. Convective events are mainly limited to the warm summer months. In contrast, convective events dominate WLE. Due to high temperatures and the variability of landuse, convective events are often limited to a small spatial extent and such events can have the character of extremes. The spatial and temporal variability of precipitation in WLE therefore is enormous and is expected to further increase in the future (IPCC, 2007). This creates challenges both for the accurate measurement of rainfall and practical management. For instance, satellite-derived rainfall estimates are known to be highly uncertain in reproducing rainfall extremes (Thiemig et al., 2013, 2012). On the other hand, even if a rainfall gauge is in place, this does not necessarily represent spatial rainfall. This is certainly an issue world-wide, but WLE have been shown to be more affected (Reason et al., 2006, 2004). If the input is uncertain, water fluxes along the SVA interface (especially those with lower contribution to the overall water balance) are difficult to quantify and separate from each other. This creates practical problems for an effective management of rain-fed agriculture and groundwater recharge estimations. Hendrickx et al. (2005) provide a straightforward explanation for the difficulties of estimating groundwater recharge depending on climatic settings:

"The determination of groundwater recharge in arid and semi-arid regions is inherently difficult for two reasons. First, the recharge estimate depends on a water balance in which actual evapotranspiration is almost equal to effective precipitation; … The recharge is thus determined by subtracting two relatively large numbers (precipitation and actual evapotranspiration) to find a small number (recharge). A small error in one of the large numbers will result in a large error in the small number." (Hendrickx et al., 2005).

Evaporation

Evaporation is the change of the state of water from liquid to the vapor phase. As long as water in its liquid form can move upwards through capillarity (i.e. soil moisture is near saturation), evaporation is completely controlled by atmospheric conditions (Brutsaert, 2014). This process is often referred to as *'stage one evaporation'* (e.g. Or et al., 2013a). If the contact of liquid water with the soil surface becomes interrupted, an air-dry layer develops in the soil in which water transport occurs in the vapor form (*'stage two evaporation'*; Brutsaert, 2014, Lehmann et al., 2008, Or et al., 2013a). For a particular soil, the thickness of this dry layer becomes steady-state after some time given no additional input of water at the soil surface. The depth of this layer is known as the zero-flux plane (*zfp*) and defined as the soil depth at which the sum of upward and downward water transport processes equals zero. The concept of the zero-flux plane is commonly accepted and widely used in unsaturated zone hydrology (Lehmann et al., 2008; Or et al., 2013a). Below this depth, water infiltrates downward by the combined effects of pressure and thermal gradients, and gravity.

Vegetation

Vegetation and their adaptation strategies play a crucial role for water transport processes in WLE. Adaptations directly affecting the below-ground water balance are, for example, particular rooting strategies (Canadell et al., 1996; Collins and Bras, 2007; Schenk and Jackson, 2002a), ways of redistributing water or nighttime transpiration (Dawson and Ehleringer, 1993; Dawson, 1993; Dawson et al., 2007; Goldstein et al., 2008; Lubczynski, 2009; Prieto et al., 2012; Schulze et al., 1998; Zou et al., 2005), dual water obtaining strategies (Burke, 2006), storage of water in the plants' tissues or co-existence with other organisms (Allen, 2007; Duddridge et al., 1980; Goldstein et al., 2008). In Figure 1.1 vegetation-induced water movements are depicted. To the authors' knowledge, none of these processes can be quantified properly until now, even though they might have a greater influence on the water balance of the unsaturated zone than previously thought (Lubczynski, 2009). The most known of all adaptations is probably the development of tap roots that grow deep (up to 70 m below ground; Canadell, 1996; David et al., 2007; Jennings, 1974) into the unsaturated zone with the ultimate goal to 'tap' the groundwater table (e.g. Moustakas et al., 2006). This basically makes the particular tree independent from droughts and thus ensures a major advantage over other species. In addition, it has been found that these tap roots are much more effective in the acquisition of water than shallow roots (Canadell et al., 1996; Reicosky et al., 1964); nevertheless quantitative evidence is lacking. Given this, the concept of accounting any water infiltrating underneath the lateral root zone of a plant groundwater recharge is questionable (Seyfried et al., 2005). There are numerous scientific publications (an appealing review on the role of trees in WLE is given in Lubczynski, 2009) on this issue.

Due to these site– and species–specific adaptations that need to be included, a proper quantification of transpiration as well as separating transpiration and evaporation remain difficult (Newman et al., 2006; Zou et al., 2005). In the recent years, researchers are advancing in respect to the latter aspect by applying methods based on stable water isotopes (e.g. Dubbert et al., 2014a, 2014b, 2013). Likewise, transpiration can be measured more accurately (refer to Lubczynski, 2009). However, potentially important processes – both from a hydrological and ecological perspective – remain difficult to quantify (Lubczynski, 2009). For instance, the uptake of water from the groundwater table (or, groundwater transpiration) or plant physiological processes such as stomata-reactions to high temperatures or currently unknown adaptation strategies remain challenging to investigate.

In essence, due to the number of different effects involved and the difficulty of quantifying these individually, vegetation can be seen as the major unknown for a complete understanding of water flow processes in WLE.

Preferential flow

Preferential flow can occur vegetation–induced (i.e. along plants' active root system or through cavities left by dead roots), due to the local geological setup (i.e. cracks and fissures) and soils. The prior aspect is not constrained to only be important for the upper part of the unsaturated zone given what was stated earlier about the possibility of deep-penetrating tap roots. Equally important for WLE are the latter two aspects, since karstic formations and calcrete are typical in dry environments (e.g. Lindenmaier et al., 2014; Miller et al., 2010) and sandy soils (even at non-vegetated locations) are prone to the development of preferential flow paths. The overall contribution to infiltration can be significant in such (Stumpp and Maloszewski, 2010). There are recent examples showing that preferential flow can be more effective in dry than wet soils (Bargués Tobella et al., 2014; Nimmo, 2012). Especially during high-intensity rainfall events with initially dry soil, preferential flow is possible (Stumpp and Maloszewski, 2010). As explained above, such events and initially dry soils are common in semi–arid environments. In addition the phenomenon of hydrophobicity – another major cause of preferential flow – is generally greater in dry soil (Nimmo, 2012). Several field methodologies for the quantification of preferential flow have been developed (refer to Allaire et al., 2009), but *'… non-equilibrium flow and heterogeneities like preferential flow can be strongly dynamic and their mathematical description is difficult to determine'* Jarvis, 2007). Consequently, quantitative studies are rare (Stumpp and Maloszewski, 2010).

Water vapor movement

The role of vapor phase water transport in WLE has been investigated intensively since many decades (Hendrickx et al., 2005; Philip and De Vries, 1957; Phillips, 1994; Phillips et al., 1988a; Scanlon, 2000, 1992; Scanlon et al., 2003; Walvoord and Scanlon, 2004; Walvoord et al., 2002a, 2002b) and the underlying physical principles are well understood and incorporated into numerical models (e.g. Saito et al., 2006; Sakai et al., 2009; Šimůnek et al., 2009). Scanlon et al. (2003) found that water fluxes in the deep unsaturated zone of WLE in the west of the USA predominantly occur as thermal vapor fluxes. Water vapor can move into all directions, following the main principles 'from warm to cold' (thermal water vapor transport) and 'from high to low concentration' (diffusive water vapor transport); i.e. a gradient in soil temperature (e.g. from the soil surface to the groundwater) or water content (e.g. from a wet soil to the atmosphere) is required. In Figure 1.1 typical temperature profiles for a sandy soil of a WLE during the dry season during day and night, respectively, are shown. Given the explanation above, it becomes clear that the directions of the thermal gradient change from day to night (and also from wet to the dry season, not shown here).

Quantitative, site-specific studies of water vapor fluxes are rare simply due to the difficulty to measure such fluxes and the complexity of the phenomenon. The magnitude and direction (refer to the explanation given above) of vapor phase fluxes can change both on an hourly to yearly timescale daily basis depending on precipitation dynamics, the soil moisture profile and temperatures which in turn affect each other. Water vapor movement can be a major contributor to overall water balance in dry environments (Barnes and Allison, 1984; Scanlon et al., 2003; Šimůnek et al., 2009).

Individual studies need to be site-specific and require long-term, multifaceted datasets (i.e. soil moisture, matrix potential and temperature at different depths including the deeper unsaturated zone) in order to derive reliable quantitative estimates.

1.1.3 SOIL AND PLANT WATER STABLE ISOTOPES IN SEMI-ARID ENVIRONMENTS

In this work the less abundant stable isotope of hydrogen in water (deuterium, ^{2}H) was mainly used as applied tracer, i.e. the concentrations used are by magnitudes higher than environmental concentrations. Specific aspects related to such artificial applications are covered in the introductory sections of the chapters three and four, respectively. For a general understanding of stable water isotopes in the unsaturated zone, this fundamental introduction is considered necessary, but will be kept brief.

Soil water stable isotopes can be used to investigate flow pathways and mixing within the unsaturated zone (Gaj et al., 2016; Garvelmann et al., 2012; Koeniger, 2003; Stumpp and Maloszewski, 2010). The main principle behind the characteristic shape of such profiles is that any water (e.g. precipitation or irrigation) reaching the ground and infiltrating into the soil is strongly affected by evaporation (refer to chapter 1.1.2). Due to the fact that the heavy water isotopes – deuterium (^{2}H) and oxygen-18 (^{18}O) – differ slightly in their physicochemical properties (i.e. higher molecular weight, lower molecular diffusivity) from the ‘common’ molecular species (^{1}H and ^{16}O, respectively), these processes result in an enrichment of heavy isotopes in the upper soil layer and hence, variations of soil water concentrations of stable isotopes (Kendall and McDonnell, 1999). The process of isotopic enrichment is commonly referred to as ‘fractionation’ and is caused by two main phenomena: *isotope exchange reactions* and *kinetic processes* (Kendall and McDonnell, 1999). Zimmermann et al. (1967) were amongst the first to show that *“…the presence of the soil effectively prevented turbulent vertical mixing, and the resulting steady-state isotope profile could be explained in terms of a balance between an upwards convective flux and a downwards diffusive flux of isotopes.”* (cited in Kendall and McDonnell, 1999). Underneath the zone of immediate influence of evaporation the isotopic composition is approaching a nearly constant value, mainly due to mixing and diffusion. As an example, a heavy rainfall event (heavy events are usually depleted in heavy isotopes) that infiltrates deep into the soil can create a short-term deviation from the steady-state constant isotopic concentration in the deep soil. Since such events are usually rare and frequent liquid water fluxes into the deep unsaturated zone are not expected (extreme events are rarely occurring), vapor phase diffusion is the main way of water transport causing a homogenization of the soil water isotopic composition over time. The major advantage of soil water stable isotopes over non-volatile tracers such as chloride or bromide is the ability to follow both liquid *and* vapor phase water movement (the prior ones become immobile in dry soils, Kendall and McDonnell, 1999).

Common applications of soil water stable isotopes are for example the determination of the origin of waters (Gat, 2008, 1995; Mayr et al., 2007), the quantification of evaporation (Gaj et al., 2016) or the estimation of groundwater recharge (Allison and Barnes, 1984; Saxena, 1984a, b). A recent review on the latter is given in Koeniger et al. (2016). Undoubtly, the studies of Allison and Barnes (Allison and Hughes, 1983, 1972; Allison, 1988, 1982; Allison et al., 1994, 1984, 1983; Barnes and Allison, 1988, 1984) improved the understanding of depth-profiles of stable isotopes in semi-arid environments essentially.

A typical soil water isotope profile of a semi-arid environment is provided in Figure 1.2. The illustration further includes a schematic description of the water cycle of stable isotopes and relevant processes affecting their distribution in soils according to the principles explained above. Note that the magnitudes of the isotopic concentrations shown in Figure 1.2 are chosen to approximately represent measured values in northern central Namibia. However, the main intention of the figure is to depict relationships between different water reservoirs rather than showing ‘real’ values.

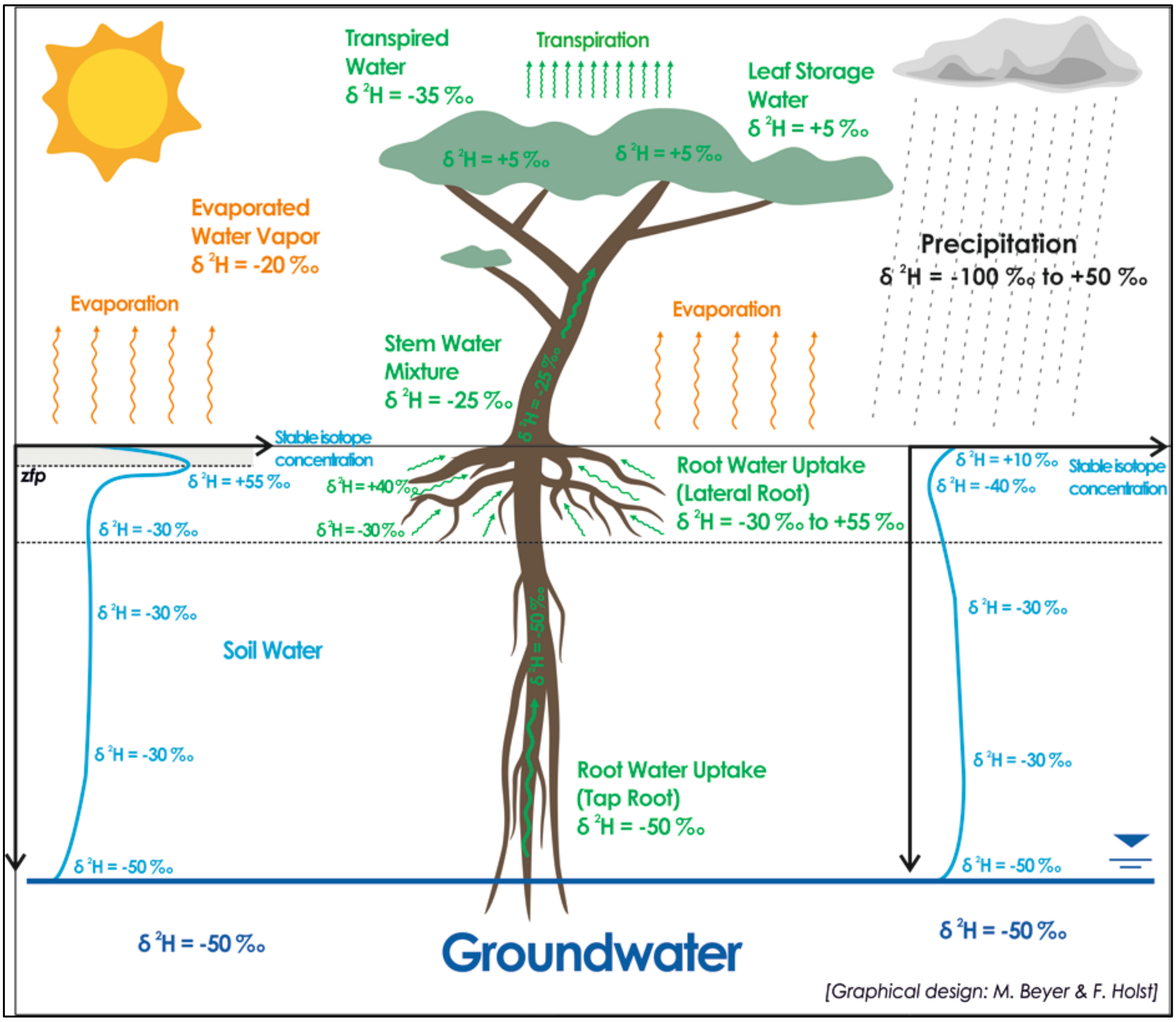


Figure 1.2: Conceptual illustration of typical relationships of the water stable isotope composition in the atmosphere, unsaturated zone and vegetation of WLE. On the left and right sides, respectively, typical profiles for a dry soil (left) and an after-rain soil (right) are depicted.

In simple terms, the characteristic soil water stable isotope profile depicted in Figure 1.2 mainly develops due to non-equilibrium transport processes (evaporation) near the surface and small differences between the physicochemical properties of the different molecular species of water. In deeper soil layers (where there is no more direct influence of evaporation), mixing processes are dominant causing a homogenization of isotopic concentrations. The soil water stable isotope profile is not influenced by vegetation (Kendall and McDonnell, 1999), i.e. the process of root water uptake is *non-fractionating*. This principle is used by many applications of SVA studies and of particular value for ecohydrological studies because it enables a separation of transpiration and evaporation fluxes (Dubbert et al., 2014b, 2013; Hsieh et al., 1998). Further applications include tracing of plant water uptake (Kulmatiski et al., 2010), rooting depths

(Jackson et al., 1999) or to identify unsaturated zone layers from which water is taken up (Ogle et al., 2004; Schulze et al., 1996). In contrast to root water uptake, isotopic *fractionation* occurs at the leaf surface (Fig. 1.2) with the atmosphere and stomata of plants being the main determinants. The processes leading to isotopic enrichment at the top soil and in the leaf of plants can somehow be compared: In both media forces of 'holding' water exist (matrix potential and leaf water potential, respectively) with a common force (the atmosphere or vapor pressure deficit) 'pulling' water from the two media. These processes are important when studying the water cycle with stable water isotopes and need to be accounted for.

1.1.4 STABLE WATER ISOTOPES AS APPLIED TRACER

This chapter contains excerpts from the publication: KOENIGER, P., GAJ, M., BEYER, M., HIMMELSBACH, T., 2016. Review on soil water isotope based groundwater recharge estimations. Hydrol. Process. doi:10.1002/hyp.10775
Any contribution taken from the above mentioned publication has been written solely by the author of this thesis.

Applied tracers are those which are added by purpose either directly to the land surface (e.g. via irrigation) or injected into the unsaturated zone (Beyer et al., 2015; Healy, 2010).

In the past the radioactive isotope tritium (^{3}H) has been used as applied tracer intensively (Rangarajan and Athavale, 2000; Saxena and Dressie, 1984; Selaolo et al., 2003; Sukhija and Shah, 1976; Wang et al., 2008; Zimmermann et al., 1967b). However, ^{3}H is radioactive and there are toxicological concerns associated with its use both during labeling and measurement (Becker and Coplen, 2001; Koeniger et al., 2010). Therefore, labeling with ^{2}H is of advantage because these concerns do not exist. Consequently, ^{3}H-labeling was replaced by ^{2}H as applied tracer to follow water movement in the unsaturated zone since its analysis has become cheaper. Deuterium is an effective tracer because it is chemically stable, non-reactive, easy to handle and cost effective (Mali et al., 2007). ^{2}H is subject to mixing with water entering the soil and is lost by evaporation as well as root water uptake. This creates a challenge for the experimental design, because the applied tracer concentration should be high enough to be detected after the desired time period (e.g. one rainy season). On the other hand, highly elevated tracer concentrations can create substantial memory effects during measurement. Hence; the experimental design has to be site-specific and carefully planned. Whereas in humid regions a small amount of tracer might be applied directly at the surface, it would cause a loss of the applied ^2H in WLE. For the determination of groundwater recharge, for example, the tracer should ideally be injected at the bottom of the root zone in order to avoid immediate loss of the tracer or enhanced dispersion of the tracer front (Blume et al., 1967; Munnich, 1983; Saxena, 1984; Sukhija et al., 2003). On the other hand, any additional artificial irrigation introduces water into the unsaturated zone which can cause an alteration of soil hydraulics and might lead to an overestimation of recharge (Beyer et al., 2015). In WLE it further proposes a challenge to apply ^2H underneath the rooting zone, which is generally deep in WLE. Blume et al. (1967) compared labeling using irrigation and sub-surface injection. An experimental procedure for the optimal design of such experiments was proposed by Munnich (1983).

In summary, ^2H is easier to use as applied tracer at the boundaries between soil, vegetation and atmosphere because it can be crossed with these interfaces. Careful planning of applied concentrations depending on the time-frame of the investigation, season and local climate is required, especially when tracer recovery is to be determined (Becker and Coplen, 2001; Speakman, 1997).

Example applications of ^2H include the investigation of soil water movement in general, studies of the validity of piston flow (Zimmermann et al., 1967a, 1967b, 1966), dispersion effects (Koeniger et al., 2010; Mali et al., 2007), preferential flow (Hangen et al., 2005; Schumann and Herrmann, 2001; van der Heijden et al., 2013) and capillary rise (Grünberger et al., 2011). From an ecohydrological perspective, root water uptake and plant physiological processes have been studied in the past (e.g. Brooks et al., 2002; Fravolini et al., 2005; Kulmatiski et al., 2010; Marc and Robinson, 2004). Lischeid et al. (2000) assessed the uncertainty of tracer experiments using multiple tracers.

1.2 OBJECTIVES

The studies presented in this thesis each stand individually but all contribute to one overall objective: The development of innovative practical, straightforward methodologies in order to investigate and quantify ecohydrologically relevant processes along the soil-vegetation-atmosphere continuum in semi-arid environments. Within this complex system, three particular aspects were selected, with each of them representing a prevailing and currently challenging scientific research problem. As for the latter two studies, another key objective is to evaluate the use of deuterium as artificial tracer in the unsaturated zone of semi-arid environments.

The focal research areas and the specific objectives of the studies are:

1. Investigate the impact of the intra-seasonal distribution of rainfall on rain-fed agriculture in the Upper Zambezi River Basin

    (a) Explore the spatiotemporal distribution of rainfall characteristics

    (b) Evaluate the impact of rainfall characteristics on agricultural yields on the example of the traditional maize crop

    (c) Identify rainfall characteristics or combinations of those crucially affecting yields using uni- and multivariate techniques

    (d) Determine most/least suitable areas for rain-fed agriculture basin wide

2. Estimate groundwater recharge through a thick unsaturated zone in northern central Namibia utilizing deuterium as artificial tracer

    (a) Investigate water movement and the longer-term (> 3 months) fate of artificially introduced ^2H_2O in the soil

    (b) Adapt the peak-displacement methodology for estimating groundwater recharge using ^2H_2O

    (c) Assess tracer recovery rates

    (d) Point out potential and limitations of using ^2H_2O in the unsaturated zone of WLE

3. Utilize ^2H_2O as artificial tracer in order to investigate rooting depths, root water uptake dynamics and water transport in the unsaturated zone of WLE

(a) Develop and test a methodology to investigate root water uptake depths in semi-arid environments

(b) Investigate depth-dependent water uptake dynamics and access of different plants to soil water reservoirs

(c) Trace water transport within the unsaturated zone, in particular to assess vapor phase movement during the dry season in a semiarid environment

1.3 STRUCTURE

This thesis begins with a description of the main processes taking place in the unsaturated zone of semi-arid environments and a brief introduction into soil water stable isotopes and relevant processes affecting their distribution **(Chapter 1)**. The centerpieces of this PhD work comprises of the three scientific publications of which the author of this thesis is the main author. These papers are already published and available within the scientific domain. Within this thesis these publications are embedded in chronological order:

In **Chapter 2** the investigation of rainfall characteristics and their impact on rain-fed agriculture is presented. The original paper is published in the *Hydrological Sciences Journal* under the doi:10.1080/02626667.2014.983519. **Chapter 3** is focusing on groundwater recharge estimation using deuterium labeling. The publication has been released in the journal *Isotopes in Environmental and Health Studies* under the doi:10.1080/10256016.2015.1076407. Finally, an experiment on the investigation of rooting depths and water transport processes in the unsaturated zone using a deuterium labeling technique is depicted in **Chapter 4**. The original paper has been published in Journal of Hydrology and can be accessed under doi:10.1016/j.jhydrol.2015.12.037.

The thesis closes with synthesis of the main findings from the three publications, which is presented in **Chapter 5**. In this chapter, ideas for further improvement – in particular for the latter two field-based studies – are compiled. Finally, opportunities for future studies and the general ways forward are summarized.

2 RAINFALL CHARACTERISTICS AND THEIR IMPLICATIONS FOR RAIN-FED AGRICULTURE: A CASE STUDY IN THE UPPER ZAMBEZI RIVER BASIN

This chapter is an edited version of: BEYER, M., WALLNER, M., BAHLMANN, L., THIEMIG, V., DIETRICH, J., BILLIB, M., 2016b. Rainfall characteristics and their implications for rain-fed agriculture: a case study in the Upper Zambezi River Basin. Hydrol. Sci. J. 61, 321–343. doi:10.1080/02626667.2014.983519

2.1 ABSTRACT

This study investigates rainfall characteristics in the Upper Zambezi River Basin and implications for rain-fed agriculture. Seventeen indices describing the character of each rainy season were calculated using a bias-corrected version of TRMM-B42 v6 rainfall estimate 1998-2010. These were correlated with maize yields obtained by applying a SVAT-model. Finally, a Self-Organizing Map (*SOM*) was trained to examine multivariate relationships. Results reveal a significant spatiotemporal variability of rainfall indices and yields with a gradient from north to south. Yields greater 1 t/ha are found to be only achievable with rainy seasons longer than 160 days. For shorter durations, the interplay of total rainfall, dry spell frequency and maximum dry/wet spell durations determines agricultural success. Using total rainfall alone or wet day frequency as estimators for yields is insufficient. Rainy seasons with abnormal patterns such as inconsistent rainy seasons (such as many wet/dry spell shifts) affect yields most negatively. Results imply profound significance in the context of agricultural planning under changing climatic conditions climatic changes and agricultural planning, as well as for the development of forecasting mechanisms.

2.2 INTRODUCTION

The foremost farming practice over most parts of Sub-Saharan Africa (SSA) is rain-fed agriculture. In fact, 97% of the total cropland in SSA is dominated by rain-fed farming (Calzadilla et al., 2013) and this agricultural practice is expected to remain the major source of staple food production for the majority of people in rural areas (Cooper et al., 2008). In these areas severe challenges are associated with the successful cultivation of the main staple crops (in particular, maize and millet/sorghum). Milgroom and Giller (2013) identify in their study four main issues related to the extremely low yields in rural SSA: (i) Non-accessibility to necessary inputs at the right time (i.e. availability of seeds, man-power or land); (ii) rainfall variability; (iii) losses in the field (i.e. elephant- or hippo- related losses) and (iv) post-harvest losses (pests). Though each of these factors being equally important, numerous studies emphasize the crucial role of rainfall and its variability (Reason et al., 2004; Tadross et al., 2005; Cooper et al., 2008, Crespo et al., 2010; Mupangwa et al., 2011; Calzadilla et al., 2013; Milgroom and Giller, 2013). In particular, over large parts of SSA, an extremely high spatiotemporal variability (Boko et al., 2007) of rainfall on an inter-annual as well as periodic basis (Tyson et al., 1975; Reason et al., 2004; Tadross et al. 2007) is reported. Induced impacts of climatic changes such as a decrease of early-rainy-season rainfall and a rising number of extreme events (Christensen et al., 2007; Kotir, 2011) further increase the risk of low yields or even yield losses. Although a seasonal forecast system is existing to support the agricultural sector (Famine Early Warning System, http://www.fews.net/), this information is not precise enough (since only delivering approximate rainfall season starting dates) and often not accessible in rural areas. As a consequence, rain-fed agriculture in rural areas is still based on a 'trial-and-error' principle: Crops such as maize or millet/sorghum are commonly planted after the first showers of the wet season, in hope that the subsequent weeks will deliver enough rainfall to allow germination and growth. If rains are not sufficient after sowing (i.e. by the occurrence of a dry spell), seeds often need to be replanted causing enormous financial damage to the farmers and might even threaten their existence.

To address these issues, several studies explicitly point out the need for a more detailed analysis of the spatiotemporal variability of rainfall (Hachigonta and Reason, 2006; Hachigonta et al., 2008; Tadross et al., 2005; Usman and Reason, 2004). Before the development and installation of any kind of forecasting system (i.e. prediction of likely onset and cessation dates), the most important characteristics are yet to identify and quantify on a smaller spatiotemporal scale.

The understanding of rainfall patterns in SSA and particularly the interconnection between rainfall characteristics and agricultural yields have been focus of past research. Numerous studies were executed that investigated the association of rainfall characteristics with synoptic patterns (El Niño-Southern Oscillation phenomena). In particular, spatial and temporal patterns of dry spells within the rainy season over southern Africa as a whole (Usman and Reason, 2004); dry and wet spell frequencies and rainy season onset dates over the Limpopo region, South Africa (Reason et al., 2005); and the variability of dry and wet spell frequency in the rainy season over Zambia (Hachigonta and Reason, 2006) have been associated to El Niño and La Niña. An effect of these phenomena on rainfall distribution was found in all of these studies, which might be a starting point for a possible forecasting method. Additionally, Tadross et al. (2005) analyzed the onset of the rainy season over South Africa and Zimbabwe. Using a Self – Organizing Map (*SOM*) approach typical rainfall patterns associated with an early/late onset were identified.

Studies relating rainfall indices to maize growth were published by Tadross et al. (2007) and Crespo et al. (2010). The former authors used daily station rainfall data and downscaled GCM scenarios to calculate a wide range of rainfall characteristics and maize growth indices over southern Africa. Results show that there have been weak trends for a later on- and earlier offsets of the rainy season in the north and thus shorter rainy season durations. Crespo et al. (2010) applied a crop modeling approach and future climate scenarios based on 10-day input data for precipitation and evapotranspiration, that maize yields are most sensitive to rainfall in the sowing decade.

However, the representativeness of the abovementioned research is partially limited by the quality of their input data. Some of the studies utilize daily station data, others use either spatially and/or temporally coarse data (e.g. 2.5°×2.5°; 5-daily), which are not able to reproduce sufficiently the high spatiotemporal variability of rainfall patterns that determine the agricultural yields (Tadross et al., 2005; Usman and Reason, 2004). This further limits the range and accuracy of rainfall indices that can be determined (e.g. in regard to precision of dry/wet spell durations or extreme events). On the other hand, several studies have been carried out using station data (Camberlin and Diop, 2003; Camberlin et al., 2009; Mupangwa et al., 2011; New et al., 2006; Raes et al., 2004; Tadross et al., 2007); hence daily data could be applied. Using station data, the spatial pattern of rainfall characteristics cannot be represented sufficiently, especially in areas with low station density. In essence, examining a new source of input data might be the crucial step forward in the understanding of the interaction between rainfall patterns and agricultural yields in semi-arid regions.

Due to a scarce network of meteorological stations and inaccessibility of information (i.e. caused by the civil wars), sufficient data allowing such analyses in a detailed manner was not available until the beginning of this century. With the emerging of satellite-based rainfall estimates (SRFE), data in an adequate spatial and temporal resolution are becoming accessible with a nearly global coverage. This enables researchers to carry out hydrological studies on catchments across different scales, regardless if ground observational data are available or not.

Nevertheless, an in-depth validation of several SRFE is required before application, to assure the selection of the most suitable SRFE for the particular target area (Dinku et al., 2007; Hong et al., 2004). The accuracy of each SRFE differs massive with used product and study area (Thiemig et al. 2012). For the target area of the present study, i.e. the Upper Zambezi River Basin (UZRB), the quality of numerous SRFE has been investigated in previous studies by Thiemig et al. (2012) and Cohen Liechti et al. (2012). Thiemig et al. (2012) found the RFE 2.0 (NOAA Climate Prediction Center, 2013) and TRMM 3B42 v6 (Huffman et al., 2007) to be the most accurate SRFE for the Zambezi River Basin (considering also CMORPH, GPROF 6.0, PERSIANN, GSMap MVK and ERA-Interim), showing a good capture of timing of heavy rainfall events, intra-seasonal variability, distribution pattern and annual rainfall amounts. In addition, the reanalysis dataset ERA-Interim (Dee et al., 2011) showed good correspondence with observed values for intra-seasonal variability and spatial distribution, whereas the number of rainy days was overestimated. Timing of heavy events was captured very well within a lag time of 0 to +1 days (point-to-pixel analysis). All SRFE showed a high uncertainty in estimating the amount of heavy rainfall events by means of general underestimation. Cohen Liechti et al. (2012) stated that the reliability of all SRFE increases with the temporal scale; hence, the chosen time step has a major influence on the quality of all products. In contrast to Thiemig et al. (2012), they found that both RFE2.0 and TRMM overestimate rainfall. This contradiction might be explained by the fact that Cohen Liechti et al. (2012) did not use the official data from stations provided by the Zambia Meteorological Department which were accessible in the study of Thiemig et al. (2012).

Summing up, there is a gap in existing research in a sense that until now either punctual accurate *or* distributed but temporally inaccurate (i.e. accumulated 5-day) data has been used to characterize rainfall patterns across SSA. Further, none of the previous studies gives a complete breakdown of the most relevant rainfall characteristics and how they affect agricultural success of rain-fed farming.

The objective of this study is a highly resolute analysis of rainfall characteristics and their impact on yields for rain-fed maize throughout a major river basin in southern Africa. As information on measured yields is only available in certain areas, an agricultural model is applied to increase the availability of data. For our research, we address the following points in order to contribute in filling gaps in existing literature:

(i) How are important rainfall characteristics distributed in time and space?

(ii) How and in which way are rainfall characteristics affecting rain-fed agricultural yields?

(iii) Which rainfall characteristics or combinations of characteristics are the determining factors for the success of rain-fed farming? Can single indicators be used as predictors?

(iv) Which regions within the study area are the most/least suitable for rain-fed agriculture?

This study provides the first complete investigation of rainfall characteristics, their spatiotemporal distribution, variability and implications for agricultural yields of maize, based on a daily time step and high spatial resolution. Regional patterns, as well as trends or shifts of them, are revealed and an identification of suitable or less suitable areas for rain-fed farming is presented. The results thus provide quantified information for farmers and local decision-makers and are based on the best available data through the combination of better spatial representation through SRFE and better point information provided by station data. We further present a methodological framework based on freely available data that combines various types of datasets and tools in order to tackle a large-scale water management problem.

2.3 MATERIALS AND METHODS

The methodological approach comprises three parts:

(i) A spatially highly resolute (0.1°×0.1°) analysis of multiple rainfall characteristics using bias-corrected SRFE data on a daily basis in the Upper Zambezi River Basin for the years 1998 – 2010;

(ii) Calibration and validation of a SVAT (Soil-Vegetation-Atmosphere-Transfer) model on daily basis to simulate rain-fed agricultural yields for maize basin-wide; and

(iii) Both uni- and multivariate analysis of rainfall characteristics vs. modeled agricultural yields in order to identify key characteristics triggering rain-fed farming.

This study combines multiple datasets, which are presented in section 2.3.1, followed by a description of the above listed methodological approaches, in sections 2.3.2, 2.3.3 and 2.3.4, respectively. The complete methodological framework is summarized in Fig. 2.1 and is arranged in the way that data sources are presented on the left side of the scheme, whereas applied methodologies and tools are placed on the right side.

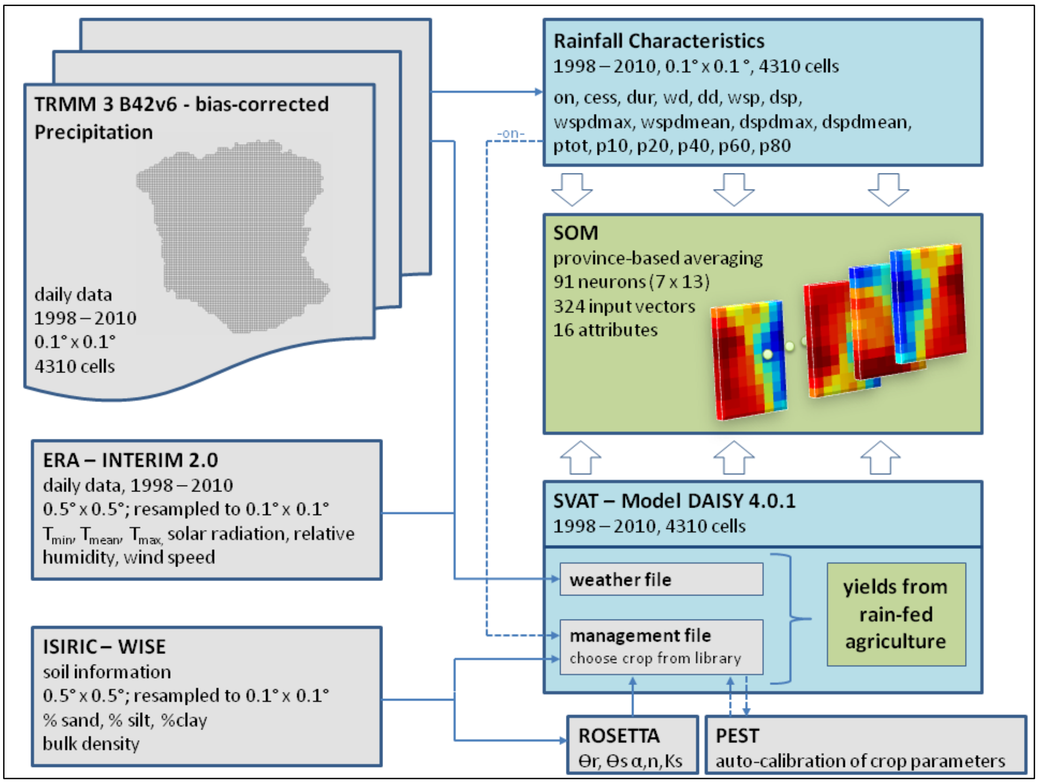


Figure 2.1: Schematic view of the research framework. The left side indicates data sources, on the right applied methodologies are depicted

2.3.1 METEOROLOGICAL, SOIL AND AGRICULTURAL DATA

Bias-corrected TRMM 3B42 v6

TRMM 3B42 v6 is a daily, near-global (50°N to 50°S) satellite-based rainfall estimate provided by NASA uninterruptedly since 01/01/1998. Estimations take advantage of various data sources, by combining calibrated MW-based estimates (TCI, SSM/I and AMSU) with IR-based estimates (Geostationary IR), which are then rescaled using monthly ground observations (CAMS and GPCP). The final product holds a spatial and temporal resolution of 0.25° and 3 h, respectively (Huffman et al., 2010, 2007). For this study, a bias-corrected version of the TRMM 3B42 v6 was used as reference data, since a previous validation study by Thiemig et al. (2012) has shown that TRMM 3B42 tends to underestimate precipitation over the target area (see Fig. 2.2a and b). Therefore, in a post-processing step, the 'histogram equalization" (HE) method – a recent bias correction method used to correct precipitation estimates from climate models (Krajewski and Smith, 1991; Piani et al., 2010) – has been applied to the original TRMM-3B42 data.

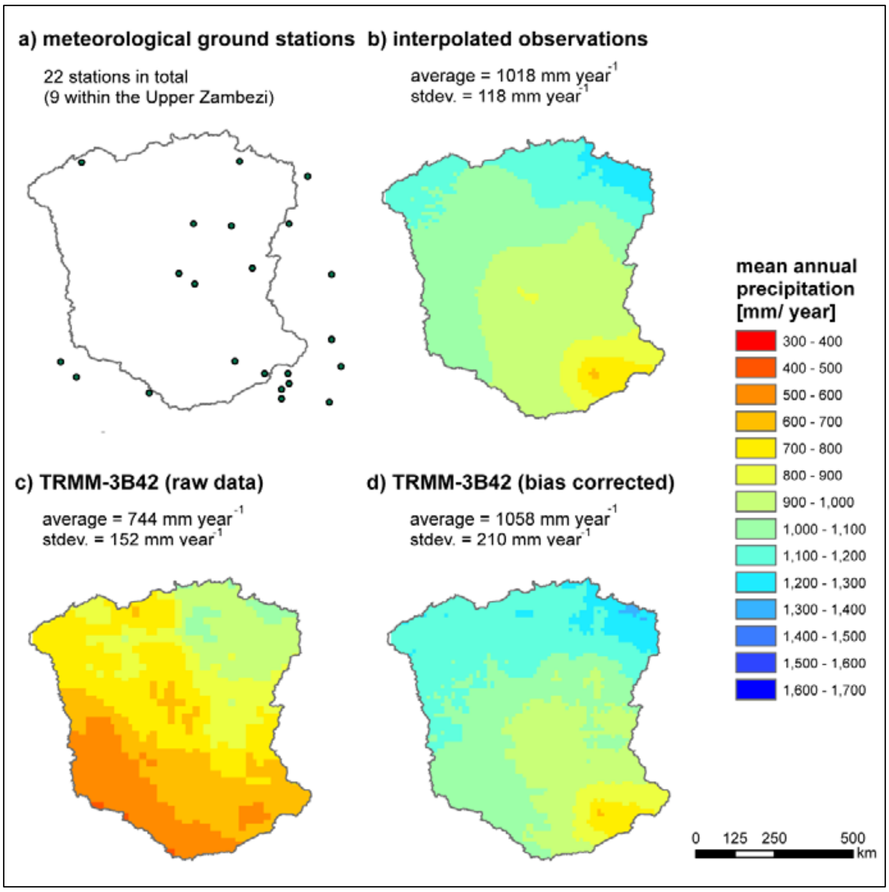


Figure 2.2: Station distribution (a) and mean annual precipitation (1998-2006), supplemented with information about average basin total and average standard deviation for the (b) KED interpolated observations, (c) original TRMM-3B42 and d) the bias-corrected TRMM-3B42

The meteorological ground observation network used as input to create the areal precipitation fields (which were then used as reference for the bias correction) consists of 96 stations, within the Zambezi River Basin, with 77% of the data provided by the Zambia Meteorological Department (Thiemig et al., 2012) and only 23% originating from the WMO GTS stations. Figure 2.2d shows the annual average of the final bias-corrected TRMM-3B42, which resembles the annual average KED-interpolated observations closely and agrees with existing literature (Shahin, 2002).

Raster-based soil data

Besides bias-corrected TRMM 3B42 v6 rainfall, two other datasets were used for this research, i.e. ISIRIC-WISE and ERA-Interim 2.0 (compare Fig. 2.1). Both are freely available online and have been utilized widely in scientific studies (Batjes, 2005).

ISIRIC-WISE global data set of derived soil properties is a harmonized, gridded (0.5°×0.5°) dataset containing soil parameter estimates for the component soil units of each terrestrial grid cell (Batjes, 2005). Each cell of the dataset can contain up to ten soil units that were derived from the analysis of about 9600 soil profiles at the *World Soil Information Centre, Wageningen*. In total, the dataset compiles 22 soil variables for top- (0–30 cm) and subsoil (30–100 cm) enabling, for example, the use for agro-ecological zoning, crop growth simulation or analysis of global environmental change (Batjes, 2005). For the study, information on the contents of sand, silt and clay as well as bulk density was extracted from ISIRIC-WISE. Due to missing data in the subsoil (30–100 cm) and generally marginal differences of top- and subsoil, only one layer (0–100 cm) was defined within the SVAT model DAISY (see section 2.3). Further, the dataset was resampled to obtain the same spatial resolution as the bias-corrected TRMM 3B42 v6 data (0.1°×0.1°).

Other raster-based meteorological data

Meteorological data other than rainfall was obtained from ERA-Interim 2.0 (Dee et al., 2011), a reanalysis of global atmospheric data provided by the *Centre for Medium-Range Forecasts*. It might be argued that mixing of two datasets, TRMM and ERA-Interim, respectively, introduces uncertainty due to the different timing rain events might be captured by the two datasets, which could create inconsistency with the other meteorological parameters. However, this fact had to be accepted because our focus is to apply the best available rainfall estimate; hence either interpolated station data or product had to be chosen. ERA-Interim 2.0 contains a large number of atmospheric variables (>30 parameters), has a spatial resolution of 0.5°×0.5° and is available up to three-hourly time steps. For the purpose of this study, the following variables were extracted on a daily basis:

- minimum, mean and maximum temperature
- solar radiation
- dew point

The setup file within DAISY requires relative humidity data; hence dew point values were converted into relative humidity. Wind speed at 2 metres was not available from ERA-Interim 2.0; therefore a wind speed of 2 m/s (model standard value if no data is available) was assigned in order to avoid involving another different dataset. As for ISIRIC-WISE, the data was resampled to a spatial resolution of 0.1°×0.1° in order to homogenize the spatial resolution with the rainfall data.

Data of measured yields

For calibration and validation of the agricultural model, observed maize yield data for rain-fed agriculture were necessary. Throughout the basin, only two reliable sources were found: i) data for the Eastern Caprivi region located in the southwestern part of the Upper Zambezi River Basin that was extracted from the 'Agricultural Statistics Bulletin 2000-2007" from the *Department of Water Affairs*, *Namibia* (Ministry of Agriculture, Water and Forestry, 2009), and ii) detailed panel survey data for the years 2001, 2004 and 2008 that was provided by the *Agricultural, Food and Resource Economics Department, Michigan State University* (Jayne, 2013).

2.3.2 EVALUATION OF RAINFALL CHARACTERISTICS

Rainfall characteristics were determined on a cell-by-cell basis for each cell and year separately. In particular, each time-series was analyzed and the defined rainfall characteristics were calculated based on the criteria summarized in Table 2.1.

Table 2.1: Definition of criteria for identification rainfall characteristics.

Description	Variable	Criteria for characteristic	References
Onset of rainy season	on	First 10 days > 25mm, no 10 consecutive dry days in next 20 days	Tadross et al.(2007), (Mupangwa et al., 2011))
Cessation of rainy season	cess	3 consecutive decades, each with less than 20 mm (after Feb 1st)	Tadross et al.(2007)
Duration of rainy season	dur	Cessation – onset date	-
Wet day	wd	Rain > 2mm	Tadross et al.(2007)
Dry day	dd	Rain < 2mm	Tadross et al.(2007)
Wet spell	wsp	5 days sum > 10mm and less than 3 days with no rain	Usman and Reason (2004), Reason at al. (2005), *adapted*
Dry spell	dsp	5 days sum < 5mm	Usman and Reason (2004), Tadross et al.(2007)
Max./mean wet/dry spell duration	$dspd_{max}/dspd_{mean}$ $wspd_{max}/wspd_{mean}$	No. of consecutive days with wet/dry spell criteria satisfied	-
Total rain in rainy season	p_{tot}	Rain sum from onset to cessation	-
No. of events above 10/20/40/60/80 mm	$p_{10}/p_{20}/p_{40}/$ p_{60}/p_{80}	Rain > threshold	-

In total, 17 rainfall characteristics were selected for evaluation. This study uses satellite-derived rainfall and station data (i.e., bias-corrected satellite derived data) to combine the high spatial resolution of the former with the more precise point information of the latter dataset. Criteria for the investigated rainfall characteristics were overtaken from existing literature and adopted whenever no general agreement on the criteria for several rainfall characteristics was achieved. For the detection of the onset of the rainy season, for example, the criterion suggested by Tadross et al. (2007) was used: a sum of 25 mm in the first 10 days not followed by 10 or more consecutive dry days in the next 20 days. Through the latter condition, detection of a ‘false” start of the rainy season is avoided (Mupangwa et al., 2011). From the same study, a threshold of 2 mm was selected for the separation of wet and dry days. Other authors use higher (e.g. Mupangwa et al., 2007) or lower (e.g. Camberlin et al., 2009) thresholds. In general, it has to be stated that the selected threshold depends on the purpose of the particular study. If looking at groundwater recharge rates, a rainfall of 1, 2 or even 5 mm might not be considered a wet day because effectively none of this water will reach the groundwater table in a region with a daily pan evaporation of 5 to 8 mm (Woltering, 2005). Since this study is focusing on crop growth, a threshold of 2 mm was considered to be suitable for supplying crops with water (Tadross et al., 2007).

A slight modification is applied to the commonly used *wet spell* criteria: Additionally to a five-day-sum of greater than 10 mm, a condition that three or more days out of these had to experience rainfall is introduced. This modification ensures that a wet spell is not only created by one or two single rain events. Durations for dry and wet spells are determined using a moving window with a length of five days. If the dry/wet spell criterion is fulfilled a duration of five is assigned to this particular spell. As long as this criterion remains satisfied when moving the window, one day is added to the dry/wet spell duration. The mean/maximum dry or wet spell can then be calculated for the rainy season under investigation.

The remaining rainfall characteristics will not be explained in detail here (refer to Table 2.1) since either previous authors are in agreement in regard to these criteria or there is no room for different interpretations.

Analysis of rainfall characteristics is performed for each year separately using the statistic programming software package R (R Core Team, 2013). As a first step, onset and cessation dates are determined and thus the time frame for the rainy season is obtained. Subsequent characteristics are only analyzed within this time frame (referred to as rainy season).

2.3.3 SVAT CALIBRATION AND VALIDATION

Agricultural yields were obtained using the Soil Vegetation Atmosphere Transfer (SVAT) model DAISY (Abrahamsen and Hansen, 2000; Hansen et al., 2012), which has been employed extensively for the simulation of physical and biological processes in agriculture. In the present work the one-dimensional version DAISY 4.01 was applied.

As input, the model requires: (i) a setup file containing information on soils (soil hydraulic parameters), crops (variety, sowing/harvesting dates) and management practices (irrigation, tillage, fertilization); and (ii) a weather file containing meteorological data (precipitation, global radiation and temperature).

Figure 2.1 visualizes how the different sources of input data were utilized within the research framework and which information was necessary for the above mentioned requirements for the DAISY model. Since the methodological approach is based on freely-available raster datasets, input files had to be created for each cell separately. The spatial resolution was chosen according to the resolution of the bias-corrected TRMM 3B42 v6 dataset (0.1°×0.1°); hence a total of 4310 pairs of weather/management files had to be prepared. Creation of these files for each cell was automated using precipitation data from the bias-corrected version of TRMM 3B42 v6, remaining meteorological data from ERA-Interim, the calculated rainfall onset date for each cell and year (defined as sowing date) and soil hydraulic properties, i.e. water retention parameters, saturated hydraulic conductivity and unsaturated hydraulic conductivity (Fig. 2.1). To obtain the latter, the software ROSETTA (Schaap et al., 2001) was applied using sand, silt and clay percentages and bulk density provided by ISIRIC-WISE. Rainfall onset dates were simply taken from the prior analysis of rainfall characteristics.

Since no information on the parameterization for local maize variety was available, the initial simulation was carried out using the standard *maize* from the library within DAISY.

Prior to the explanation of the calibration and validation procedure itself, important assumptions for the modeling approach are summarized as follows:

(1) Simulated yields for each year are calculated with a sowing date equal to the onset date that was calculated before. This implies that the modeled yields are based on an optimum decision of a farmer in terms of when to start sowing. As for other external influences on yields, such as elephants destroying the harvest, flooding, losses induced by pests or socio-economic aspects, which are infeasible to implement in a SVAT model, this introduces a great challenge for calibration of DAISY.

(2) The maize variety calibrated throughout all catchments is traditional maize (*Zea mays*), although in certain parts of SSA also genetically modified varieties are grown.

(3) It is possible that not in all areas modeled maize is actually grown (J. Mendelsohn, personal comment). The current study focuses on the main question ‘How and by what magnitude do different rainfall characteristics affect the successful growth of maize in the UZRB?’ Therefore aspects such as flooding, wetlands or elevation are neglected.

The relevant parameters of the model were calibrated automatically using PEST (Parameter ESTimation, Doherty 2005), a software for parameter estimation and uncertainty analysis that is suitable for automatic calibration for a wide range of models. PEST itself will not be explained here in greater detail; thus the cited literature is suggested for further information. Table 2.2 summarizes the parameters used for calibration in PEST.

Table 2.2: Parameters chosen for calibration of DAISY and their corresponding default and calibrated values for maize.

Module	Parameter	Description (unit)	Default	Calibrated
Devel (phenology and development)	EmrTSum	Soil temp. sum at emergence (°C)	300.0	327.3
	DSRate1	Development in vegetative stage (d^{-1})	0.024	0.015
	DSRate2	Development in reproductive stage (d^{-1})	0.015	0.010
Leaf_phot (photosynthesis module)	Fm	Maximum assimilation rate (g CO_2 × $(m^2\ h)^{-1}$)	6.0	3.5
	Qeff	Quantum efficiency at low light ((g CO_2 × $(m^2\ h)^{-1}$)/(W × m^{-2}))	0.040	0.055
Canopy (canopy info)	DSLAI05	Development stage at crop area index = 0.5 (-)	0.250	0.251
	SpLAI	Specific leaf weight ((m^2 × m^{-2})/(g DM × m^{-2}))	0.0100	0.0083
	PARext	Photosynthetic active radiation extinction coefficient (-)	0.800	0.852
Root (root system)	maxPen	Penetration at emergence (cm)	120	95
Water_stress (effect of water stress)	y_half	Effect of water stress (-)	0.200	0.001

In Table 2.2, the parameters of the main sub modules of the vegetation module are represented (for details refer to Abrahamsen and Hansen, 2000). These have been proven suitable as calibration parameters in related studies (Hansen et al., 2012; Seidel, 2012). Especially the inclusion of the parameter *WSE*, an optional component regulating the effect of water stress on the crop was seen as crucial, since an effect of water stress on the maize growth was expected in this semi-arid climate. Five out of the eight years with available data on measured yields from the Caprivi region were selected as calibration parameters, whereas the remaining data comprised basis for validation.

2.3.4 Investigation of relationships between rainfall characteristics and modeled agricultural yields

For univariate analysis, simple regression was used. On the other hand, multivariate relationships between yields and rainfall characteristics were investigated by applying a Self – Organizing map (*SOM*) approach.

The SOM method is an unsupervised artificial neural network developed by Teuvo Kohonen (1982). In brief the algorithm projects high dimensional input data into a lower, generally two-dimensional, output lattice (for details refer to Kohonen 1982, Kohonen 1990 and Wallner et al., 2013). Input data with similar characteristics are grouped in neighboring regions of this output space. This output space is arranged in a hexagonal structure, as depicted in Figure 2.3.

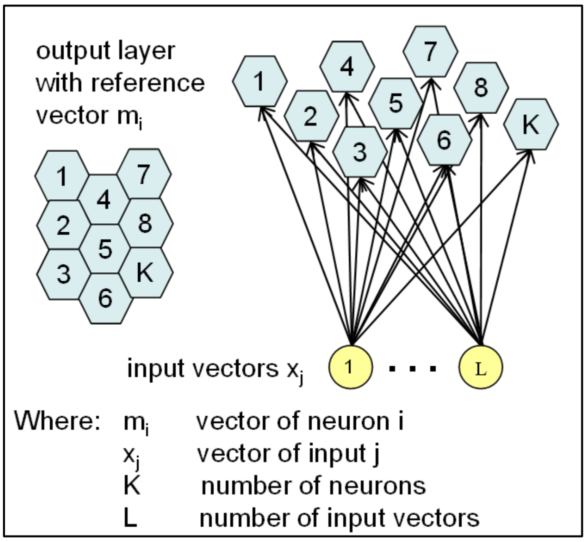


Figure 2.3: Structure of a Self-Organizing Map (Wallner et al., 2013)

The main advantage of *SOM* is the ability to provide a user-friendly representation of large, multi-dimensional datasets; hence, similarities and relationships can directly be derived by interpreting the two-dimensional output space and the associated component planes.

In the present research, the trained *SOM* is visualized in three different ways:

(1) component planes, illustrating the distribution of the particular variables on the map;

(2) the unified distance matrix (U-matrix) showing the neuron population based on the input dataset and distances between neighboring neurons (Rivera et al., 2011), and

(3) k-mean-clustered U-matrix dividing the input into six groups (based on the identifier ‘yield” from marginal to very high).

The size of the *SOM* is mainly set based on the character of its input data. According to López García and Machón González (2004), the number of output neurons is equal to five times the square root of the input data. This is implemented and automated within the SOM toolbox in MATLAB (Kohonen, 1995; Vesanto et al., 2000). For the purpose of this research, the algorithm generated a *SOM* with 91 neurons (7×13) after external averaging of yields and rainfall characteristics for each of the regions within the study area.

2.4 STUDY AREA

With a total area of 1.37 million km² the Zambezi River Basin is the fourth largest river basin in Africa and the largest in the Southern African Development Community (WorldBank, 2010; Thiemig et al. 2013) . Its location is in Southern Africa between 9°-20° S and 18°-36° E. The basin is shared by 8 countries (Angola, Zambia, Namibia, Botswana, Zimbabwe, Malawi, Tanzania, Mozambique) and hence has a highly transboundary importance in regard to water resource management not only because of the different contributions of these sub basins to the overall runoff of the Zambezi River but also because of the very high variability of climate in space and time and major differences in sub basin characteristics. The Upper Zambezi River Basin, on which this research focuses, compromises the basin upstream of Victoria Falls (Fig. 2.4) and has a total size of 514.000 km² (WorldBank, 2010).

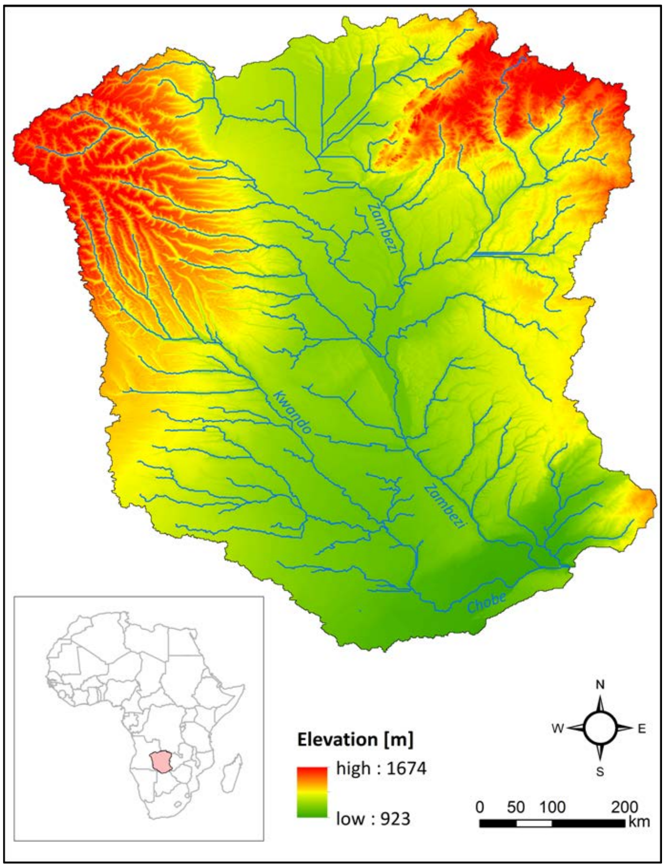


Figure 2.4: The Upper Zambezi River Basin (UZRB)

Annual rainfall varies between 500 mm in the southern part of the catchment to up to 1400 mm in the northern Zambian and Angolan regions (MacDonald, 2007). The rainy season shows a very high seasonal, inter-annual and decadal variability, which implies a challenge for water resources management (Conway et al., 2009; Goulden et al., 2009; New et al., 2006; Tyson et al., 1975). In the past extended drought and flood periods affected the whole basin: the years 1907-1945 are characterized as a dry period, whereas 1946-1964 showed an above normal runoff behavior with extensive flooding (WorldBank, 2010). From 1981-1997 the basin experienced a severe drought period that caused the drying up of wetlands, floodplains (which are usually flooded yearly). Since 1998 up to now, major extended flooding has occurred indicating the presence of a novel wet period. For agricultural outputs and livestock production, rainfall reliability is the over-riding issue. In the Upper Zambezi Basin, there is almost no irrigated agriculture developed yet, which stresses the dependence on rainfall even more.

Temperature across the basin varies highly with elevation (ranging between 800 m in the southern parts to 1500 m in northern Zambia) even though there are slight differences between different latitudes as well (MacDonald, 2007). Finally, from a geological perspective, Kalahari sands (deposited and non-deposited) are present throughout the whole basin (WorldBank, 2010). It is believed that in most areas these are underlain by Basalt stone (BGR, 2005).

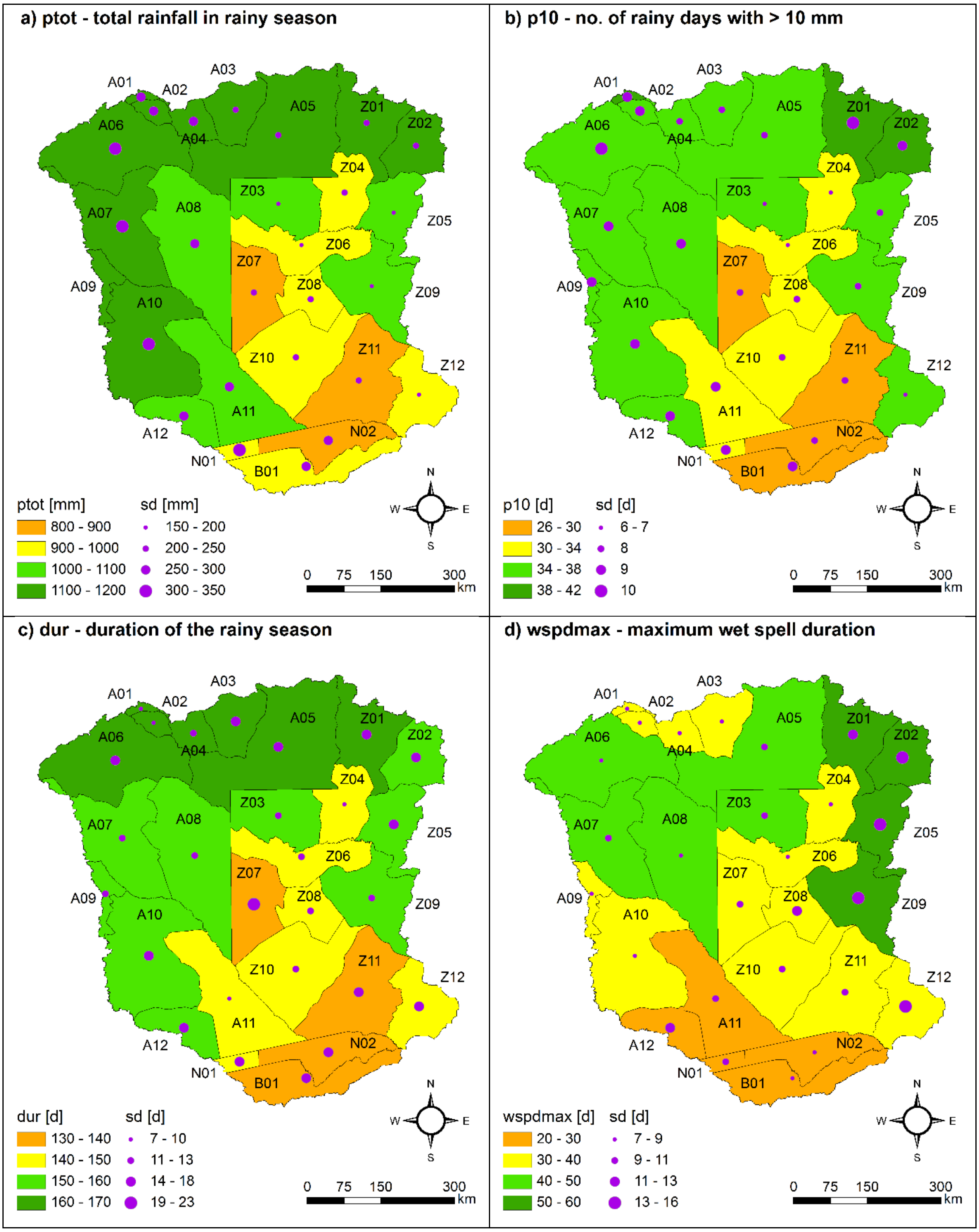
2.5 RESULTS

2.5.1 RAINFALL CHARACTERIZATION

Statistics of the rainfall characteristics are presented here in two ways: first, as mean maps for administrative regions over the whole period of investigation and second, for each year and cell separately. Local decisions in SSA are often made based on the administrative region or even smaller units; a presentation in this way therefore makes great sense. The second way of analyses is more suitable for an in-depth analysis of regional patterns or distinctive features of a particular rainy season. The taxonomy used in the interpretation of results is ordered as a letter representing the country one region belongs to (A – Angola, B – Botswana, N – Namibia and Z – Zambia) followed by a region identifier.

a) Mean over regions

As shown in Figure 2.5, most rainfall characteristics reveal a northwest to southeast gradient. Rainy season totals are the highest in Angola and the north of Zambia (see Fig. 2.5a). However, the western Angolan part of the catchment is also the one with the greatest variability. The northern areas of Angola and Zambia (A03 – Lucano; A05 – Alto Zambeze; Z01 – Mwinilunga and Z02 – Solwezi) are the most stable by means of total rainfall with high annual amounts and low variability. The central part of the UZRB, on the other hand, displays less favorable conditions. Along the flat plains of Barotse, the Namibian parts of the basin and also Botswana, total rains are notably lower whilst the variability continues to increases the further one looks towards the south. Despite of this, mean rain amounts from the detected onset to cessation would allow a successful cultivation of maize throughout the basin (according to FAO, maize needs 500 to 800 mm of water depending on the climate; http://www.fao.org/nr/water/cropinfo_maize.html). However, the high coefficients of variation (*cv*) of up to 0.4 (i.e. administrative region N01) and the fact that the recent period has been particularly wet should be noted. Nevertheless, looking at rainfall totals throughout the rainy season alone does not explain the low yields in most parts of the catchment. Maize is described as sensitive to water logging and in the flowering and yield formation period also prone to water stress (FAO, http://www.fao.org/nr/water/cropinfo_maize.html); thus, the intraseasonal distribution of rainfall is a crucial aspect and focused subsequently.


a) ptot - total rainfall in rainy season
ptot [mm]
800 - 900
900 - 1000
1000 - 1100
1100 - 1200
sd [mm]
150 - 200
200 - 250
250 - 300
300 - 350
b) p10 - no. of rainy days with > 10 mm
p10 [d]
26 - 30
30 - 34
34 - 38
38 - 42
sd [d]
6 - 7
8
9
10
c) dur - duration of the rainy season
dur [d]
130 - 140
140 - 150
150 - 160
160 - 170
sd [d]
7 - 10
11 - 13
14 - 18
19 - 23
d) wspdmax - maximum wet spell duration
wspdmax [d]
20 - 30
30 - 40
40 - 50
50 - 60
sd [d]
7 - 9
9 - 11
11 - 13
13 - 16
A01
A02
A03
A04
A05
A06
A07
A08
A09
A10
A11
A12
Z01
Z02
Z03
Z04
Z05
Z06
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0
75
150
300
km

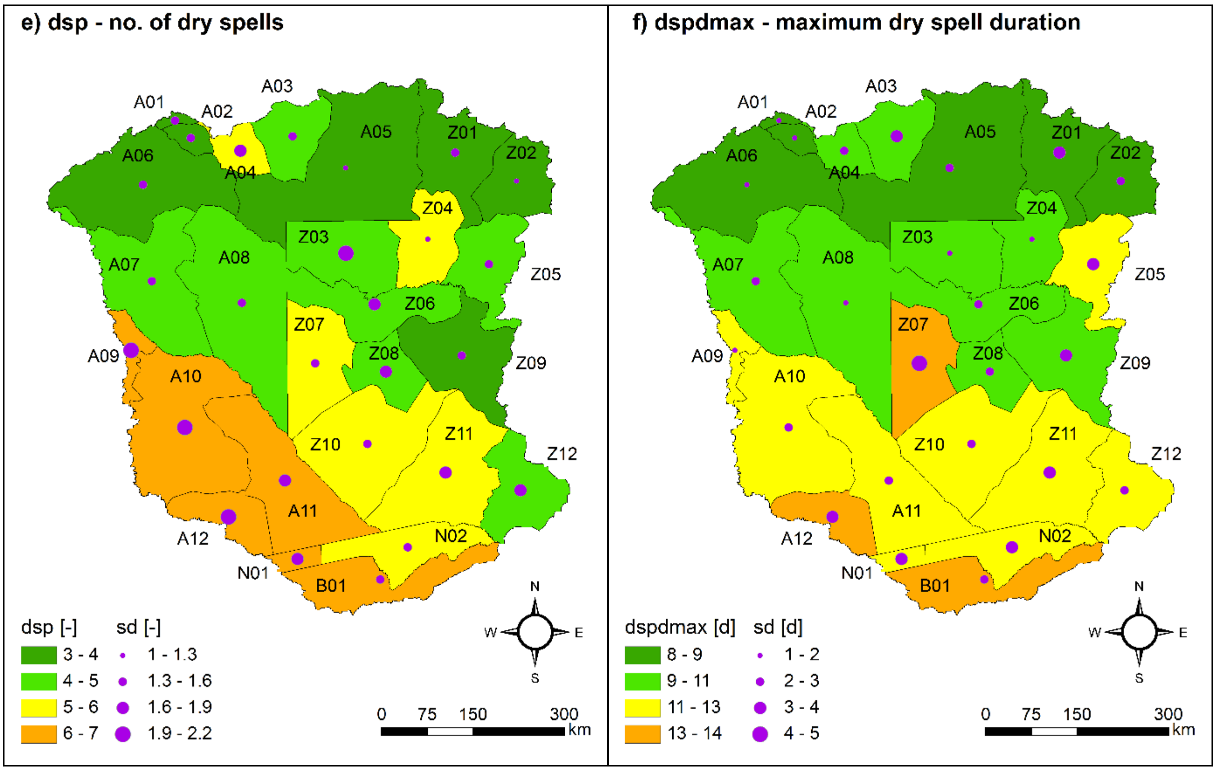

Figure 2.5: Mean and standard deviation of selected rainfall characteristics averaged over administrative regions for the years 1998 – 2010; (a) p_{tot} – total rainfall in rainy season, (b) p_{10} – no. of rainy days with >10mm, (c) dur – duration of the rainy season, (d) wspd$_{max}$ – maximum wet spell duration, (e) dsp – no. of dry spells, dspd$_{max}$ – maximum dry spell duration

The regional pattern of the number of days with more than 10 mm accumulated rainfall (p_{10}; Fig. 2.5b) and duration (*dur*; Fig. 2.5c) of the rainy season appears quite similar to that of total rainfall (p_{tot}). The former characteristic is commonly referred to as 'productive rainfall' and therefore of great importance for plant growth (Mendelsohn et al. 2013). As for p_{tot}, the northern and western parts of the catchment experience a mean of at least 34 days with more than 10 mm and duration of at least 150 days. These are the highest means throughout the basin. However, variability is considerable even in these areas (Fig.2.5 a-c). The central region displays a pattern similar to that of p_{tot} – shorter duration of the rainy season and a lower number of p_{10} compared to the north and northwest. The southernmost parts of the basin (N01, N02 and B01) as well as parts of Zambia (Z07 and Z11) show the least favorable conditions with short growing seasons and numbers of productive rains. At the same time, the variability in these areas is the highest for all rainfall indices.

Characteristics related to the consistency of the rainy season (i.e. number and length of wet and dry spells), as shown in Fig. 2.5d to f, display different spatial patterns. A clear north – south gradient is apparent dividing the catchment in two, nearly equal-sized portions with exception of the regions A01 to A04. The northern part of the basin is characterized by a high number of wet spells (*wsp*) and long maximum wet spell durations ($wspd_{max}$; Table 2.3 and Fig. 2.5d). This implies more favorable conditions for rain-fed crops than in southern part, where the opposite is the case. At the same time, however, the regions with a very high $wspd_{max}$ are most likely those where the big flooding such as in 2009, 2010 and 2011 were created. An interesting pattern is revealed if one looks at the variability of $wspd_{max}$: whereas the northern Angolan areas are more consistent, variability of this particular characteristic is very high (*sd* of 13-16 days) in northeastern Zambia. These particular areas (Z01, Z02, Z05, Z09) in the head-catchments of the Zambezi River might have a major impact on the magnitude and frequency of flooding downstream (i.e. in Caprivi). In terms of rain-fed agriculture, the long wet spells in the north could also be harmful for those crops being sensitive to water logging. In regard to dry spell characteristics (*dsp* and $dspd_{max}$; Fig. 2.5e and 5f), the northern half of the UZRB is less prone to droughts within the rainy season. A dry spell duration of 10 days, as identified even in the most consistent regions could still be sufficient to cause significant losses of harvest. In the south of the catchment, preconditions for rain-fed agriculture appear to be less favorable (Table 2.3 and Fig. 2.5d to e). As for the previously discussed indicators, a 'dry corridor' in the central part of the UZRB is clearly visible. Additionally to the Namibian, Botswanan and southern Zambian provinces, also parts of Angola (A10 to A12) experience short (<40 days) maximum wet spells, a high number (>5 per rainy season) of dry spells and a long maximum dry spell duration (>11 days) based on average numbers. Most of these areas display a high variability at the same time, making them the most vulnerable for rain-fed farming.

Table 2.3: Mean values and standard deviations (1998-2010) of selected rainfall characteristics averaged over administrative regions.

ID	Region	on	cess	p_{tot}	p_{10}	p_{40}	dsp	$dspd_{max}$	wsp	$wspd_{max}$
A01	Camanongue	297 ± 12	96 ± 9	1156 ± 277	38 ± 9	3 ± 3	4 ± 1	8 ± 1	10 ± 3	39 ± 9
A02	Leua	297 ± 10	94 ± 9	1131 ± 286	36 ± 9	3 ± 3	4 ± 2	8 ± 2	11 ± 2	38 ± 8
A03	Lucano	295 ± 10	91 ± 14	1103 ± 231	35 ± 7	4 ± 2	5 ± 2	10 ± 3	12 ± 2	37 ± 8
A04	Cameia	295 ± 10	92 ± 11	1129 ± 254	35 ± 7	5 ± 3	5 ± 2	11 ± 3	12 ± 2	36 ± 8
A05	A. Zambeze	297 ± 9	91 ± 16	1103 ± 225	37 ± 8	3 ± 1	4 ± 1	9 ± 2	10 ± 1	47 ± 10
A06	Moxico	298 ± 10	93 ± 11	1139 ± 305	37 ± 10	3 ± 2	4 ± 1	8 ± 2	9 ± 2	44 ± 8
A07	Luchazes	299 ± 9	93 ± 10	1117 ± 305	36 ± 9	3 ± 3	5 ± 2	10 ± 2	9 ± 2	43 ± 10
A08	Lumb. Ng.	302 ± 6	90 ± 11	1038 ± 268	34 ± 9	3 ± 2	5 ± 1	10 ± 2	10 ± 1	40 ± 8
A09	Cuito Cuan.	301 ± 10	93 ± 11	1155 ± 389	36 ± 9	4 ± 4	6 ± 2	11 ± 2	10 ± 2	36 ± 8
A10	Mavinga	303 ± 7	90 ± 12	1102 ± 317	36 ± 9	4 ± 3	6 ± 2	12 ± 3	10 ± 2	33 ± 9
A11	Rivungo	307 ± 7	87 ± 10	1016 ± 293	33 ± 9	4 ± 3	6 ± 2	12 ± 2	10 ± 2	30 ± 9
A12	Dirico	305 ± 8	91 ± 14	1063 ± 290	34 ± 9	4 ± 3	7 ± 2	14 ± 3	11 ± 2	29 ± 12
B01	Botswana	311 ± 8	83 ± 17	911 ± 280	29 ± 9	4 ± 2	7 ± 1	13 ± 3	10 ± 2	25 ± 7
N01	Kavango	309 ± 11	88 ± 19	981 ± 302	31 ± 9	5 ± 3	7 ± 2	12 ± 3	10 ± 3	26 ± 10
N02	Caprivi	312 ± 8	77 ± 18	808 ± 256	27 ± 8	3 ± 2	6 ± 1	13 ± 3	9 ± 1	27 ± 8
Z01	Mwinilunga	298 ± 12	92 ± 14	1146 ± 234	40 ± 10	2 ± 1	3 ± 1	8 ± 3	8 ± 2	56 ± 12
Z02	Solwezi	301 ± 9	92 ± 10	1199 ± 238	41 ± 9	3 ± 2	3 ± 1	9 ± 3	7 ± 2	60 ± 15
Z03	Zambezi	301 ± 9	87 ± 10	1051 ± 191	35 ± 6	3 ± 2	4 ± 2	10 ± 2	10 ± 2	41 ± 10
Z04	Kabompo	308 ± 7	87 ± 5	1049 ± 198	36 ± 8	2 ± 1	4 ± 2	10 ± 3	8 ± 2	52 ± 15
Z05	Mufumbwe	305 ± 9	93 ± 7	1070 ± 191	37 ± 8	3 ± 1	4 ± 1	11 ± 3	8 ± 2	51 ± 16
Z06	Lukulu	306 ± 6	88 ± 7	994 ± 177	33 ± 6	3 ± 1	5 ± 2	10 ± 3	10 ± 1	39 ± 9
Z07	Kalabo	308 ± 11	77 ± 19	953 ± 237	31 ± 7	3 ± 2	5 ± 1	10 ± 2	10 ± 1	35 ± 7
Z08	Mongu	307 ± 7	86 ± 7	976 ± 233	33 ± 8	3 ± 2	5 ± 2	10 ± 2	9 ± 2	39 ± 12
Z09	Kaoma	304 ± 7	92 ± 7	992 ± 185	34 ± 7	3 ± 1	5 ± 2	11 ± 3	9 ± 2	40 ± 14
Z10	Senanga	308 ± 8	87 ± 8	967 ± 240	32 ± 8	3 ± 2	5 ± 2	11 ± 3	9 ± 2	34 ± 10
Z11	Sesheke	308 ± 7	80 ± 14	856 ± 223	29 ± 8	2 ± 1	5 ± 2	12 ± 3	9 ± 2	33 ± 10
Z12	Kalomo	307 ± 11	88 ± 8	807 ± 245	27 ± 8	2 ± 2	5 ± 1	13 ± 5	9 ± 2	32 ± 11
UZRB		303 ± 9	89 ± 11	1037 ± 254	34 ± 8	3 ± 2	5 ± 2	11 ± 3	10 ± 2	39 ± 10

b) Region-specific analysis

For a detailed analysis of a particular year or region, the annual maps of the rainfall onset dates (*on*), number of rainy days above 20 mm (p_{20}) and maximum wet spell duration ($wspd_{max}$) for an average (2001/02), dry (2004/05) and wet (2007/08) rainy season were chosen for in-depth analysis (Fig. 2.6). The statements from the analysis of regional means might be true for characterizing the average behavior over one region; however, all characteristics vary greatly in both time and space if investigating on smaller scales. It becomes clear that variability is the overriding issue within most areas of the basin. The rainy season 2001/02 (average by means of total rainfall), for instance, displays a homogeneous pattern of the onset of rains over the whole UZRB, whereas in 2004/05 (dry) and 2007/08 (wet) the spatial distribution is highly heterogeneous (Fig. 2.6a). Similarly, the difference of p_{20} in time and space is enormous (Fig. 2.6b). In 2001/02, major disparity between northern and southern parts of the catchment is visible. In contrast the spatial pattern in 2004/05 and 2007/08 is more or less consistent, but the amount of p_{20} differs significantly. The pattern of $wspd_{max}$ (Fig. 2.6c) reveals a gradient from east to west in this characteristic rather than from north to south, as it is the case for most other indices. The illustration (Fig. 2.6) points out how challenging agricultural planning is for local farmers. An early onset of the rains does not necessarily coincide with a good rainy season by means of total rainfall. This stresses the importance of a prediction system for rainy season onset and related characteristics within the UZRB.

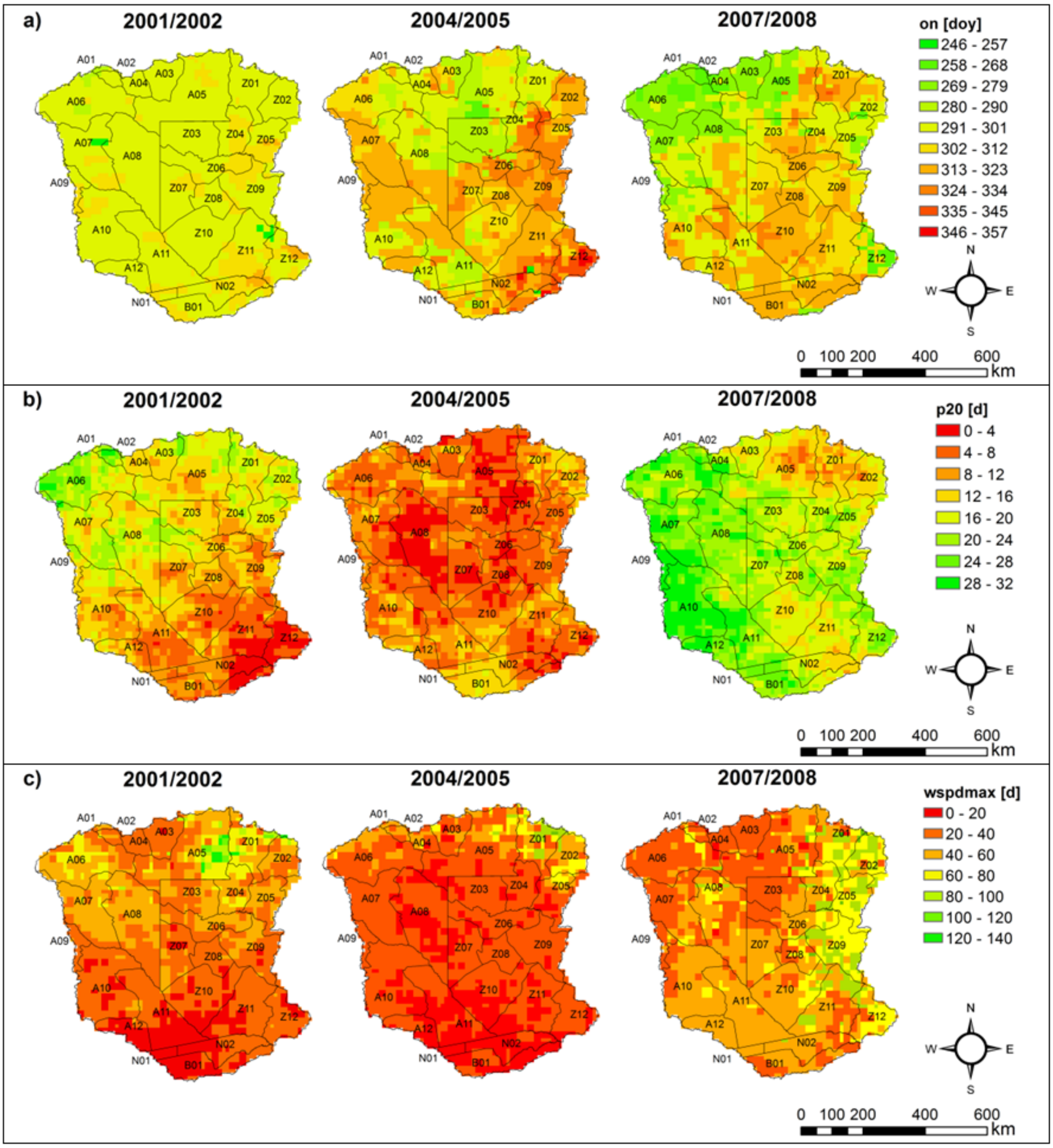

Figure 2.6: Detailed maps of (a) rainfall onset, (b) number of rainy days with more than 20mm and (c) maximum wet spell duration for the rainy seasons 2001/02 (P_{total} = 1009mm), 2004/05 (P_{total} = 718mm) and 2007/08 (P_{total} = 1388mm)

2.5.2 SPATIOTEMPORAL ANALYSIS OF YIELDS

The scatter-plot in Figure 2.7 shows the results for calibration and validation of DAISY.

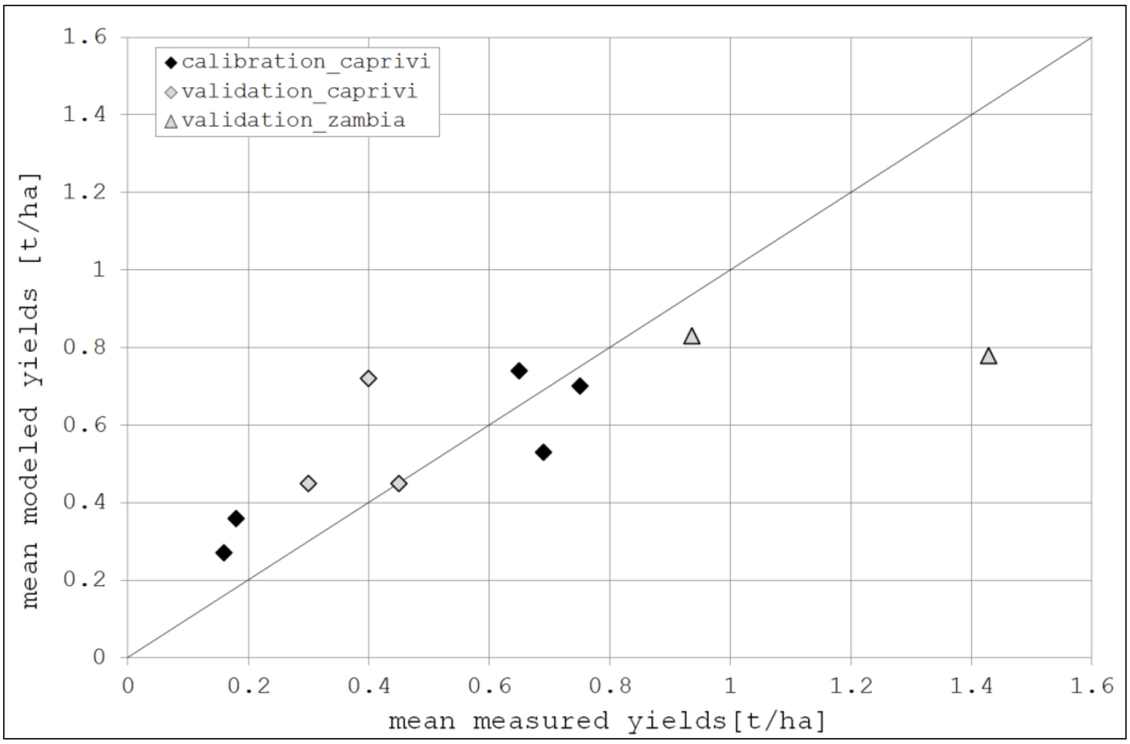

Figure 2.7: Mean measured vs. modeled maize yields

With exception of one year (2008), modeled yields are generally in agreement with the measured. Considering uncertainty introduced by the remotely sensed information that was used, calibration results are satisfactory. A higher availability of data for calibration and validation perhaps could have improved the results. The model was calibrated mostly in a region with generally low yields (compare Fig. 2.8). In order to calibrate these low yielding years (i.e. the rainy seasons of 2002 and 2003), the automated calibration resulted in a combination of parameters reacting very sensitive to dryness. This might have caused the low modeled yields over certain regions of Zambia, particularly in 2008. Due to these facts, uncertainty in the results has to be considered and is acknowledged here explicitly. By means of suitability for simulation of plant-growth in semi-arid areas, DAISY showed a good performance. Induced losses through drought stress were captured by the model accurately and growth of maize as well as harvesting dates was reproduced realistically.

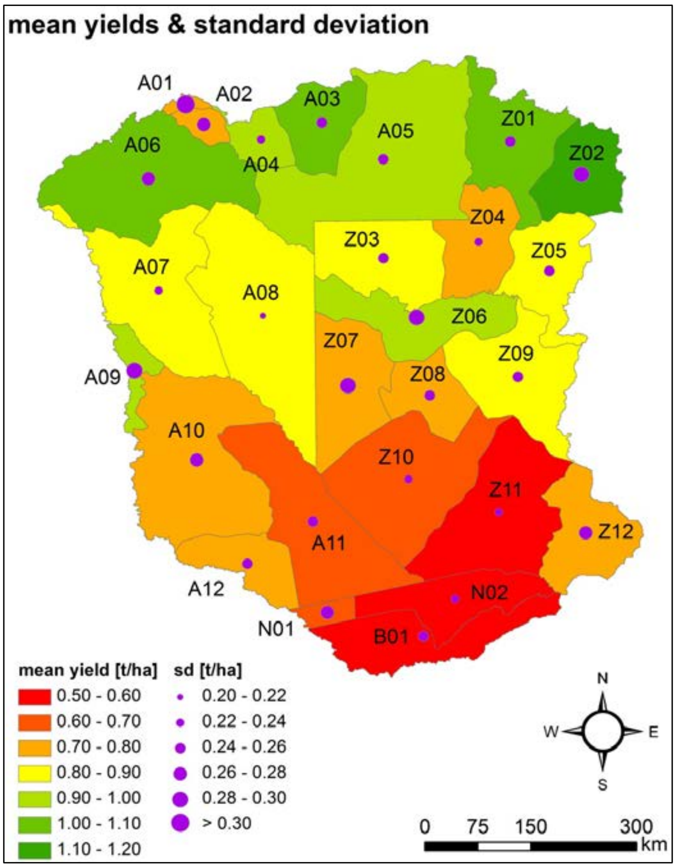

Figure 2.8: Mean and standard deviation of modeled yields for the studied regions for the period 1998 – 2010

Generally, yields throughout the UZRB are very low and variability is extremely high. Mean modeled yields over the basin, as depicted in Fig. 8, reveal a clearly decreasing gradient from north to south, which is in coincidence with the pattern for many rainfall characteristics. The area with the highest yields is Solwezi (Z02) in the northeastern border of the UZRB reaching mean yields of 1.1 to 1.2 t/ha. Analysis of rainfall characteristics shows that Solwezi is the region with the highest mean rainfall during the rainy season (p_{tot}), highest 'productive' rain events (p_{10}), least dry spells (*dsp*) and the longest maximum wet spell durations ($wspd_{max}$). However, variability in this region is notable with a standard deviation greater than 0.3 t/ha and; thus, a *cv* of slightly above 0.25. Lowest harvests, on the other hand, were modeled for regions B01 (Botswana), N02 (Caprivi) and Z11 (Sesheke), with mean yields not exceeding 0.6 t/ha. Absolute variability in these areas (Fig. 2.8) is low, but taking into account *cv*, variability is in ranges up to 0.5 (i.e. region B01). B01, N02 and Z11 can thus be categorized as the most vulnerable regions; hence, these are least suitable for rain-fed agriculture. Often, high *sd* and *cv* of harvests are related to a high degree of variability in one or more of the rainfall characteristics. For example, Z12 (Kalomo) has the most unreliable rainy season by means of the characteristic *dur* with a mean of 135 days and a standard deviation of 23 days which might cause the high *cv* of 0.38 for modeled yields. Clearly sticking out are also two small areas in the north of Angola, A01 (Camanongue) and A02 (Leua). Surrounded by regions with relatively high yields, mean harvests in these are significantly lower. Analyzing the rainfall characteristics, it becomes obvious that in A01 and A02 the *dd* (number of dry days) is very high; at the same time, the mean dsp (number of dry spells) is low. This indicates that rains in both regions are more erratic, i.e. wet and dry days alternate extensively affecting yields negatively. Most stable yields are obtained in the northern part of the catchment. A04 (Cameia), A07 (Luchazes) and Z01 (Mwinilunga) achieve the lowest coefficients of variation with less than 0.25.

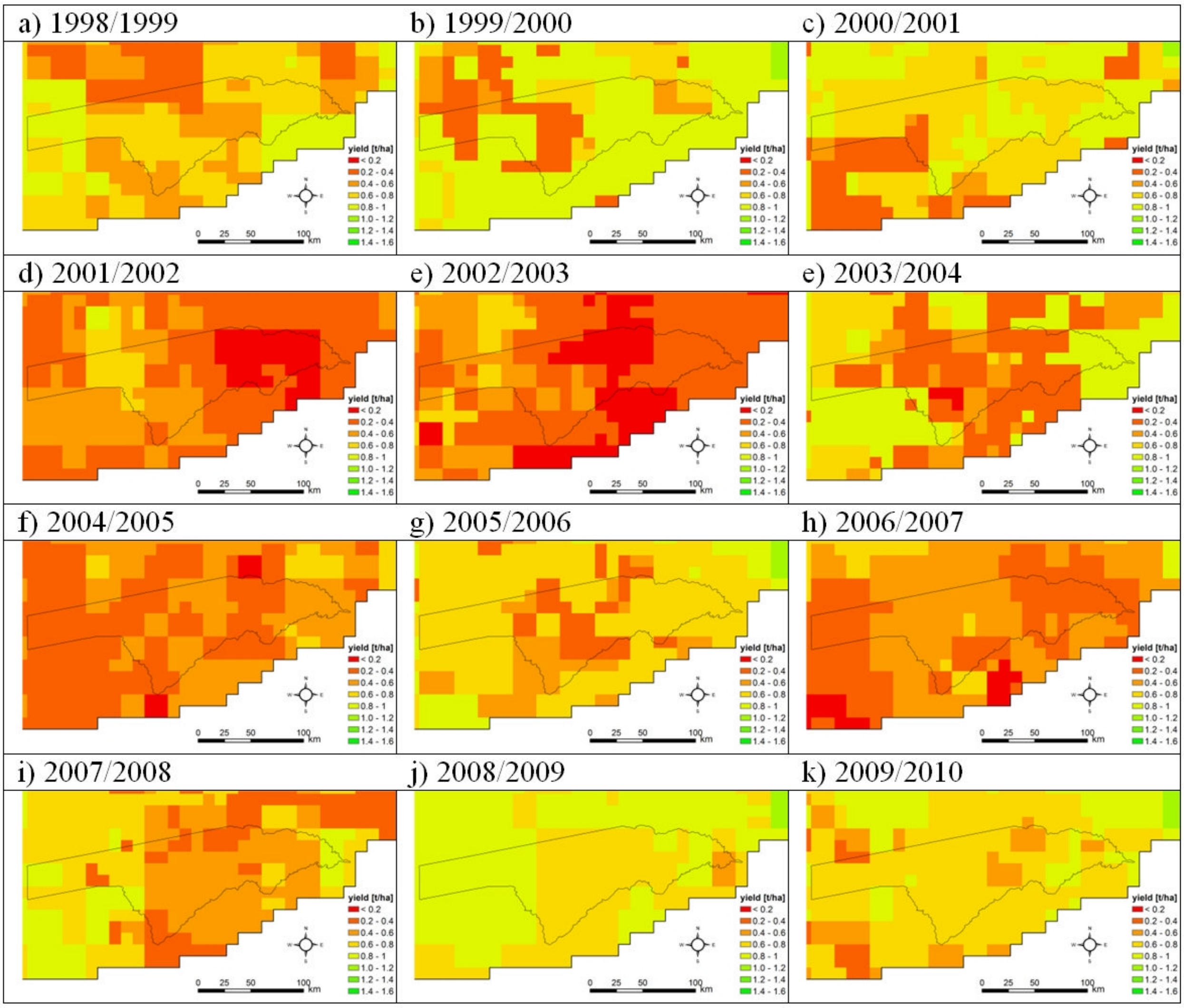

Figure 2.9: Distribution of modeled yields for the years 1998-2010 over the Caprivi region (N02)

In Fig. 2.9, a detailed map for the N02 (Caprivi) over the study period is shown. Here, the interplay between rainfall, flooding and agriculture is particularly complex and challenges are vast. Both the Zambezi and Chobe Rivers can leave up to one third of the Caprivi flooded bringing both a blessing (fishing and recession agriculture) and a curse (destructive character of floods) to the region, depending on the rainfall characteristics in their head catchments . Furthermore, the elephant density here is significant, creating an additional problem for farmers. As revealed by the image, even in ‘good’ years the maize yield does not exceed 1 t/ha. In recent years, yields were slightly higher due to a series of ‘good’ rainy seasons. However, both spatial and temporal variability is great and needs to be considered additionally. No temporal trends or spatial consistencies can be identified which leads to the conclusion that both rainfall characteristics and yields can be considered as somewhat random. Increased climatic variability (Christensen et al., 2007) is very likely to worsen this issue. In Mendelsohn and Roberts (1997), soils in the Caprivi are defined as ‘moderately to good”. However, if not considering additional factors such as the ones mentioned above, this could lead to wrong decision-making. The results further reveal the controversy that in a region with generally high availability of water people are not able to cultivate their crops successfully. It is in these areas, where adaptation and improvement is achievable with relatively low cost (i.e. rain/flood water harvesting, channel systems).

2.5.3 UNIVARIATE ANALYSIS OF YIELDS VS. RAINFALL CHARACTERISTICS

The univariate analysis was carried out in order to identify single rainfall characteristics affecting yields most, without taking into account interactions with others. For the regression analysis, mean modeled yields over each administrative region for the whole period of investigation were plotted against all characteristics. In a previous attempt (not shown here), all 4310 cells were used; however, the scattering did not result in any significant correlation due to the high amount of single outliers (i.e. data errors in the TRMM data for single cells) or local anomalies. In Figure 2.10, a scatter plot of selected rainfall characteristics is illustrated. For further validation of modeled yields, the analysis was also conducted using measured data from the regions where data was available. These results, together with the correlation coefficients of rainfall characteristics, are summarized in Table 2.4.

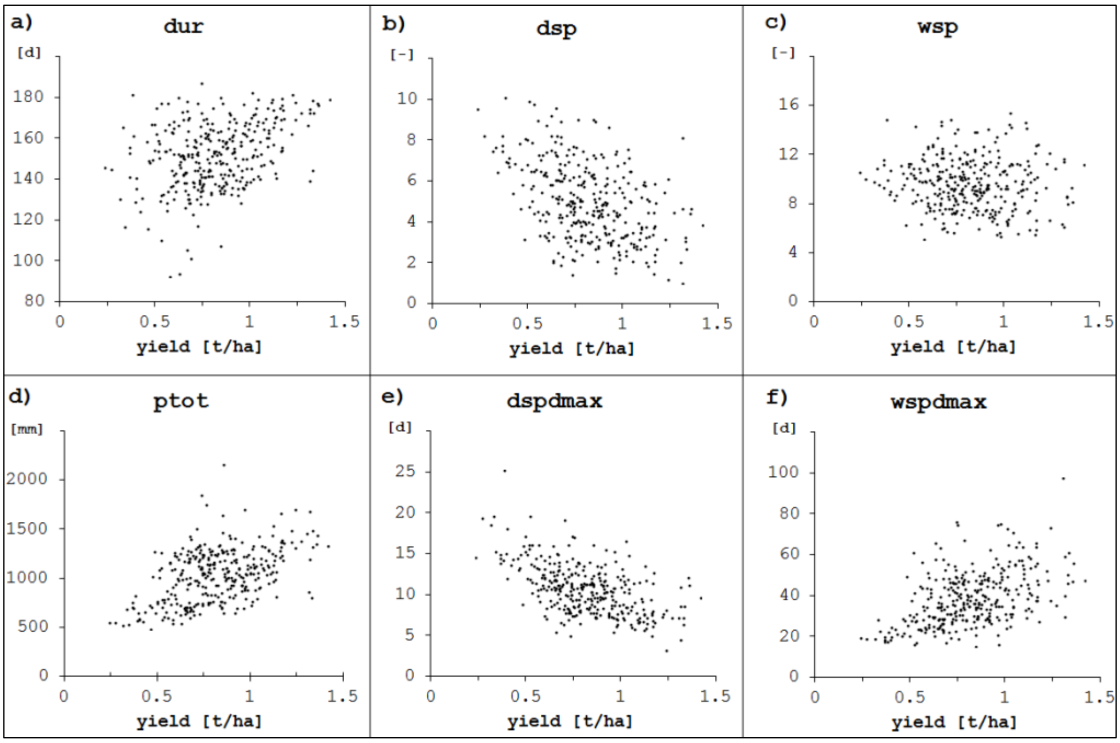

Figure 2.10: Scatter plots of selected rainfall characteristics vs. yield

In Figure 2.10 it is clearly visible that the three indicators in the lower part of the graphic (p_{tot}, $dspd_{max}$ and $wspd_{max}$) are less spread; therefore, these have a higher impact on yields than the ones in the upper part (*dur*, *dsp* and *wsp*). In general, characteristics describing ‘duration’ show higher correlation than those describing ‘frequency’. The highest correlation of modeled yields are with $dspd_{max}$ / $dspd_{mean}$ (-0.56), p_{10} (0.51), $wspd_{max}$ / $wspd_{mean}$ and p_{tot} (0.48 for all three). Nevertheless, no investigated relationship between the criteria and yield reached a correlation coefficient greater than 0.8; hence, these results indicate that any unique characteristic can potentially be used as a predictor for the outcomes of rain-fed agriculture. It further strengthens the statement that the total rainfall amounts per rainy season do not determine the success of rain-fed farming, but interplay of several indicators. Unexpected, but easily explained can be the high correlation for dry days (0.36): characteristic *dd* is strongly related with *dur;* for this reason, a longer rainy season automatically means more dry and wet days, spells and total rainfall. Unlike dry spells, single dry days seem to have no negative effect on yields. Characteristics as *wd*, *wsp* and extreme events (p_{40}, p_{60} and p_{80}) show no strong interconnection with yields. Especially the low, even negative correlations for *wd* and *wsp* are surprising. If one compares the correlations of wet days (-0.01) and the number of rainy days above 10 mm (0.51), it becomes obvious that the selected threshold of 2 mm for a wet day is not sufficient in relation to agricultural yields. This result strengthens the assumption of defining rainy days above 10 mm as ‘productive rainfall events’ (Mendelsohn et al., 2013). However, it might be interesting to investigate this criterion further, since it is possible that a strong correlation appears by using 4, 6 or 8 mm as threshold. The low relationship of *wsp* indicates that not the number of wet spells, but rather their duration has a strong impact. For the extreme events, a rather negative impact on yields would be expected if their number increases. However, this is not the case indicating either there is no significant effect or that the model does not react to it.

Table 2.4: Comparison of measured and simulated yields for calibration and validation of DAISY.

Rainfall characteristic	rxy modeled	rxy measured
p_{tot}	0.48	0.64
dur	0.36	0.57
wd	-0.01	0.14
dd	0.34	0.56
dsp	-0.45	-0.44
$dspd_{max}$	-0.56	-0.16
$dspd_{mean}$	-0.56	-0.08
wsp	-0.08	-0.07
$wspd_{max}$	0.48	0.54
$wspd_{mean}$	0.48	0.50
p_{10}	0.51	0.66
p_{20}	0.33	0.61
p_{40}	0.20	0.39
p_{60}	0.15	0.17
p_{80}	0.13	0.08

The comparison of rainfall characteristics with measured yields resulted in similar findings for most indicators (Table 2.4). Whereas correlations of the 'wet' characteristics with yield show similar magnitudes, stronger connections to agricultural outputs are found for p_{tot}, p_{10}, p_{20}, p_{40}, *dur* and *dd*. Major differences between modeled and measured correlations with harvest are encountered in $dspd_{max}$ / $dspd_{mean}$. Whereas yields in the simulation react sensitive to these indicators, the relationship is much lower, in reality. A possible explanation for this could be that, through the parameterization of the model, results are strongly affected by water stress and, therefore, longer dry spells have a greater effect. It seems also possible that some kind of manual irrigation is carried on the fields out during long dry spells, or soils in some parts of the study area are moister than modeled through flooding.

2.5.4 MULTIVARIATE ANALYSIS OF YIELDS VS. RAINFALL CHARACTERISTICS

In this study, the input data comprises of 16 selected rainfall characteristics plus the modeled yield for each cell and year. During the training of the SOM, similar input data would then be grouped into common neighborhoods in the output space. The component planes obtained from the SOM algorithm and the results of the subsequent clustering are visualized in Figure 11. Six clusters were identified by the k-means algorithm. Combining the information of the component planes, these classes are characterized as follows:

(1) Marginal yield: short rainy season; relatively high number of wet and dry days; very high number of wet and dry spells; very long wet spell duration; short wet spell duration; very low number of rainy days above 10 mm; very low number of extreme events; very low total rainfall;

(2) Very low yield: short rainy season; low number of dry days; high number of wet and dry spells; dry spell duration in medium range; low number of rainy days above 10 mm; low number of extreme events; short wet spells; low total rainfall;

(3) Low yield: short rainy season; low number of dry days; low number of dry days; medium number of dry spells; low number of rainy days above 10 mm; high number of extreme events; medium wet spell duration; total rainfall in medium range;

(4) Normal yield: short rainy season; low number of dry days; low number of dry spells; medium number of wet spells; short dry spells; medium number of rainy days above 10 mm; medium number of extreme events; medium duration of wet spells;

(5) High yield: mid-range length of rainy season; low number of wet days; low number of dry spells; short dry spells; long wet spells; high number of rainy days above 10 mm; high number of rainy days above 20 mm; medium number of extreme events above 40 mm/d; high total rainfall; long wet spells and

(6) Very high yield: long rainy season; high number of wet and dry days; very low number of dry spells; very short dry spells; very long wet spells; very high numbers of rainy days above 10 mm; high number of events above 60 mm; high total rainfall.

Although being purely qualitative, this classification allows gaining an understanding of combined effects of rainfall characteristics on yields. Quantitative information can be obtained by studying the component planes in detail.

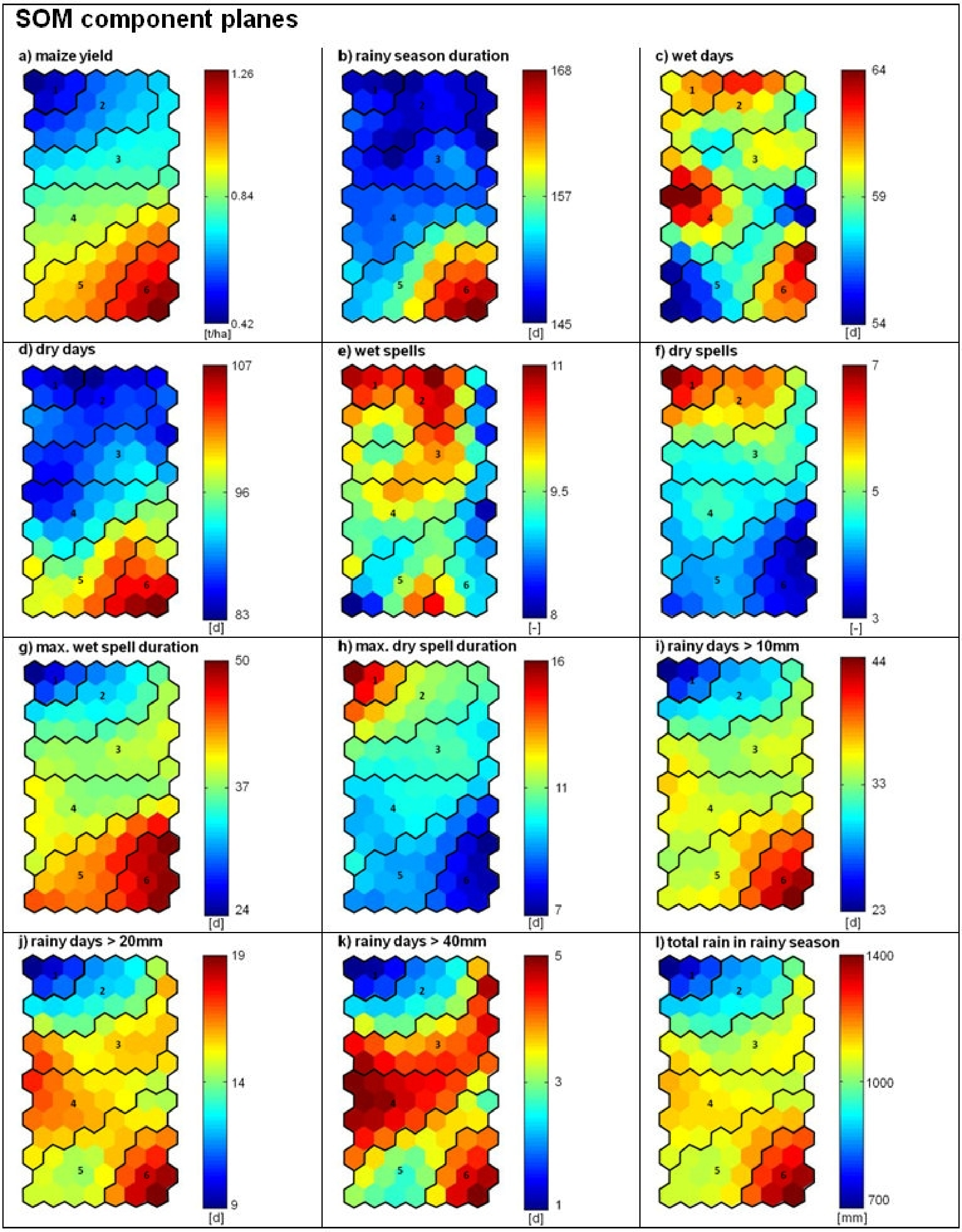

Figure 2.11: Component planes for yields and selected rainfall characteristics derived by the SOM – algorithm. Clusters are indicated as (1) marginal yield, (2) very low yield, (3) low yield, (4) normal yield, (5) high yield and (6) very high yield

One aspect revealed by the component planes is the great importance of *dur* (Fig. 2.11b). According to the image, 'good' maize yields (classes 5 and 6) can only be achieved with a rainy season longer than 160 days. In all other classification units, *dur* varies only slightly; hence, differences in yields are then determined by differences in other characteristics. In particular, differences in *dsp*, $dspd_{max}$, $wspd_{max}$ as well as, to a certain degree, p_{tot} and p_{10}, define the maize yield (Fig. 2.11). In addition to a short rainy season, the two lowest yielding groups (clusters 1 and 2) are further described by many but short wet spells, and many but long dry spells. Surprisingly, the number of wet days (*wd*) is relatively high in the low yielding clusters; hence, it does not correlate at all with yields. In comparison, the component plane for p_{10} (Fig. 2.11i) shows a distribution that is in greater agreement with maize yields. Again, this indicates a threshold of 2 mm for a rainy day is not sufficient in relation with rain-fed agriculture. The distribution of extreme events (only p_{20} and p_{40} shown here) reveals an interesting pattern. High and very low yielding clusters show a clear distribution; contradictory, a high number of extreme events are also encountered in clusters 3 and 4. Although a clear explanation for this remains difficult, there might be a relation with the higher magnitudes of *wsp* and *dsp* in combination with shorter wet spells (Fig. 11g) in these clusters. This would be in agreement with the previous finding that many changes of wet and dry spells affect yields negatively. Another possibility could be the high number of extreme events directly impacting yields.

In the component plane for *wd*, one area in the middle with a very high number of wet days is clearly standing out (Fig 11c). Interestingly, more than 60 percent of the input vectors in this area are from the western part of the catchment (Angola). This region within the component planes also experiences more extreme events and a higher rainfall total. Again, the high number of extreme events could be the reason for the lower yields. Also, specifics in soil type or local climatology might be an explanation.

Finally, a measure for the evaluation of especially suitable (or unsuitable) regions for rain-fed agriculture within the studied catchment was introduced. This was achieved by simply calculating a ‘class status’ (*CS*) as weighted mean of the class to which one region is belonging in accordance to the classification presented previously. For example, if the input vectors of a region are classified into class 1 in three years and class 2 for 9 years, the class status will be $(3\times1 + 9\times2)/12 = 1.75$. The higher the class status of a region, the higher is its suitability for rain-fed agriculture. This allows one to directly derive the dominant combination of rainfall characteristics present in one region and also enables quantitative analysis using the component planes. The final results are summarized in Figure 2.12. Additionally to *CS*, the table also includes information about the number of input vectors from a region in each of the classes.

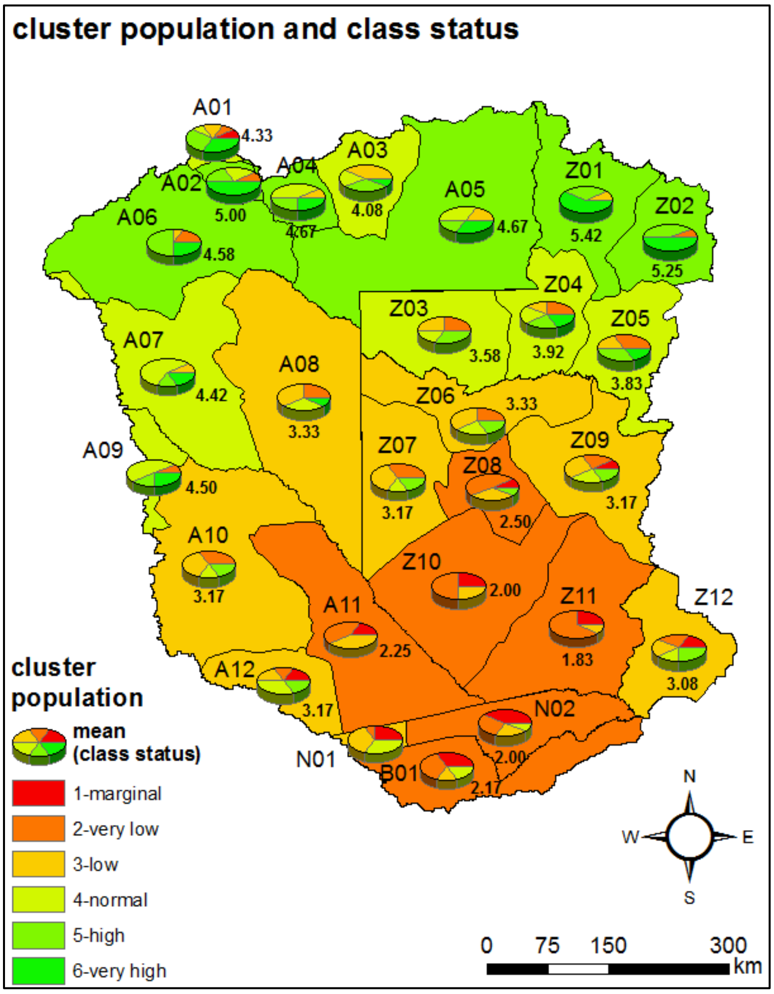

Figure 2.12: Class population for each cluster per region and class status (mean class population). The pie chart visualizes the class population distribution for each region between 1998 and 2010. The background color and the numbers refer to the class status.

The most suitable regions for rain-fed agriculture are, in general, the north- Zambian and Angolan regions, such as Mwinilunga (Z01; *CS* = 5.42), Solwezi (Z02; *CS* = 5.25) and Leua (A02; *CS* = 5.00); Worst conditions, on the other hand are present in Sesheke (Z11; *CS* = 1.83), Senanga (Z10; *CS* = 2.00) and Caprivi (N02; *CS* = 2.00). It is in these regions where vulnerability and, thus, the need for adaptation is the highest, in order to deal with future climatic changes, which might worsen the situation.

2.6 CONCLUSIONS AND DISCUSSION

This study investigated the rainfall characteristics over the Upper Zambezi River Basin and their implications for rain-fed agriculture on the example of *Zea mays*. Measured yields were reproduced successfully using the SVAT model DAISY and mapped for the period 1998–2010. Finally, the relationship between rainfall characteristics and maize yields was analyzed utilizing both a uni- and multivariate approach (*SOM*).

It is found that yields and all investigated rainfall characteristics exhibit significant spatiotemporal variability over the UZRB. A clear gradient from north to south is identified in most rainfall characteristics: the northern parts of the basin receive more total rainfall over the wet period, and experience longer rainy seasons, more productive rainfall events, longer wet spells and shorter and less dry spells. Mean yields from rain-fed maize farming range from 1.2 t/ha in the northern to only 0.5 t/ha in the southern part of the basin. The southernmost areas, in particular the Namibian, Botswanan and southern Zambian regions, display the least favorable preconditions for rain-fed farming.

By means of connection between yields and rainfall characteristics it is found that using total rainfall over the rainy season alone as an indicator for good yields is not sufficient. The highest correlation found is -0.56 between yields and the maximum dry spell duration ($dspd_{max}$), followed by the number of days with more than 10 mm of rain (p_{10}; 0.51), total rainfall and maximum/mean wet spell duration (p_{tot}, $wspd_{max}$, $wspd_{mean}$; 0.48) and the number of dry spells (*dsp*; -0.45). The number of wet days and spells (*wd* and *wsp*) as well as the frequency of extreme events higher than 20 mm do not affect yields directly. The multivariate analysis using a *SOM* revealed the importance of the indicator ‘duration of the rainy season’ (*dur*): Yields higher than 1 t/ha can only be achieved with rainy season duration longer than ~160 days. This is an important finding, having in mind that only a few of the investigated regions reach that threshold regularly. For durations shorter than ~160 days, the interplay of p_{tot}, *dsp*, $dspd_{max}$ and $wspd_{max}$ (the indicators with the highest correlation coefficient) determines the success of rain-fed agriculture in a particular year. An inconsistent rainy season (such as many shifts of wet and dry spells) was found to affect yields negatively. In terms of adaptation, a key could be to cultivate faster growing varieties or to introduce small-scale water storage systems (i.e. rainwater harvesting) to extent water availability or bridge dry periods. Furthermore, it was identified that using *dd* and *wd* as well as *wsp* as indicators for agricultural success is not appropriate. As stated before, the *wd* criteria (> 2mm of rain) showed no correlation with yields whilst one of the highest correlations was found for p_{10}. This clearly shows that small rains do not provide sufficient moisture for maize to enhance yields significantly. The threshold when interested in farming yields should thus be further investigated (i.e. by analyzing from which threshold on a high correlation is found). By means of succession potential for rain-fed farming of maize, the regions Mwinilunga (Z01), Alto Zambeze (A05), Solwezi (Z02) and Cameia (A04) have the highest potential whilst Caprivi (N02), Botswana (B01), Mongu (Z08), Kavango (N01), Rivungo (A11), Sesheke (Z11) and Senanga (Z10) are the least suitable areas.

This investigation using the best available dataset for the region by means of spatial and temporal representativeness enables decision-makers, water resource managers, researchers and farmers to carry out region-specific analyses of rainfall characteristics and to develop adaptation measures, i.e. those identified and summarized by Milgroom and Giller (2013). Further interpretation of local experts who are more familiar to the particular area of interest than any outside researcher could be is recommended. This study and the examination of patterns solely included rainfall. It should be stated at this point that maize is not grown primarily all over the UZRB (personal comment by J. Mendelsohn, 2013) and was rather chosen to have a unified ‘scale’ to evaluate and compare climatic suitability. However, over large parts of the basin maize remains the number one staple crop having also cultural importance for the people.

Even though the parameterization and calibration of the SVAT model could be improved with increased data and information on measured yields, the usefulness of intensified research on rainfall characteristics is pointed out by this study. Rain-fed agriculture is, and will remain to be, challenging even in the areas identified as most suitable. However, with knowledge of length of typical dry periods, for example, a first step towards adaptation can be made. Results also reveal that rainfall variability is the overriding issue for local farmers. The effect of intra-seasonal and seasonal variability is discussed in the present research in-depth. For an investigation of decadal variability, on the other hand, the time period of 12 years is not sufficient. There is evidence that decadal cycles of climate are present and should be further investigated (Conway et al., 2009; Tyson et al., 1975; WorldBank, 2010). In addition, this problem further complicates the identification of trends and impacts of climatic changes. Using the criteria and indicators suggested by this study consequently for the future, trends might be detectable. In a recent investigation, Ines and Hansen (2006) observed that wet day frequency and intensity distributions were used to improve GCM predictions, which generally predict too many rain events of too low intensity. Integrating such innovative approaches into the present study might allow the design more precise forecasting systems.

The great variability also hinders many efforts to predict probable rainy season onset dates. Still, there is a pressing demand for such (Reason et al. 2006). Using neural network approaches such as *SOM*, which are capable of identifying relationships in highly complex and large datasets with a high number of parameters, allows advancement in this regard (as shown by Rivera et al. 2011 in their study of central Chile). Connecting the spatial patterns of rainy season characteristics with synoptic patterns might be a step towards a forecasting system. Extended examination of the connection between the studied rainfall characteristics (i.e. how does an early/late onset of rains affect the remaining indicators?), an analysis over different stages of maize growth as well as scenario studies with other varieties or even crops are only a few possibilities for future applications. Especially investigating the effect of rainfall characteristics on phenological aspects, such as the sensitivity of maize in its different development stages, is worth examining further. Finally, the results of this investigation are not only limited to rain-fed agriculture, but can be very useful for studying flood creation and groundwater recharge, as well as an additional information for hydrological models.

Acknowledgements

We would like to express our gratitude to the Agricultural, Food and Resource Economics Department of Michigan State University for providing their detailed data on agricultural yields over Zambia from their panel survey and the Zambia Meteorological Department. Matthias Beyer wants to thank J. Mendelsohn for sharing valuable insights and local knowledge over the past three years and D. Rivera for fruitful discussions on data mining and SOM's. Finally, we thank the reviewers for helping to improve this paper. We appreciate their effort to provide many useful comments and recommendations.

3 ESTIMATION OF GROUNDWATER RECHARGE VIA DEUTERIUM LABELING IN THE SEMI-ARID CUVELAI-ETOSHA BASIN, NAMIBIA

This chapter is an edited version of: BEYER, M., GAJ, M., HAMUTOKO, J.T., KOENIGER, P., WANKE, H., HIMMELSBACH, T., 2015. Estimation of groundwater recharge via deuterium labelling in the semi-arid Cuvelai-Etosha Basin, Namibia. Isotopes Environ. Health Stud. 51, 533–52. doi:10.1080/10256016.2015.1076407

3.1 ABSTRACT

The stable water isotope deuterium (^2H) was applied as an artificial tracer (^2H_2O) in order to estimate groundwater recharge through the unsaturated zone and describe soil water movement in a semi-arid region of northern central Namibia. A particular focus of this study was to assess the spatiotemporal persistence of the tracer when applied in the field on a small scale under extreme climatic conditions and to propose a method to obtain estimates of recharge in data-scarce regions. At two natural sites that differ in vegetation cover, soil and geology, 500 ml of a 70 % ^2H_2O solution was irrigated onto water saturated plots. The displacement of the ^2H peak was analyzed 1 and 10 days after an artificial rain event of 20 mm as well as after the rainy season. Results show that it is possible to apply the peak displacement method for the estimation of groundwater recharge rates in semi-arid environments via deuterium labeling. Potential recharge for the rainy season 2013/14 was calculated as 45 mm a^{-1} at 5.6 m depth and 40 mm a^{-1} at 0.9 m depth at the two studied sites, respectively. Under saturated conditions, the artificial rain events moved 2.1 and 0.5 m downwards, respectively. The tracer at the deep sand site (site 1) was found after the rainy season at 5.6 m depth, corresponding to a displacement of 3.2 m. This equals in an average travel velocity of 2.8 cm d^{-1} during the rainy season at the first site. At the second location, the tracer peak was discovered at 0.9 m depth; displacement was found to be only 0.4 m equaling an average movement of 0.2 cm d^{-1} through the unsaturated zone due to an underlying calcrete formation. Tracer recovery after one rainy season was found to be as low as 3.6 % at site 1 and 1.9 % at site 2. With an *in situ* measuring technique, a three-dimensional distribution of ^2H after the rainy season could be measured and visualized. This study comprises the first application of the peak displacement method using a deuterium labeling technique for the estimation of groundwater recharge in semi-arid regions. Deuterium proved to be a suitable tracer for studies within the soil–vegetation–atmosphere interface. The

results of this study are relevant for the design of labeling experiments in the unsaturated zone of dry areas using $^{2}H_2O$ as a tracer and obtaining estimations of groundwater recharge on a local scale. The presented methodology is particularly beneficial in data-scarce environments, where recharge pathways and mechanisms are poorly understood.

3.2 INTRODUCTION

Over large parts of semi-arid Sub-Saharan Africa (SSA), where population growth rates are high and industrialization is progressing, pressure on water resources is steadily increasing. Groundwater resources are therefore becoming progressively more important as they can act as a secure source of freshwater, for example, during periods of drought or during the dry season. In order to manage aquifers sustainably, an accurate determination of recharge rates is crucial. Groundwater recharge is widely acknowledged as being the most important parameter for the management of aquifers (Kinzelbach et al., 2002). At the same time, it is the parameter that is most difficult to determine (Beekman and Xu, 2003). Consequently, many researchers are developing methods for the quantification of groundwater recharge. Tracer-based methods are amongst the most precise methods for groundwater recharge studies (Scanlon et al., 2002). However, quantitative studies on groundwater recharge using stable isotope methods are difficult and rather rare (Allison et al., 1994; Gaye and Edmunds, 1996).

The peak displacement method (Leibundgut et al., 2009; Saxena and Dressie, 1984) has been proven to be a suitable technique for a quantitative estimation of groundwater recharge. Even though processes such as dispersion and preferential flow are difficult to tackle, the method is a simple approach to obtain estimations of recharge. The technique has been successfully applied in areas where a significant seasonal variation of the concentration of the stable isotopes deuterium (^{2}H) and oxygen-18 (^{18}O) in precipitation is present and is reflected in the soil water stable isotope profiles (Adomako et al., 2010; Saxena and Dressie, 1984). Numerous precedent studies utilized the peak displacement method using tritium (^{3}H) in the past. Tritium was imprinted into the rain and subsequently soil water by thermonuclear bomb testing, and successfully used to derive groundwater recharge rates in semi-arid regions (Allison and Hughes, 1978, 1972; Butler and Verhagen, 2001; Gaye and Edmunds, 1996; Ruifen and Keqin, 2006, 2001; Selaolo et al., 2003). A complete review is given by Koeniger et al. (2015). Furthermore, tritium has been used as an artificial tracer in numerous studies in various climatic regions using different experimental procedures (Athavale et al., 1980; Bahadur et al., 1977;

Jin et al., 2000; Rangarajan and Athavale, 2000; Rao, 1983; Sukhija et al., 2003; Wang et al., 2008; Zimmermann et al., 1967a, 1966).

Within the last decade, only a few studies using the peak displacement method, using either environmental isotopes or artificial labeling, have been conducted due to several reasons. Even though a seasonal variation of isotopic composition of ^{2}H and ^{18}O might be detectable in the rain, this signal is often lost within the soil profile due to dispersion effects and mixing (Allison, 1988; Allison et al., 1994). An application of the method using environmental tracers, in particular in semi-arid regions, is therefore often not possible. In the southern hemisphere in particular, the impact of the thermonuclear tests was much less pronounced than in the northern hemisphere. Tritium concentrations have returned to close to environmental concentrations and are hence not practically useful for this method anymore. Within the unsaturated zone, the peak concentrations resulting from the thermonuclear tests can only be found in greater depths (>20 m). Hence, sampling and analysis of soil profiles become very labor intensive and no longer feasible. Tritium is toxic if used in high concentrations and therefore of concern to both the environment and health. This limits its practicability. Transient flow and transport models are now available to account for the whole spectrum of involved processes (e.g. dispersion, preferential flow) and can be applied where detailed information on soil hydraulic properties is available.

Recently, artificial applications of the stable isotope deuterium are becoming increasingly popular in the fields of hydrology and ecohydrology. Labeling with $^{2}H_2O$ is of advantage because it is not radioactive and there are no toxicological concerns during both labeling and measurement (Becker and Coplen, 2001). Being part of the water molecule, ^{2}H is considered a conservative tracer and thus suitable for studies in the unsaturated zone (Lischeid et al., 2000). It can be measured in very low concentrations (Becker and Coplen, 2001); therefore only small amounts of tracer are necessary and applications become economically feasible.

In numerous studies, $^{2}H_2O$ is applied as an artificial tracer to investigate water movement in the unsaturated zone. In their pioneer efforts, Zimmermann et al. (1966, 1967) used deuterium for the study of soil water movement. They found in their experiments that in sandy soils water transport occurs layered, that is, if new water infiltrates into a soil, the old water is simply pushed downward (Becker and Coplen, 2001). They investigated dispersion effects and quantified recharge in a humid region in Sweden over a period of several months based on peak displacement. A comparison of deuterium, bromide and chloride during an irrigation experiment to assess the uncertainty of tracer experiments under similar boundary conditions was presented by Lischeid et al. (2000). An investigation of preferential flow through a forest-reclaimed lignitic mine soil was conducted by Hangen et al. (2005). Results showed that deuterium and bromide showed similar transport behavior and were considered as suitable tracers for studying preferential flow. Similarly, Schumann and Herrmann (2001) identified preferential flow paths during an irrigation experiment. Mali et al. (2007) studied water movement through the unsaturated zone using $^{2}H_2O$ and dye tracer. The authors were able to quantify travel velocities and vertical dispersion and concluded that deuterium is a useful tool for unsaturated zone studies and more suitable than dye tracer for such applications. Koeniger et al. (2010) applied ^{2}H, ^{18}O and uranine in column and field studies. They estimated flow rates through the unsaturated zone and compared the tracers. Mean transport velocities for deuterium were found to be higher and dispersion coefficients lower compared to uranine in the column experiments. The authors confirmed $^{2}H_2O$ to be a suitable water tracer extending possibilities for field studies in the field of biogeosciences. Recently, Grünberger et al. (2011) was able to quantify capillary rise from a shallow aquifer using deuterium as an artificial tracer.

As shown, many precedent studies deal with water movement in the unsaturated zone. Studies focusing on the quantification of recharge via labeling with $^{2}H_2O$ are rare, in particular within the unsaturated zone of semi-arid regions. The fate of deuterium applied as an artificial tracer within the unsaturated zone of soils in semi-arid climates over a longer period (e.g. one rainy season) has not been investigated. Such climates are characterized by high evaporation rates, the presence of a dry season, heterogeneous soils and specialized vegetation. In addition, groundwater tables are generally far from the surface. This imposes additional challenges for both experimental design and theoretical considerations of recharge studies. The potential of using $^{2}H_2O$ for the purpose of quantifying deep percolation and estimating recharge in such environments has not been assessed yet. In fact, there is currently no established method for the quantification of groundwater recharge in semi-arid climates based on stable isotopes of water. The persistence of artificially introduced $^{2}H_2O$ in the unsaturated zone of such areas is yet to be studied, and the necessary input concentrations and methods of application are poorly understood. Becker and Coplen (2001) explicitly state that 'further research is required to better understand how isotopic exchange affects the behavior of deuterated water over the time scale of a tracer experiment'. Additionally, it is in (semi-)arid areas where the portfolio of available methods for recharge estimation is further limited due to scarcity of data, lack of infrastructure or high spatiotemporal variability.

The main objective of this study is to adapt the method developed by Saxena (1984a, b) for the direct quantification of potential annual groundwater recharge through the unsaturated zone in the Cuvelai-Etosha Basin (CEB) using artificial deuterium labeling. We aim to investigate water movement in the unsaturated zone and fate of $^{2}H_2O$ introduced by an artificial rain event over the course of an entire rainy season. A further focus is set on challenges regarding the experimental design of such experiments under extreme climatic conditions.

3.3 STUDY AREA

The CEB is a transboundary endorheic watershed shared almost equally by Angola and Namibia with a total size of 173,000 km^2. A digital elevation model of the CEB is presented in Figure 3.1.

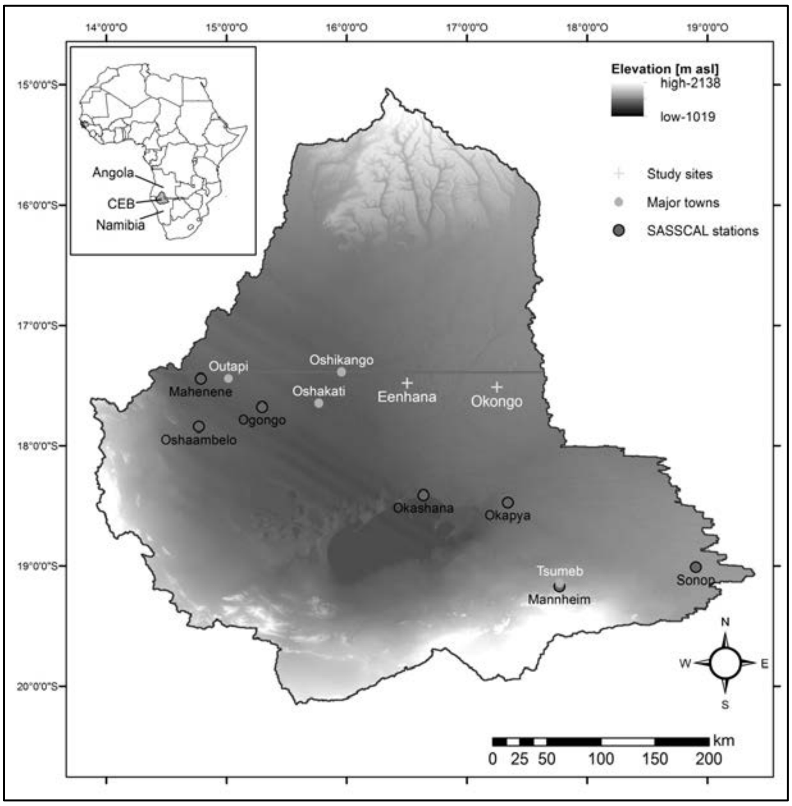

Figure 3.1: Digital elevation model (DEM) of the transboundary Cuvelai-Etosha surface water Basin (CEB). Marked are the locations of major towns, climate stations established in the framework of South African Science and Service Center for Climate Change, Agriculture and Landuse (SASSCAL) and the study sites for the presented research. The grey line marks the borders of Namibia and Angola.

The Cuvelai-Etosha region is home to a large number of people both on the Namibian and Angolan sides, mainly because of the presence of shallow groundwater and relatively fertile soils in many areas (Lindenmaier et al., 2014). The basin has a vivid hydrogeological history as both the deltas of the Cunene and Okavango Rivers were once situated within the CEB (Lindenmaier et al., 2014; Miller et al., 2010). In recent history, a deep aquifer containing fresh water was discovered in the northeastern part of the basin (Lindenmaier et al., 2014). At present all of the surface water is either draining towards the Etosha Pan, a salt pan in the southern part of the CEB, or remains in surface depressions (locally called *iishana*) that are forming a vast, partly inter-connected channel-like system north-west of the Etosha Pan (Mendelsohn et al., 2013). No perennial river exists, and the basin receives all of its water concentrated over the rainy season from November to April. Mean annual precipitation varies between 200 and 600 mm a^{-1} along a distinct rainfall gradient from the west to the east of the basin (Mendelsohn et al., 2013). Temperature average throughout the basin is higher than 22 °C with maximum values reaching up to 40 °C in summer (Mendelsohn et al., 2013). In winter, temperatures can drop to around zero at night. Evaporation rates can reach up to 3000 mm a^{-1} and exceed yearly rainfall by a factor of five. In Figure 3.2, long-term rainfall records from the station Ondangwa and rainfall distribution of 2013/2014 at Elundu school, Eenhana constituency, are shown. Groundwater recharge processes are poorly understood due to the complex discharge and rainfall patterns and the high spatial variability of soils, vegetation and geology. *Iishana*, ephemeral river beds, a high number of pans, dunes and calcrete formations create direct and indirect recharge paths which until now have been difficult to describe.

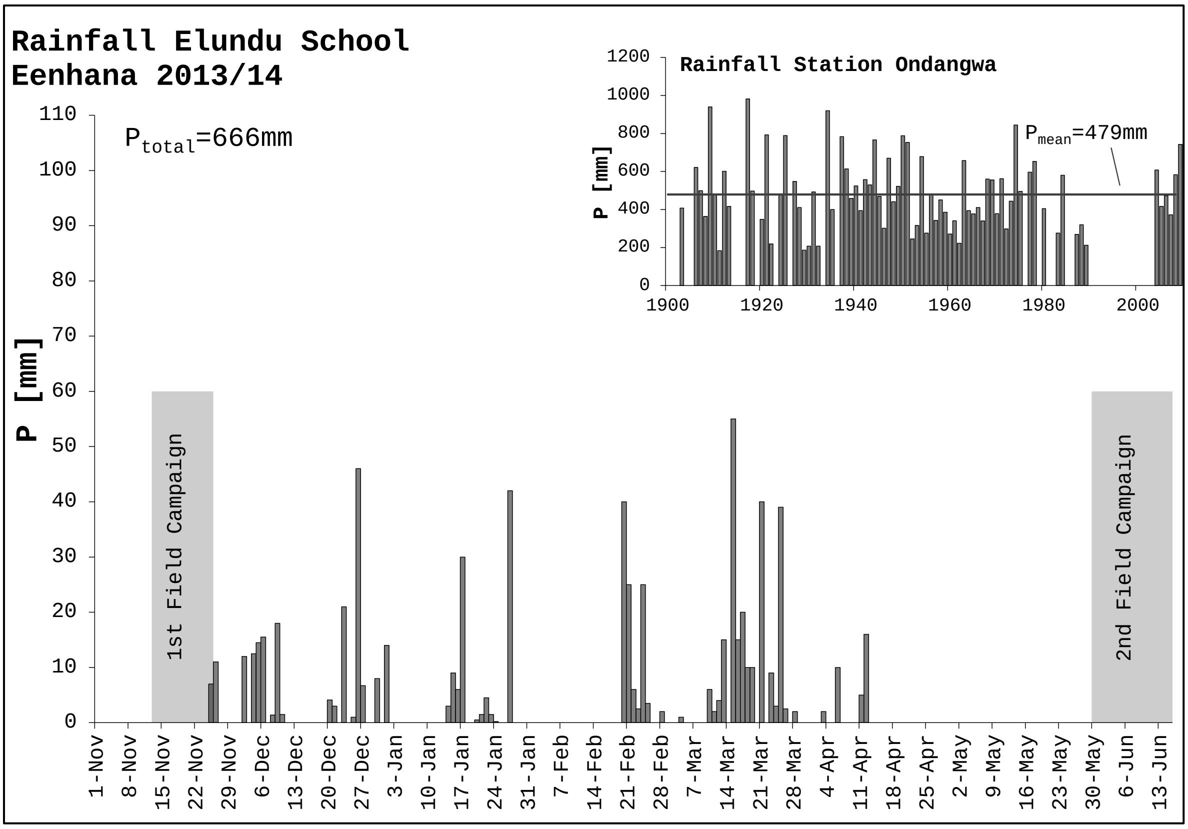

Figure 3.2: Rainfall for the rainy season 2013/2014 measured at Elundu school, Eenhana and long-term rainfall at the station Ondangwa (inset graphic). Note that gaps in the long-term series at Ondangwa represent missing years.

Two sites differing in soil type, geological set-up and vegetation within the CEB were chosen for this study: (1) Eenhana – a forested site on deep Kalahari sand and (2) Okongo – a site with woodland and shrubs on loamy sand underlain by a thick calcrete layer. The selected study sites represent major land forms throughout the CEB. At both sites, soils are classified as arenosols (Mendelsohn et al., 2013). The groundwater table at these two sites is 30 and 20 m below the surface, respectively. Around the Eenhana site (site 1), the pure sand can reach depths of several hundred metres, and deep infiltration of rain water can be expected. Resulting from visual inspection and preliminary irrigation experiments, no hydrophobic behavior of the soils was observed. At the top layer (first 3 cm), a biological soil crust was identified which likely developed due to extreme temperatures and dryness during the Namibian winter in combination with microbiological activity. Within the first 20 cm below surface, finger-like flow was observed. The soil is homogeneous and, according to its soil hydraulic properties, highly permeable (Table 3.1). At the Okongo site (site 2), none of these effects was observed. Soils in this area contained generally more silt and clay, and hydraulic conductivity is lower than at site 1 (Table 3.1). The hydraulic behavior of the thick (often more than 10 m) calcrete layer is unclear. Double-ring infiltrometer tests on top of the calcrete showed no immediate infiltration of water. After using a well camera at several hand-dug wells on-site, cracks and macropores potentially enhancing recharge became visible. Information on soils and local vegetation are summarized in Table 3.1. The latter aspect plays an important role within the hydrological cycle of (semi-)arid environments as it was recognized as a main factor controlling deep drainage and groundwater recharge (Seyfried et al., 2005). A conceptual description of common rooting strategies in such regions is incorporated in Figure 3.3. The tree species present throughout the study area (e.g. *A. erioloba.*, *B. plurijuga*, *C. collinum*; Table 3.1) are known to be capable of adaptations to particularly dry conditions, such as the development of deep tap roots (Canadell et al., 1996; Seymour and Milton, 2003). We refer to the discussion section for a comprehensive analysis of the impact of local vegetation on the genesis of groundwater recharge.

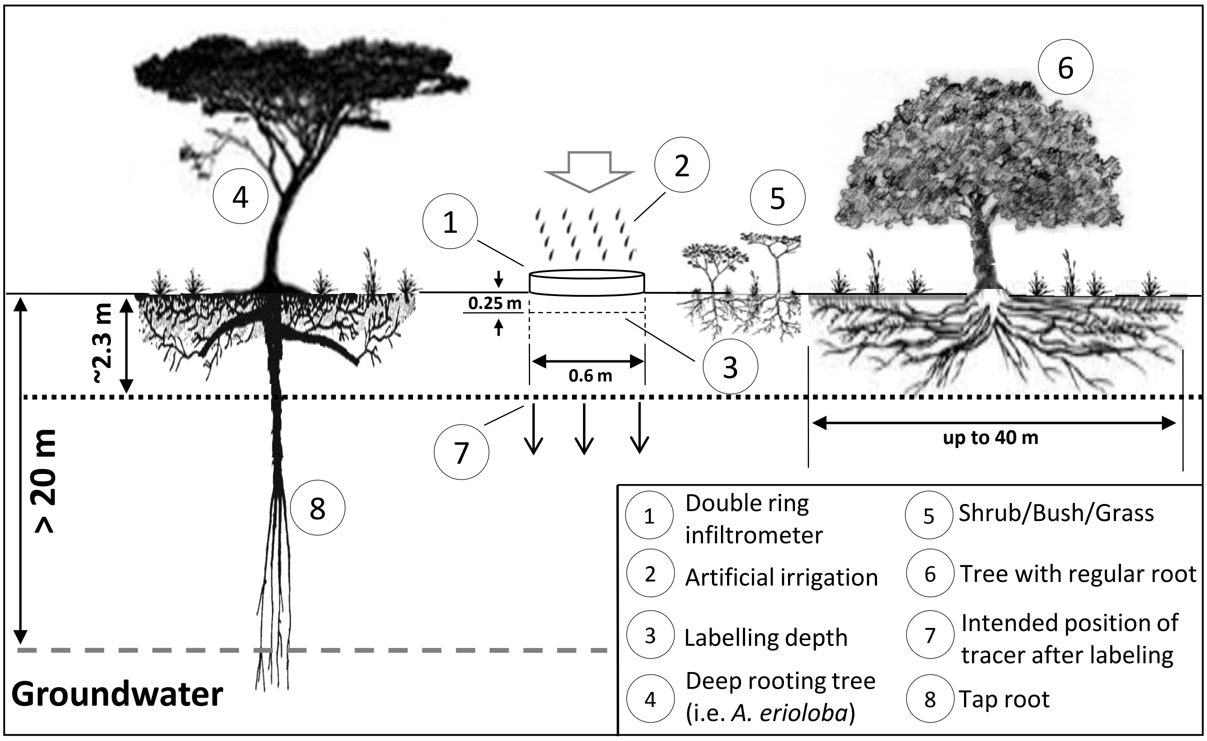

Figure 3.3: Experimental design and typical characteristics of vegetation in semi-arid and arid environments.

3.4 METHODS

3.4.1 EXPERIMENTAL DESIGN

For the design of the experiments, special attention has to be paid towards the amount and method of tracer application. The main objective for this research is to inject the ^2H_2O before the start of the rainy season and detect it during the subsequent dry season. The two major requirements to achieve this are (i) to prevent the tracer from evaporating and (ii) not to lose the entire tracer solution via root water uptake through plants. As a consequence, the tracer needs to be either injected or moved to a depth where root activity is at minimum or at least markedly reduced and transpiration is close to zero. This is of great importance to assure that the tracer signal would be detectable after the rainy season. Diffusion effects are of minor importance when looking at purely sandy soil (compare soil hydraulic properties in Table 3.1) during the rainy season since vertical water transport is dominating. To fulfill the above mentioned prerequisites, an experimental procedure was developed as follows.

First, typical rainy season conditions (wet soil) within the experimental plot comprising an area of 0.27 m^2 were established and saturated conductivity (*ks*) derived by performing a double-ring infiltrometer test. After gentle excavation of the sand until the target depth of 25 cm, 1.85 mm (500 ml) of 70 % ^2H_2O was distributed uniformly using drip irrigation with an average intensity of 0.75 mm min^{-1}. Finally, after carefully refilling the soil, an artificial rain event of 20 mm was irrigated onto the plot with a mean intensity of 2.5 mm min^{-1}. To examine the position of the tracer front, one soil profile each with a vertical sampling resolution of 10 cm was taken using an *Eijkelkamp* hand auger 1, 2 and 10 days after the application of ^2H_2O until a maximum depth of 2.6 m (site 1). At the second site, profiles were taken after 1, 2 and 5 days. After the rainy season, samples were taken up to a maximum depth of 7.4 m. The soil was collected in headspace glass vials that were sealed with a crimping tool immediately after sampling. From these samples, the isotopic composition, water content and grain size distribution were determined in the laboratory (refer to laboratory methods). Additional plant samples were taken at site 2 since during the course of the field experiment, fresh grass was growing directly on the experimental plot and similarly analyzed for isotope ratios.

A recent development allowed the measurement of stable isotopes in soils directly in the field and was helpful to decide on the maximum sampling depth. Even though this method is still in an experimental stage, the approximate magnitude of ^2H values gave an idea as to whether there was a tracer in the samples and at which depth the values would return to the background concentration. For this *in situ* measurement of ^{2}H and ^{18}O, commercially available soil gas probes (BGL-30, *Umweltmesssysteme (UMS), Munich*) were connected to a laser spectrometer (OA-ICOS, *Los Gatos Research, DLT100*). A laptop communicating with the OA-ICOS was programmed to control the measurement cycle and to mimic the behavior of a laboratory auto sampler. In essence, the step involving the vaporization of a liquid sample was skipped and the soil gas directly sent to the measuring cavity of the OA-ICOS. Measurements of stable isotopes were accordingly taken at a resolution of 30 cm horizontally and 20 cm vertically starting from the centre of the experimental plot. This resulted in 22 field measurements that were interpolated using the statistic software R (R Core Team, 2013). The procedure enabled creating a highly resolute image of the deuterium distribution above the calcrete layer and a quasi-3D visualization of the spatial ^{2}H distribution after the rainy season at site 2.

3.4.2 LABORATORY ANALYSIS

Gravimetric water content was determined after drying the samples for 24 h at 105 °C. The grain size distribution was derived by dynamic image analysis. For fine soils the grain size distribution smaller than 63 µm was analyzed by sieving and sedimentation (Altuhafi et al., 2013). Soil hydraulic properties, that is, water retention parameters and saturated as well as unsaturated conductivities, were obtained using the evaporation method (Becher, 1971; Schindler et al., 2010; Wind, 1966) and subsequent fitting of retention curves with the software ROSETTA(Schaap et al., 2001). Saturated conductivity was also examined in the field using a double-ring infiltrometer. In Table 3.1, the most important parameters describing the soil hydraulic behavior of both soils are compiled.

Table 3.1: Rainfall, vegetation and soil characteristics as well as parameters determined in the laboratory for experiments conducted at the Eenhana and Okongo sites in the CEB, Namibia.

		Eenhana	Okongo
total rainfall 2013/14	[mm a^{-1}]	660	660*
vegetation type	[-]	forest	woodland
dominant plant species	[-]	*Combretum collinum; Acacia erioloba; Baikiea plurijuga*	*Collinum apiculatum; Collinum zeyheri; Ricinodendron rautenii*
rooting depth (lateral root zone)	[m]	2.3 - 2.4	1.0 - 2.0
soil type			
0 – 100 cm	[-]	sand	loamy sand
sand/silt/clay	[%]	98/1/1	94/3/3
>> 100 cm	[-]	sand	calcrete
sand/silt/clay	[%]	97/2/1	79/7/14
bulk density	[g/cm^3]	1.59	1.53
porosity	[-]	0.35	0.40
field capacity (pF =2.5)	[vol.-%]	3.5	5.13
residual water content	[vol.-%]	3.3	4.50
saturated water content	[vol.-%]	35.3	39.5
saturated hydraulic conductivity (lab)	[cm day^{-1}]	2490	1184
saturated hydraulic conductivity (field)	[cm day^{-1}]	2304	1872
size of plot	[m^2]	0.27	0.27
depth of ^2H_2O injection	[m]	0.25	0.25
amount of tracer irrigated	[ml]	500	500
amount of tracer irrigated	[mm]	1.85	1.85

*Approximated. Distance between Eenhana rain gauge and Okongo study site is about 100 km.

For the extraction of soil water, a cryogenic vacuum distillation was used, which is described in detail by West et al. (West et al., 2006) and was modified for higher throughput by Koeniger et al. (Koeniger et al., 2011). Despite recent developments of measuring stable isotopes *in situ* (Gaj et al., 2016; Soderberg et al., 2012; Volkmann and Weiler, 2013), cryogenic vacuum extraction still is the most commonly used method and applied to extract water from soil, xylem and plant samples (Hangen et al., 2005; Koeniger et al., 2011; West et al., 2006). In the present study, two replicate samples for each depth with approximately 10 g of soil were prepared and vacuum extracted at 105 °C. Even for the driest samples, a minimum of 0.1 ml of water could be extracted from those.

The extracted water samples were analyzed for ^2H concentrations using a Picarro L2120-i cavity ring-down (CRD) water vapor analyser after vaporisation, and can be expressed in the unit [$10^3\,\delta^2H$] following the definition of Coplen (Coplen, 2011) given in Equation (3.1):

$$10^3\delta^2H = \left(\frac{R_{Sample}}{R_{Standard}} - 1\right), \qquad \text{(eq. 3.1)}$$

with R_{Sample} being the ratio ($^2H/^1H$) of the less abundant to the more abundant isotope in the sample and $R_{Standard}$ the ratio ($^2H/^1H$) in a standard. For high concentrations it is advantageous to express the concentrations in parts per million (ppm), as given in Kendall and McDonnell (Kendall and McDonnell, 1999):

$$^{2}H\ (ppm) = \left(\frac{\delta^{2}H}{1000} + 1\right) * 156. \qquad \text{(eq. 3.2)}$$

This notation will be used throughout the manuscript.

3.4.3 ESTIMATION OF LOCAL GROUNDWATER RECHARGE AND TRACER RECOVERY

In the 1960s, a method was developed to quantify groundwater recharge rates in sandy soils by tracing natural ^{18}O and injected tritium profiles (Zimmermann et al., 1967a, 1967b). Saxena and Dressie (Saxena and Dressie, 1984) define the downward movement of soil moisture as the shift of the peak concentration of the tracer in the case of artificial labeling, and as the mean depth of the depleted isotope layer when looking at the seasonal variability of stable isotopes. The rate of soil moisture movement was calculated using Equation (3.3):

$$v = \frac{z_2 - z_1}{t_2 - t_1}, \qquad \text{(eq. 3.3)}$$

where v [L T^{-1}] is the velocity of soil moisture movement from the tracer depth (as defined above) z_1 to z_2 [L] during the time span between t_1 and t_2 [T]. The amount of water stored within the soil S [L] during this period is then simply calculated by multiplying the soil moisture θ [–] with the vertical extent of the particular soil layer:

$$S = \theta \cdot \Delta z. \qquad \text{(eq. 3.4)}$$

Assuming the tracer peak is located underneath the root zone and water surpassing the root zone is not subject to further effects, recharge through the unsaturated zone R_{un} [LT^{-1}] can be determined as follows:

$$R_{un} = \frac{\int_{z_0}^{z_n} \theta(z) \cdot dz}{T}, \qquad \text{(eq. 3.5)}$$

where z_0 and z_n [L] represent the soil depths of the tracer peak after injection of the tracer and after a certain time period T (i.e. one rainy season). In our study, we follow the above-described approach with two adaptations to the methodology: Since there is no rain during the dry season, the influence of summer rain can be neglected (Saxena, 1984a, b). Hence recharge can be calculated from the position of the tracer peak before (t_1) and after (t_2) the rainy season. In order to avoid the overestimation of the calculated recharge due to the initial saturated conditions, a correction of water contents was introduced. We use as a threshold water content at pF 2.5 (i.e. the lower end of field capacity) and define any water with a lower pF as draining water. From the clearly visible peak in water content caused by the artificially introduced water, the difference between field capacity and observed water content is calculated for each soil layer (Equation 3.6):

$$I_{corr} = (\theta_{obs} - \theta_{fc}) \cdot \Delta z, \qquad \text{(eq. 3.6)}$$

where I_{corr} [L] represents the water depth that is to be corrected for, θ_{obs} is the observed water content and θ_{fc} the water content at field capacity for the particular soil layer. By implementing Equation (3.6) into Equation (3.5), the final equation for the estimation of recharge through the unsaturated zone R_{un} can be expressed as:

$$R_{un} = \frac{\int_{z_0}^{z_n} \theta(z) \cdot dz}{T} - \int_{z_b}^{z_e} I_{corr} \cdot dz, \qquad \text{(eq. 3.7)}$$

where z_b and z_e [L] represent the depths of the beginning and the end of the artificially introduced event, respectively.

The calculated recharge rate represents the amount of water infiltrating underneath the lateral root zone. We subsequently refer to this as ‘potential recharge’ because of the possibility that this water is subject to effects (e.g. water vapor transport) during the dry season.

When introducing artificial water into a soil, the movement of subsequent rain events might occur at an accelerated rate due to the relationship of hydraulic conductivity and water content (i.e. higher water content in the soil profile leads to higher hydraulic conductivity). At both study sites, however, the upper 30 cm of the soil profile dried out within less than three days. In semi-arid areas, the typical evapotranspiration rate is 5–8 mm d^{-1} (Kendall and McDonnell, 1999). Therefore, the hydraulic connectivity between the artificially introduced water and the rain is lost very quickly. A major rain event would then be needed to re-establish this connection. Hence, for the presented study, the impact of the artificially introduced water is reduced to a minimum. Keeping track of the soil water balance in such places can help determine the impact of the artificially introduced water.

To assess the persistence of ^2H_2O in the unsaturated zone, tracer recovery was calculated according to the procedure described by Speakman (Speakman, 1997). An assumption had to be made that only the volume underneath the irrigated plot was considered, that is, lateral movement of the tracer was neglected. Homogeneity of ^2H concentrations was assumed for the complete soil layer where the sample was taken.

3.5 RESULTS

3.5.1 CHARACTERIZATION OF WATER MOVEMENT DISTRIBUTION OF 2H2O AT EENHANA FOREST SITE

Volumetric water content profiles 1 and 10 days after tracer injection as well as after the rainy season are presented in Figure 3.4a. Downward movement of the introduced ‘package’ of water can be clearly observed. One day after the injection of ^2H_2O, the event water has already infiltrated to a depth of more than 1 m. In the subsequent days, excess water travels slower through the drier media below. For the period between the application of the tracer and the 10-day profile, the infiltration rate equals 23 cm d^{-1}. Measurements after the rainy season indicate that the soil moisture is constantly below field capacity from the soil surface until about 2.3 m below the surface, which reveals the effect of evapotranspiration. Notably, a clear increasing step-shift of moisture content at 2.4 m is observed, which is due to the end of the root zone. This has been further investigated and proved by both visual inspection of the depth profiles and further tracer experiments. Underneath 2.4 m the sand at the investigated site has an almost white color with no visual signs of organic contamination. The average travel velocity over the whole rainy season resulting from the after rainy season profile is 2.8 cm d−1. At a depth of around 6 – 6.5 m, the water content drops to almost dry marking the end of moisture front of the rainy season 2013/2014. The elevated soil moisture contents near the surface 1 and 10 days after the irrigation are caused by overnight rain events.

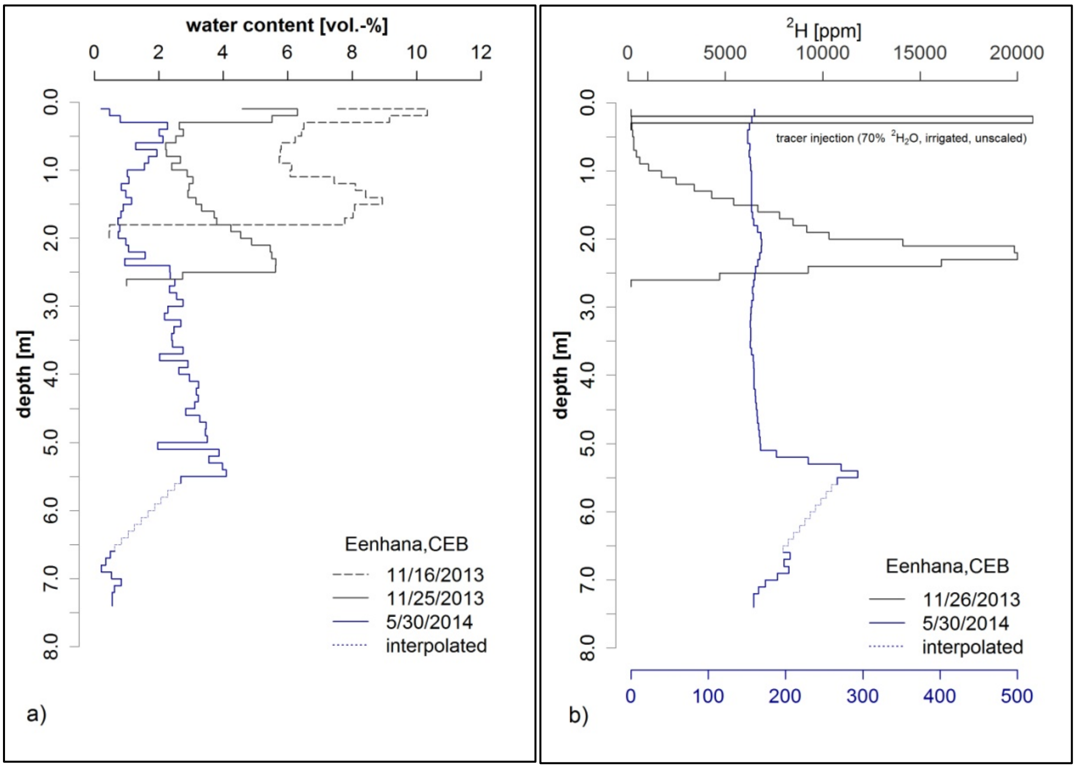

Figure 3.4: (a) Water content profiles during the experiment for the Eenhana site. (b) Deuterium concentrations during the experiment for the Eenhana site. Note that two different axes are used for ^{2}H concentrations for better visualization. The upper x axis belongs to the profile prior to the rainy season (26 November 2013) and the lower x axis belongs to the after rainy season profile (30 May 2014).

The ^{2}H profiles prior to and after the rainy season (Fig. 3.4b) provide a clear picture of the displacement of soil moisture during the rainy season. A Dirac-like type of pulse of the tracer injection is reflected within the soil profile as a sharp peak in the 10-day profile. Advection (downward displacement) as well as dispersion (tailing of the tracer front) effects can be observed in the post rainy season profile. In the upper 5 m below ground, the tracer concentrations remain constant and at similar concentrations as the non-tracer-influenced parts of the shallow (pre rainy season) profiles with two exceptions: (i) the after rainy season profile (Figure 3.4b) also shows that the artificially introduced ^2H_2O must have remained at that depth for a certain time. An elevated deuterium concentration can still be identified at that depth, which might indicate an exchange with immobile water; and (ii) a clear evaporation effect is visible in the upper 0.3 m. The peak tracer concentration after the rainy season (~300 ppm) at 5.5 m is reduced by a factor of 70 compared to the peak concentration of the 10-day profile (~21,000 ppm). The after rainy season profile shows that precipitation during the rainy season shifted the peak downwards to 5.5 m below ground. This corresponds to a peak displacement of 3.2 m. At 7.4 m depth, the deuterium concentration moves back to background concentration

(158 ppm) marking the end of the tracer front. It was found that 10 days after the tracer application 26.2 % of the input was still present within the soil. After the rainy season, the number of ^2H molecules present in the soil profile equals only 3.6 % of the input.

3.5.2 CHARACTERIZATION OF WATER MOVEMENT DISTRIBUTION OF ^2H_2O AT OKONGO SHRUB–WOODLAND SITE

At the second study site, a significantly different infiltration behavior of the moisture front was observed (Figure 3.4a). One day after the tracer injection, significant peaks in soil moisture are present at ~0.3 and 0.7 m. A further increase of water content due to impoundment is pronounced towards the beginning of the calcrete layer. The majority of the infiltrated water is, however, found between 0.3 and 0.4 m depth. This indicates that water movement at the Okongo site is much slower and processes are different from those at the Eenhana site. Five days after labeling, the (now homogenized) moisture front introduced is clearly visible at a depth of approximately 0.9 m. For this period, infiltration velocity equals 0.13 cm d^{-1}, which is almost half of that at the Eenhana site. This is in accordance with observed differences in soil hydraulic characteristics between the two sites (Table 3.1). Similar to changes in water content, deuterium transport was restricted to the upper part of the profile. Peak concentrations of deuterium five days after the tracer injection are found at 0.5 m. The tracer peak after the rainy season is found at 0.9 m depth. This corresponds to a peak shift of only 0.4 m or an average travel velocity of 0.2 cm d^{-1}, being much smaller than those for the Eenhana site. Tracer recovery was calculated from the post rainy season profile, and it was found that 1.9 % of the tracer applied remained within the soil underneath the experimental plot. No infiltration of water underneath the root zone was observed, which is due to the calcretic layer starting at 1.2 m depth hampering deeper sampling. The water content on top of this layer is significantly above field capacity, and the impounding water is expected to evaporate, be taken up by roots, or infiltrate into the groundwater via potentially existing preferential flow paths along plant roots or cracks and fissures within the calcrete layer. These results imply consequences for the application of the peak displacement method at this site as discussed below. The recovery rate of the tracer was calculated as 1.6 % after the rainy season.

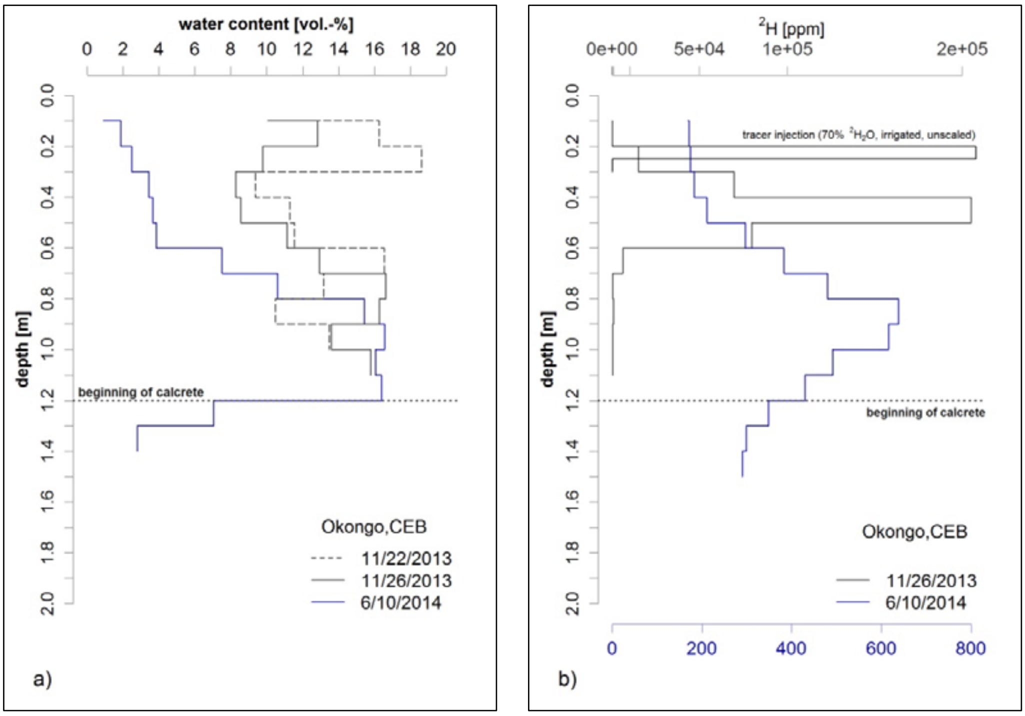

Figure 3.5: (a) Water content profiles during the experiment for the Okongo site. (b) Deuterium concentrations during the experiment for Okongo. Note that two different axes are used for ^{2}H concentrations for better visualization. The upper *x* axis belongs to the profile prior to the rainy season (26 November 2013) and the lower *x* axis belongs to the after rainy season profile (10 June 2014).

3.5.3 SPATIAL DISTRIBUTION OF THE TRACER

In order to examine the spatial distribution of the remaining tracer after the rainy season, Figure 3.6 presents an x–z and x–y plot of the distribution of ^{2}H at Okongo.

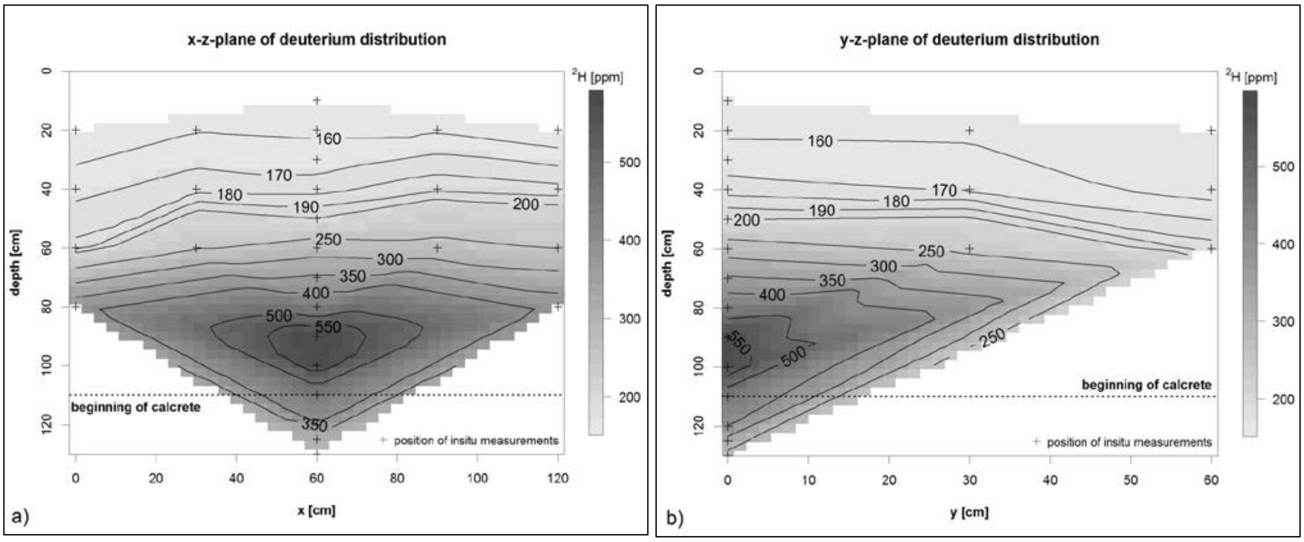

Figure 3.6: (a) Spatial distribution of ^2H_2O after the rainy season at the Okongo site in x–z direction. (b) Spatial distribution of ^2H_2O after the rainy season at Okongo site in y–z direction.

The following insights for the presented experiment as well as for the further application of ^2H_2O as tracer in the unsaturated zone can be derived:

i) Over the course of the rainy season, a significant portion of the applied tracer was retained in the soil matrix. This fact is surprising since one would expect a loss of the tracer in hot climates, where evaporation and transpiration loss is high and plants are flourishing during the rainy season. This demonstrates that 500 ml of 70 % ^2H_2O was a sufficient amount of tracer for this study.

ii) Diffusion and mixing effects distributed the tracer over a much larger area than the initial irrigated plot which was 60 cm in diameter. Horizontally, ^2H concentrations greater than 300 ppm can still be found more than 60 cm from the centre of the plot. In the upward vertical direction, the influence of the tracer reaches up to ~20 cm below the surface. An upward transport of the tracer by evaporation is the most probable reason for this.

iii) Highest tracer concentrations were found at 90 cm depth directly underneath the area of tracer application. Maximum concentrations of 500–550 ppm in x direction coincide with the dimensions of the experimental plot. In the z direction these maximum concentrations were found over a smaller length (25 cm), which is most likely due to a non-uniform spread of the tracer during application or heterogeneities in the soil matrix such as root channels or locally occurring calcrete accumulations.

iv) The centre of mass of ^2H_2O did not reach the calcrete layer. This is possibly caused by a slight change of soil hydraulic properties towards the pure calcrete and is dependent on the genesis of the calcrete layer. Lateral movement of water at this depth might become more dominant. However, this cannot be further evaluated due to missing *in situ* measurements below 60 cm.

3.5.4 CALCULATION OF GROUNDWATER RECHARGE

The calculation of potential groundwater recharge rates follows the methodologies described above (Section 3.4.3). At the Eenhana site, a correction for the artificially introduced water was necessary due to the fact that the increased soil moisture starting at 1.7 m depth (Figure 4a) is expected to cause infiltration underneath the root zone. Hence, this portion of water had to be accounted for. After this correction, the direct groundwater recharge rates through the unsaturated zone were calculated as 45 mm for the rainy season 2013/14 at this site corresponding to 7 % of the rainfall. According to these results, the deep sands around Eenhana comprise a potential recharge area of the CEB.

At Okongo, a potential recharge of 40 mm was estimated. However, due to the impermeable layer at around 1.2 m, the tracer peak had to be applied within the root zone. We use the term 'potential recharge' in this case since the majority of this water is still available for plants and potentially exposed to evaporation during the dry season. Explicitly stated, it is possible that practically none of this water might reach the groundwater table. Table 3.2 summarizes the results for both studied sites.

Table 3.2: Rainfall, vegetation and soil characteristics as well as parameters determined in the laboratory for experiments conducted at the Eenhana and Okongo sites in the CEB, Namibia.

		Eenhana	Okongo
total rainfall 2013/14	[mm a^{-1}]	660	660*
vegetation type	[-]	forest	woodland
dominant plant species	[-]	*Combretum collinum; Acacia erioloba; Baikiea plurijuga*	*Collinum apiculatum; Collinum zeyheri; Ricinodendron rautenii*
rooting depth (lateral root zone)	[m]	2.3 - 2.4	1.0 - 2.0
size of plot	[m^2]	0.27	0.27
depth of ^2H_2O injection	[m]	0.25	0.25
amount of tracer irrigated	[ml]	500	500
amount of tracer irrigated	[mm]	1.85	1.85
depth of tracer peak before rainy season	[m]	2.3	0.4
depth of tracer peak after rainy season	[m]	5.5	0.9
groundwater recharge	[mm y^{-1}]	45	41
percent of precipitation	[%]	~7	~6

*Approximated. Distance between Eenhana rain gauge and Okongo study site is about 100 km.

3.6 DISCUSSION

3.6.1 SOIL WATER MOVEMENT AND DISTRIBUTION OF ^2H_2O

The presented profiles of soil water movement and tracer movement enable a site-specific characterization of the unsaturated zone water movement. With the combination of tracer and soil moisture profiles, quantification of water fluxes is possible. Especially at Eenhana, we emphasize the importance of the intra-seasonal distribution of rainfall for the movement of water through the unsaturated zone and the creation of groundwater recharge in semi-arid environments, which is discussed in earlier studies (Beyer et al., 2016b). From further experiments on-site, it was determined that a rainfall event as high as 60 mm did not infiltrate deeper than 40 cm on a dry soil (data not shown herein). Looking at the soil hydraulic properties of the soil at the Eenhana site (Table 3.1), it becomes clear how low the water-holding capacity of the media is. For longer wet periods and extreme events, infiltration of water underneath the root zone can be expected. It is therefore crucial for recharge estimates to investigate the rainfall characteristics of the rainy season when evaluating groundwater recharge. An analysis of these characteristics according to the criteria defined in Beyer et al. (2016b) was performed for the rainy season 2013/14. Indicators which are believed to be related to groundwater recharge such as maximum wet spell duration, number of events above 10 mm and rainfall during the core rainy season (Beyer et al., 2016b) were found to be in an upper range: rainfall within the core rainy season was 615 mm, and the maximum wet spell duration equaled 22 days. Furthermore, 19 events exceeding 10 mm were recorded (rainfall events >10 mm are commonly considered as productive rainfall events, (Mendelsohn et al., 2013). It is these events that create conditions for deep infiltration of water (Kendall and McDonnell, 1999). Only four events reached magnitudes greater than 40 mm. These results imply that in this particular rainy season, longer wet periods rather than extreme rain events caused the deep infiltration of water and thus, recharge. For further research this points out the potential of such field experiments which can be combined with transient flow and transport modeling and analysis of rainfall distribution within the rainy season. In addition to soil moisture, including tracer transport and distribution into model calibration will lead to more robust models and could potentially be used for developing local empirical relationships for the estimation of groundwater recharge (Allison et al., 1994).

The after rainy season profile at Eenhana shows how soil moisture increases with depth. In this case, it was possible to identify the end of the lateral root zone at around 2.3–2.4 m depth. However, the role of deep-rooting tree species, which are utilizing a tap root (compare Figure 3.2) to support the tree with moisture during the dry season, has to be further investigated. Such tree species (e.g. *A. erioloba*, *B. plurijuga*) can potentially reach groundwater tables as deep as 60 m (Burke, 2006; Palgrave, 2003). This has to be accounted for when quantifying groundwater recharge. To our knowledge, little is known on the volume of water 'pumped' from the groundwater table by these region-adapted plant species. In addition, it is not clarified until now if such roots are able to utilize water in greater depths of the unsaturated zone. This issue could be tackled by injecting ^2H_2O into the root of such trees and quantify dry season transpiration using the tracer concentration breakthrough curve during future research activities.

Whereas at Eenhana the interpretation of the combined $^{2}H_2O$ and soil moisture profiles provided clear evidence, difficulties arise when interpreting the results for the Okongo site. From the soil moisture profiles one and five days after injection of $^{2}H_2O$, respectively, one could infer that the zone of main root activity is probably located between a depth of 0.3 and 0.5 m. The after rainy season profile reveals an impoundment of water at the calcretic formation. Below this layer, water content decreases with depth, which might be due to either very little infiltration or a decrease in porosity. Comparing the peak of the soil moisture with the one of ^{2}H, it becomes obvious that these measurements do not coincide. Only a slightly elevated concentration of deuterium is found at the position of maximum soil moisture. This could be interpreted as follows: the main amount of water was introduced artificially by the preliminary water saturation of the soils. This 'unlabelled' water represents the moisture front in the five-day profile. The actual tracer application and subsequent artificial rain event only reached a depth of 0.5 m with a small portion of the tracer reaching the pre-saturation-induced moisture front via preferential flow paths causing the small increase of $^{2}H_2O$ at 0.9 m. Another indicator for the presence of preferential flow is the difference in field and laboratory determined saturated hydraulic conductivity ks (see Table 3.1). In addition, we used a dye tracer and visually inspected its distribution after several irrigation experiments. Preferential flow within the upper 50 cm could clearly be identified. However, another explanation might be that 'old' water simply is pushed downwards.

3.6.2 Tracer recovery

With 3.6 % at Eenhana and 1.9 % at the Okongo site, tracer recovery determined after one rainy season was very low at both sites. Nevertheless, the peak concentrations of ^{2}H were clearly detectable (Figures 3.3 and 3.4). Loss of tracer can be attributed to the combined effects of evaporation, transpiration and lateral flow. At Eenhana, almost 75 % of the applied tracer disappeared already 10 days after the application. We believe this is caused mainly by evapotranspiration. The root zone at the Eenhana site extends deeper than at Okongo. If irrigating the tracer, it first has to surpass the root zone and is therefore subject to transpiration. Furthermore, the experiments took place during the flowering season, where transpiration demand is very high. Upward transport could be verified by sampling and analysis of fresh grass growing on top of the experimental plot and xylem samples of shrubs nearby at Okongo. The results show that all grass samples which were taken two and five days after the application of $^{2}H_2O$ showed considerably elevated concentrations (>200 ppm) of ^{2}H indicating an upward transport of the tracer to the surface (the background concentration is ~155 ppm). Samples of shrubs approximately 1 m from the plot that were taken two days after the experiment showed no enrichment (155 ppm). A slightly elevated concentration of ^{2}H (~160 ppm) was found in a grass sample outside of, but close to, the experimental plot indicating lateral transport of the tracer. The fact that at both studied sites the tracer concentration was well within the detectable range confirms the suitability of $^{2}H_2O$ for experiments under semi-arid conditions.

3.6.3 UNCERTAINTY AND SHORTCOMINGS OF RECHARGE ESTIMATES USING PEAK DISPLACEMENT

The groundwater recharge rates determined in this study at both sites agree well with the range of values that were found in previous studies (between 20 and 100 mm, Struckmeier and Richts, 2008). It should be noted that the determined recharge is a direct recharge for a year with exceptionally high rainfall at the study site. Therefore, the value of 45 mm a^{-1} should rather be seen as an upper percentile and does perhaps not represent the mean recharge which might be lower. In addition, it has to be kept in mind that the determined recharge through the unsaturated zone does not necessarily coincide with recharge at the groundwater table. This is only the case if no other effects such as water vapor transport from greater depths or uptake of deep soil water through tap roots of specialized plants are present. The presented methodology, although being the most direct way of quantifying recharge, is subject to a certain degree of uncertainty due to a number of factors:

i) Heterogeneity and the contribution and potential effect of preferential flow must be acknowledged. If sampling in the field occurs along a preferential pathway, this will result in an overestimation of groundwater recharge because the tracer would penetrate much deeper. Similarly, if preferential pathways are present, but the sampling does not occur along it, recharge would be underestimated. This issue has been pointed out by several authors (Scanlon et al., 2006; Sukhija et al., 2003). A possible way of overcoming this problem might be to compare the results with estimations based on the chloride mass balance method (de Vries et al., 2000; Kinzelbach et al., 2002). Sampling multiple profiles in the field within the experimental plot, labeling at more than one plot per site and an identification of lateral flow, might further help distinguish between preferential and matrix flow. Hence, the uncertainty of the method can be lowered by taking into account local heterogeneities.

ii) Any irrigation is introducing artificial water into the soil column. Hence, any water possibly contributing to infiltration has to be accounted for. Furthermore, following the principles of soil sciences, soil hydraulic conductivity is increasing with a higher water content potentially causing a change of initial conditions for the rainy season. In the example of Eenhana, this turned out to be of minor consequence because in the 10 days after the injection of the deuterium, 51 mm or 5.6 mm d^{-1} was lost within the soil profile due to evapotranspiration. Soil hydraulic connectivity between the artificial rain event and the top soil was cut, that is, the top soil already had dried out up to a depth of 1.5 m (Figure 4a). However, for future research a different experimental design not using irrigation should be considered. Currently, a punctual application of deuterium in depth is tested causing no disturbance of the experimental plot and applying only a minimum amount of water.

Since the development of the peak displacement method (Saxena and Dressie, 1984; Zimmermann et al., 1966), no considerable methodological advances have been reported to account for non-mobile water or heterogeneities. In the original technique (Saxena and Dressie, 1984), the water content between the position of the tracer peak after application and after a certain time is used to calculate recharge. But in fact, not all water within a soil profile is mobile, that is, there is always a residual portion of water which is not contributing to recharge per se. If the soil hydraulic properties of the site under investigation can be determined precisely, the residual water content should be subtracted and included in Equation (3.5).

Very little research has been conducted on the uncertainty of the method. In existing studies (Cook et al., 1994; Gvirtzman and Magaritz, 1986; Munnich, 1983; Rangarajan and Athavale, 2000), uncertainty for the method ranges in between 1 and 20 %. Considering applied laboratory and field methodologies of the presented study, our estimation is confidently within that range. A challenge is that even if water is infiltrating underneath the primary root zone, it could potentially be lost through upward water vapor transport during the dry season. In addition, the role of deep groundwater table penetrating roots should be investigated further as this comprises a potential sink component of the groundwater balance.

Finally, uncertainty of the method could be introduced by the set-up and calibration of transient flow and transport models. These types of model are becoming increasingly popular and have been applied successfully in the past (Adomako et al., 2010; van der Heijden et al., 2013). Advantages of such models are the ability to incorporate effects such as dispersion, preferential flow or water vapor transport. Several researchers are working on the development of models which are able to simulate fractionation processes of stable isotopes of water (Braud et al., 2009, 2005; Haverd and Cuntz, 2010). This will contribute to improve process understanding, in particular in (semi-)arid environments. However, for data-scarce countries, the non-availability of necessary input data might limit the applicability of such detailed approaches. In addition, numerical modeling in such environments is challenging due to rapid changes in dry–wet conditions. Currently, models are being developed for the presented study sites. This might enable a quantification of local recharge over a longer period of time and investigating favorable conditions for the creation of recharge as well as improving process understanding within the unsaturated zone of semi-arid environments.

3.7 CONCLUSIONS

We proposed a method for a quantification of direct groundwater recharge in semi-arid areas using a single-tracer experiment following the peak displacement method. A cost-efficient and easily applicable experimental framework was used, which is delivering reliable estimations of direct recharge and allows a hydraulic characterization of the unsaturated zone.

As concluding remarks, we state the following:

We presented a methodology to apply peak displacement utilizing ^2H_2O as a tracer to determine annual groundwater recharge on a local scale. Deuterium is an appropriate tracer for such applications. Hence, the portfolio of methods for estimating groundwater recharge in data-scarce environments can be extended with such field experiments. A very low amount of tracer is required (less than 500 ml) to obtain reliable results for recharge on deep soils.

At sites with a near-surface impermeable layer, the methodology is difficult to apply due to the fact that at such infiltration underneath the root zone does not take place. It can be expected that during the dry season this water will be utilized by the local vegetation and evaporation. Care needs to be taken when interpreting data at such sites. However, when having the opportunity to gain further insight into processes within the calcretic layers, for example, by deeper drilling, the method might still be useful.

With combined moisture and tracer profiles, calibration and parameterization of transient flow and transport models can be improved in the future potentially leading to more robust models for dry climates and increase understanding of (eco)hydrological processes in complex environments.

The experimental design can be improved in future studies by punctual application of the tracer underneath the root zone. This would eliminate the issues arising with the introduction of artificial water into the soil.

The role of deep-rooting plant species and preferential flow paths for the estimation of groundwater recharge needs to be investigated further, especially in dry climates where plants are adapted to local conditions. This requires interdisciplinary research (e.g. the application of ground penetrating radar or transient electro-magnetic systems). The contribution of preferential flow might be quantified by taking multiple soil cores within the experimental plot. Set-up and calibration of transient flow and transport models will help to quantify such processes. Further research should also be carried out in regard to theoretical considerations of the methodology, in particular to account for heterogeneities within the unsaturated zone. Finally, the potential effect of site-specific upward transport of water should be investigated to decrease the uncertainty of the method further and increase understanding of hydrological processes in semi-arid regions in general. ^2H_2O as a tracer, potentially combined with others, provides opportunities for future studies.

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4 A DEUTERIUM-BASED LABELING TECHNIQUE FOR THE INVESTIGATION OF ROOTING DEPTHS, WATER UPTAKE DYNAMICS AND UNSATURATED ZONE WATER TRANSPORT IN SEMI-ARID ENVIRONMENTS

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4.1 ABSTRACT

Non- or minimum-invasive methods for the quantification of rooting depths of plants are rare, in particular in (semi-)arid regions; yet, this information is crucial for the parameterization of SVAT (Soil – Vegetation – Atmosphere Transfer) models and understanding of processes within the hydrological cycle. We present a technique utilizing the stable isotope deuterium (^{2}H) applied as artificial tracer to investigate the vertical extent of the root zone, characterize water uptake dynamics of trees and shrubs at different depths and monitor transport of water through the unsaturated zone of dry environments.

One liter of 35% deuterated water ($^{2}H_2O$) was punctually applied at several depths (0.5 m, 1 m, 2 m, 2.5 m and 4 m) at six different plots at a natural forested site in the Cuvelai – Etosha Basin (CEB), Namibia/Angola. Subsequently, uptake of the tracer was monitored by collecting plant samples (xylem and transpired water) up to seven days after tracer injection. Soil profiles at the plots were taken after the campaign and again after six months in order to evaluate the transport and distribution of ^{2}H within the unsaturated zone.

Of 162 plant samples taken, 31 samples showed clear signals of artificially introduced ^{2}H, of which all originate from the plots labeled up to 2 m depth. No artificially injected ^{2}H was found in plants when tracer application occurred deeper than 2 m. Results further indicate a sharing of water resources between the investigated shrubs and trees in the upper 1 m whilst tree roots seem to have better access to deeper layers of the unsaturated zone. The soil profiles taken after six months reveal elevated ^{2}H-concentrations from depths as great as 4 m up to 1m below surface indicating upward transport of water vapor. Purely diffuse transport towards the soil surface yielded an estimated 0.4 mm over the dry season.

Results are of particular significance for a more precise parameterization of SVAT models and the formulation of water balances in semi-arid areas. The developed methodology is beneficial for site-specific investigations in complex and data scarce environments, where the root zone plays a major role for the overall water balance. For arid and semi-arid environments experiencing low recharge rates, water transported in its vapor phase is found to play an important role for the overall soil water balance. The use of ^2H_2O is cost – effective and provides the opportunity to investigate multiple effects along the soil – vegetation interface that have been difficult to deal with previously.

4.2 INTRODUCTION

In recent history, two scientific articles raised the recognition of the role of plants within the hydrological cycle to a new level. Jasechko et al. (2013) stated that "transpiration is the largest water flux from Earth's continents, representing 80 – 90 percent of terrestrial evapotranspiration" (Jasechko et al., 2013). One year later, McDonnell (2014) published his idea of what he called *"two water worlds"* hypothesis which is based on the findings that in certain watersheds streams and trees return different pools of water to the hydrosphere (McDonnell, 2014). Even though heavily debated and partially rectified (e.g. Coenders-Gerrits et al., 2014; Schlaepfer et al., 2014), both studies – amongst a number of others (Casper et al., 2003; Hipondoka et al., 2003; Kulmatiski et al., 2010; Verweij et al., 2011) – emphasize the urgent need for an increased number of studies along the soil – plant – atmosphere interface. Despite of advances in applied techniques, measuring root activity is recognized as one of the greatest challenges in plant ecology (Casper et al., 2003; Kulmatiski et al., 2010; Schenk, 2008) and ecohydrology in general. In dry environments, where plant adaptations to the local conditions such as the development of deep tap roots or hydraulic redistribution are common (Canadell et al., 1996; Dawson, 1993; Richards and Caldwell, 1987), it is crucial to obtain information on the lateral and vertical extent of the root zone in order to parameterize SVAT (Soil Vegetation Atmosphere Transfer) and climate models (Schulze et al., 1996). Furthermore, the knowledge of rooting depth and distribution is critical for the calculation of deep percolation and for the identification of thresholds of precipitation duration and intensity that support groundwater recharge (Seyfried et al., 2005). From an ecohydrological perspective, the dominance of certain functional groups (e.g. trees, shrubs, herbaceous plants) or species (Canadell et al., 1996) and effects such as bush encroachment (Hipondoka et al., 2003) or hydraulic redistribution (e.g. (Dawson, 1996, 1993; Prieto et al., 2012; Schulze et al., 1998) are of particular interest. Information on rooting depth and distribution is also highly beneficial for any investigation along the soil – vegetation – atmosphere interface because water is the limiting factor in arid and semi-arid environments (Canadell et al., 1996; Oliveira et al., 2005; Schenk and Jackson, 2005, 2002b; Schulze et al., 1996; Seyfried et al., 2005).

An overview of studies on maximum rooting depths of plants is presented by Canadell et al. (1996). The authors pointed out that plants from environments experiencing a long dry season on average have deepest roots (15 ± 5.4 m). The deepest recorded rooting depths were found in the Kalahari (*Boscia albitrunca* – 68 m, *Acacia erioloba* – 60 m; (Jennings, 1974). Deepest roots can be expected where thick sandy soils are present (Canadell et al., 1996). For such soils, a dependence of maximum rooting depth on rainfall amount and distribution has been found previously (Burke, 2006; Schenk and Jackson, 2002a). On a global scale, results from existing studies have been used in order to map the global distribution of deep roots in relation to climate and soil characteristics (Schenk and Jackson, 2005), to derive parameters for modeling (Zeng, 2001) or to investigate the lateral zone of influence of plants (Casper et al., 2003). Schenk and Jackson (2002b) evaluated existing data and derived relationships for below- and aboveground allometries in water-limited ecosystems.

Different approaches for investigating rooting depths

Traditionally, approaches for investigating root structure and functioning included manual digging, excavation techniques and even the use of dynamite throughout the 20th century (Canadell et al., 1996). Schulze et al. (1996), for example, excavated trenches of 5-10 m length and 3 m depth to investigate rooting depths in Patagonia. Jennings (1974) made a rather coincidental finding during borehole drilling in Botswana: They found roots of *B. albitrunca* and *A. erioloba* at 68 m and 60 m depth, respectively. In contrast, Ringrose et al. (2000) found no evidence of roots appearing deeper than 6 m in a similar environment (Ringrose et al., 2000). Since the beginning of the new century, innovative techniques have developed with different approaches.

Ground-penetrating radar (GPR), for instance, has been utilized in several studies (Bassuk et al., 2011; Butnor et al., 2003; Hruska et al., 1999; Raz-Yaseef et al., 2013; Stokes, A. et al., 2002). The technique was shown to be a reliable, non-invasive method for the location of roots and the determination of bulk root densities. However, bulk root density has been found to be not a good indicator for root activity (Kulmatiski et al., 2010). Jackson et al. (1999) used caves and DNA to derive ecosystem rooting depths and were able to assign roots to plant species up to 65 m depth (Jackson et al., 1999). Regardless of these recent developments, traditional methods are still common (Hipondoka and Versfeld, 2006; Rings et al., 2013) and challenges remain.

Approaches based on stable isotopes of water

Techniques utilizing stable isotopes of water (deuterium, ^{2}H and oxygen-18, ^{18}O) as environmental or artificial tracer (subsequently, we refer to as 'labeling') have been found to be particularly suitable for plant-related studies and are used extensively (Casper et al., 2003). In early studies, Allison et al. (1984) evaluated the effect of climate and vegetation on water stable isotope composition (Allison et al., 1984). Other applications of environmental isotopes include the identification of water use strategies of certain species (i.e. Brunel et al., 1995; Chimner and Cooper, 2004; Edwin et al., 2014; Li et al., 2007), changes in water-use strategies (Wu et al., 2013), quantifications of preferential flow (Stumpp and Maloszewski, 2010) and investigations on hydraulic lift (Ceperley et al., 2014). Dawson et al. (2007) used measurements of stable isotopes in woody plants to identify nighttime transpiration (Dawson et al., 2007).

Artificial applications of the stable isotope deuterium (^{2}H) are only now becoming increasingly popular in hydrology and soil sciences. Labeling with deuterated water ($^{2}H_2O$) is of advantage because it is not radioactive and has no toxicological concerns during both labeling and measurement (Becker and Coplen, 2001), compared to the previously used tritium (^{3}H). Being part of the water molecule, ^{2}H is considered a conservative tracer and therefore ideal for studies in the unsaturated zone (Koeniger et al., 2010). It can be measured in very low concentrations (Becker and Coplen, 2001); therefore only small amounts of tracer are necessary and experiments become economically feasible. It has been shown previously that the use of artificial ^{2}H enables a quantification of transpiration (i.e. Calder et al., 1986, 1992; Lambs and Saenger, 2011; Marc and Robinson, 2004). Meinzer et al. (2006) used $^{2}H_2O$ to study the dynamics of water transport in conifers and found maximum sap flow velocities of 2.4 – 5.3 m d^{-1} (Meinzer et al., 2006). Studies directly related to root distribution are, however, rare and limited to shallow depths (e.g. Bishop and Dambrine, 1995; Hawkins et al., 2009; Peñuelas and Filella, 2003; Plamboeck et al., 1999; Sternberg et al., 2005). Only one attempt was made to use artificial $^{2}H_2O$ to investigate the spatiotemporal distribution of plant water use of trees and grasses in a tropical savanna (Kulmatiski et al., 2010) to a maximum depth of 120 cm. It is this latter investigation by Kulmatiski et al. (2010) that prompted the idea for the present study. The authors injected ^2H_2O at four different depths (5, 20, 50 and 120 cm) and analyzed plant samples taken from up to five meters distance from the labeled plots in order to test the two-layer hypothesis (Walter, 1971). This theory suggests that woody plant species develop deep roots to escape competition with grasses at shallow depths. The findings by Kulmatiski et al. (2010) do not support this theory and are of high relevance for future research. Based on their studies, one could also investigate water uptake by plants from deeper regions of the unsaturated zone (which is essentially the purpose of this study).

In numerous studies ^2H_2O was applied as artificial tracer to investigate water movement in the unsaturated zone. Applications include studies of preferential flow (Hangen et al., 2005; Schumann and Herrmann, 2001; van der Heijden et al., 2013), transport velocities (Blume et al., 1967; Koeniger et al., 2010; Mali et al., 2007; Saxena, 1984a, b; Zimmermann et al., 1966) and capillary rise (Grünberger et al., 2011). Koeniger et al. (2010) conclude ^2H_2O to be a suitable water tracer extending possibilities for field studies in the field of biogeosciences. Allison et al. (1994) state that in dry areas with sandy soils and high porosity water vapor transport might diffuse a tracer into soil and groundwater systems (Allison et al., 1994). Similarly, several researchers studied the possibility of upward water vapor transport, but clear experimental evidence from the field is lacking (DePaolo et al., 2004; Dincer et al., 1974; Phillips et al., 1988b; Scanlon, 1992; Soderberg et al., 2012; Walvoord et al., 2002a, 2002b).

In the past ^2H_2O has primarily been used at shallow depths. Experimental setup is difficult for deeper application of the tracer, which might enable investigating water uptake dynamics not only in lateral direction, but also in the vertical direction. As shown above, a number of processes within the soil – vegetation – atmosphere interface of arid and semi-arid environments have been difficult to investigate and describe in the past. In particular, the determination of rooting depth and water uptake dynamics remains challenging, especially with non- and minimally invasive methods. Although it is possible to investigate bulk root mass with currently available methods (i.e. ground-penetrating radar techniques), water transport mechanisms remain challenging to characterize mainly because bulk root mass has been found to not be a good indicator of root activity (Kulmatiski et al., 2010). Rooting depth and depth-specific applications of ^2H_2O, on the other hand, provide a measure for root activity; hence, any advance in quantifying rooting depth and evaluating water uptake from different depths is beneficial.

The scope of our investigation is to combine a comprehensive analysis of depth-dependent water uptake dynamics and monitoring water transport through individuals of multiple plant species and within the unsaturated zone using a minimally invasive experimental procedure employing ^2H_2O as an artificial tracer. In particular, our objectives are:

i) to propose and test a methodology to investigate rooting depths in semi-arid environments;

ii) to investigate depth-dependent water uptake dynamics and access of different plants to soil water reservoirs; and

iii) to monitor water transport within the unsaturated zone, in particular to assess vapor phase movement during the dry season in a semi-arid environment.

The experimental design and sampling strategy further allows as a sub goal to iv) investigate if indicators for processes such as hydraulic redistribution (e.g. displacement of tracer towards shallow depths) can be identified at the studied site. To our knowledge, deuterium labeling has not yet been carried out deeper than 2 m below ground. Similarly, the tracer has not been used to quantify rooting depths before.

4.3 MATERIALS AND METHODS

4.3.1 STUDY AREA

The Cuvelai – Etosha Basin (CEB) is a transboundary endorheic watershed shared almost equally by Angola and Namibia with a total size of 173,000 km^2. A digital elevation model of the CEB is presented in Figure 4.1. The Cuvelai – Etosha region is home to a large number of people both on the Namibian and Angolan side, mainly due to the fact that shallow groundwater and relatively fertile soils are accessible to many areas (Mendelsohn et al., 2013). The basin has vivid hydrogeological history as both the deltas of the Cunene and Okavango Rivers were once situated within the CEB (Lindenmaier et al., 2014; Miller et al., 2010). In recent history, a deep aquifer containing fresh water was discovered in the northeastern part of the basin (Lindenmaier et al., 2014), likely a remainder of the former Okavango Delta. At present all of its surface water is either draining towards the Etosha Pan, an enormous salt pan in the southern part of the CEB, or remains in surface depressions (locally called *iishana)* that are forming a vast, partly inter-connected channel-like system north-west of Etosha Pan. No perennial river exists and the basin receives all of its water concentrated over the rainy season from November to April. Mean annual precipitation on the Namibian side varies between 200 and 600 mm y^{-1} along a distinct rainfall gradient from the west to the east of the basin (Mendelsohn et al., 2013). In the Angolan Highlands, mean rainfall can reach up to 1500 mm y^{-1} (Mendelsohn et al., 2013). Temperature average throughout the basin is greater than 22°C with maximum values reaching up to 40°C in summer (Mendelsohn et al., 2013). In winter temperatures can drop to around zero at night. Evaporation rates can reach up to 3000 mm y^{-1} and exceed yearly rainfall by a factor of five.

The study site chosen for our experiment (Elundu) is situated in the Eastern Sand Zone (Figure 4.1). It is characterized by deep Kalahari sand (locally up to 400 m deep), a remainder of the former Okavango Delta. Around the study site the pure sand can reach depths of several hundred meters and deep infiltration of rain water can be expected. Resulting from visual inspection and preliminary irrigation experiments, no hydrophobic behavior of the soils was observed. At the top layer (first 3 cm) a biological soil crust was identified which likely developed due to extreme temperatures and dryness during the Namibian winter in combination with microbiological activity. Within the first 20 cm below surface fingered like flow was observed during irrigation experiments using dye tracer. The soil is homogeneous and according to its soil hydraulic properties highly permeable (refer to Table 4.2). In this area rainfall is higher than anywhere else on the Namibian side of the catchment and can reach up to 700 mm y^{-1}. Figure 4.2 shows the mean monthly precipitation for the closest meteorological station with long-term records, namely Ondangwa. Over time these favorable conditions in terms of rainfall allowed a forest with trees as high as 20 m to develop. Mendelsohn et al. (2013) categorize the vegetation type as north-eastern Kalahari woodland (Mendelsohn et al., 2013). Tree species consist of *A. erioloba (Camelthorn), Baikiaea plurijuga (Zambezi teak), Combretum collinum (Red bushwillow)* and, in a lower abundance, *Terminalia sericea (Silver cluster leaf), Ochna pulchra (Mermaid tree)* and *Erythrophleum africanum (Ordeal tree).* Especially the large trees are often almost circular surrounded by a high number of *Salacia luebertii (Wild mango)*, which is the dominating shrub throughout the forest. Even in the rainy season no grass cover can be found, which might be explained by overgrazing and subsequent bush encroachment (Hipondoka et al., 2003). The groundwater table on site (also called 'perched aquifer') is situated approximately 30 m below surface (Lindenmeier et al., 2014; Miller et al., 2013). The recently discovered deep, artesian aquifer (namely Ohangwena II) is located at greater depths. The origin of water in this deep freshwater reservoir is not known until now (Lindenmaier et al., 2014); hence, extensive research is conducted currently to determine its recharge areas and mechanisms.

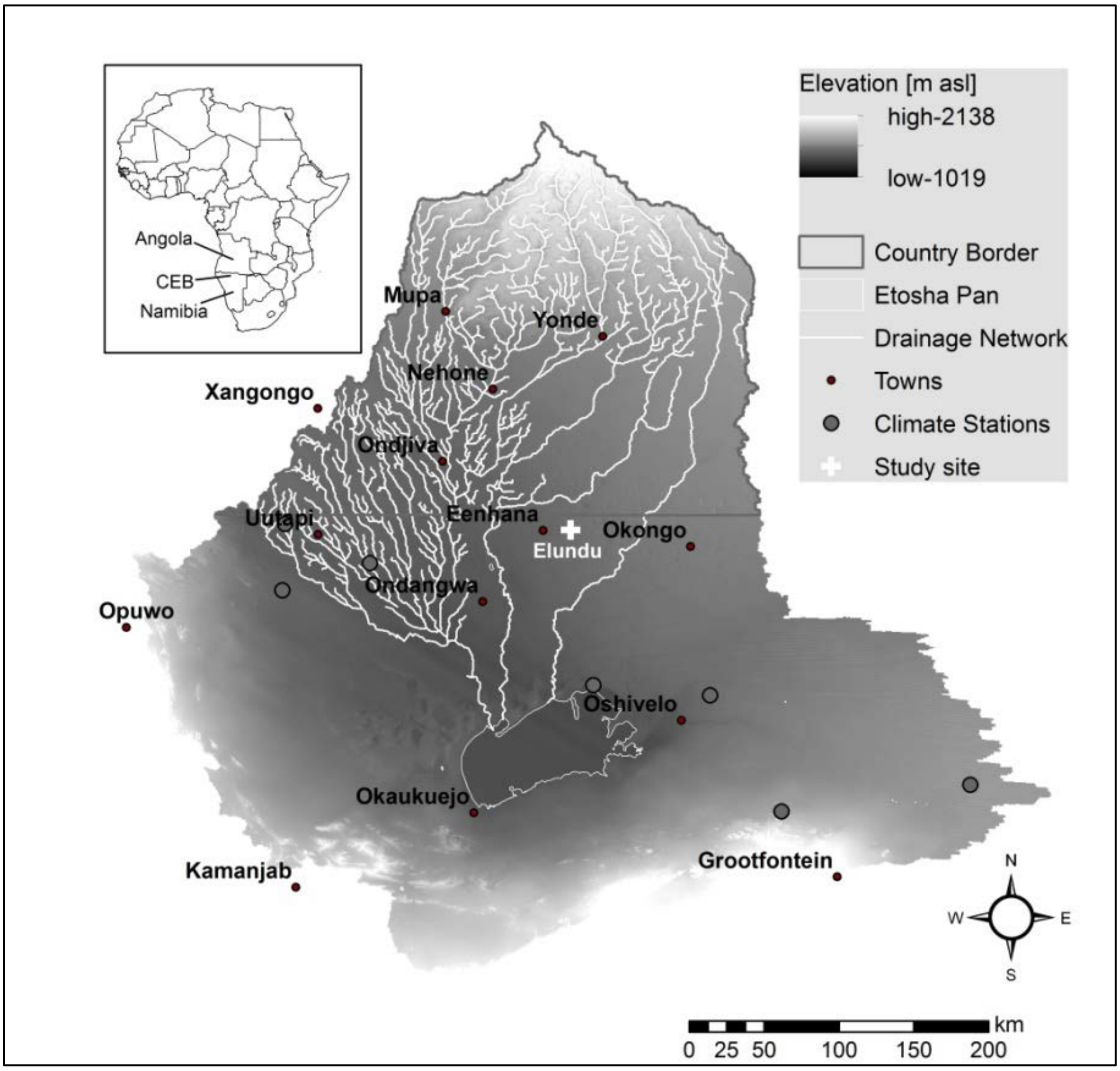


Figure 4.1: Digital Elevation Model (DEM) and drainage network of the Cuvelai–Etosha Basin (CEB). The study site (Elundu) is located in the Eastern Sand Zone. Marked are climate stations implemented within the framework of SASSCAL (Southern African Science Service Centre for Climate Change and Adaptive Land Management) and major towns.

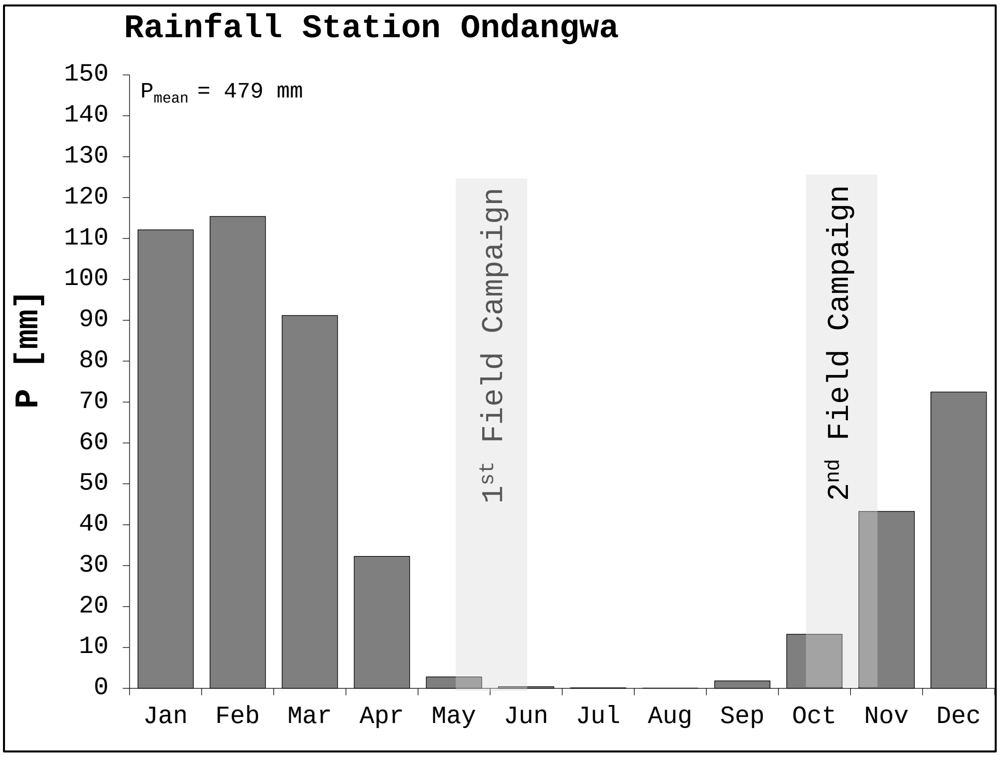


Figure 4.2: Mean monthly precipitation at the closest meteorological station with longer term records (1902 – current). The two field campaigns relevant for the present study took place at the beginning and end of the dry season, respectively.

4.3.2 ^2H_2O TRACER EXPERIMENT: SETUP, TRACER INJECTION, SAMPLING PROCEDURE AND ANALYSIS

Six quadratic plots (1 m²) were chosen within the study area. When establishing the plots, it was desired to have at least one individual of the main species under investigation (which are the most abundant: *B. plurijuga*, *A. erioloba* and *S. luebertii*) around each of the plots. However, this was practically difficult and could not be achieved for all plots (see Appendix A). We also aimed on choosing trees with similar heights at the plots to allow comparability. For the main species under investigation, preferably adult individuals were chosen. A minimum distance of 100 m between the plots was assigned, so that the tracer injection at the treated plots would not interfere with one another. This assumption neglects the possible occurrence of mycorrhizal fungi, which have been associated to water transport through soils (Allen, 2007; Duddridge et al., 1980; Plamboeck et al., 2007). Considering the time-scale of this experiment, however, transport over distances greater than 100 m seems unlikely. Hence, we treat potentially present fungal species as a major unknown, since micobiological feedbacks are not the scope of this research. The targeted injection depths (0.5, 1, 2, 2.5 and 4 m) were assigned randomly to the plots. An additional plot with a targeted injection depth of 4 m was established close to a *B.*

plurijuga surrounded by numerous individuals of *S. luebertii*. This additional plot was established because at the initial 4 m plot, no individual of *B. plurijuga* was present, but this species was one of the targeted. In addition we observed that individuals of *B. plurijuga* (and *A. erioloba*; compare the second plot with 4 m target depth) were often surrounded by a circle of *S. luebertii*, a small shrub that is well-supplied with water even at the end of the rainy season, when top soils are already dry. One explanation for this could be some kind of hydraulic redistribution through the roots (tap root or lateral) of *B. plurijuga*. In order to examine this, a label was placed close to the stem. If hydraulic redistribution occurs within the experimental time-frame, the upper part of the soil would display elevated concentrations of ^2H.

At each plot (with exception of the above mentioned additional plot), three holes were drilled until the target depth using a hand auger. The extracted soil was stored separately for each hole. A schematic illustration of the plots and plant distribution around each plot is depicted in Appendix A.

Subsequently, five small balloons were filled with a 35% ^2H_2O solution using a custom-made syringe. Each balloon had a capacity of ~ 65 ml resulting in a total amount of ~ 325 ml per hole or ~1 l per plot, respectively. The balloons were attached to a thin cord and then inserted into the holes. A wooden stick with a metal tip was then used to destroy the filled balloons at the target depth. Prior investigations carried out on site to explore the labeled volume showed that per cord or injection hole (five balloons) surrounding soil was wetted 20 cm in horizontal and 30 cm in vertical direction. This corresponds to a total labeled soil volume of 0.14 m^3 (144000 cm^3) for the plots with three holes and 0.048 m^3 (48000 cm^3) for the plot with one hole, respectively. After the labeling procedure the soil taken out with the hand auger was carefully re-inserted into the holes. This setup allows investigating for each plot, if the surrounding plants sampled have access to the injected water, i.e. if a plant root would be present in the labeled soil compartment, immediate uptake can be assumed due to the fact that the rest of the soil is dry. We explicitly aim at the investigating the vertical extent of the lateral root zone and exclude a potentially present deep, groundwater-penetrating tap root which has been found by previous researchers (Canadell et al., 1996; Schulze et al., 1996). The importance of such deep roots differs depending on the ecosystem. In the Amazonian forests, for example, the impact of deep roots has been shown to be significant (Nepstad et al., 1994; Oliveira et al., 2005). In a mesic savanna the effects of severing deep taproots were found to be rather small in recent studies (Verweij et al., 2011). The method presented here is not suitable for the investigation of deep tap roots, mainly because of the limitation to which holes can be dug using a hand auger. Figure 4.2 illustrates the experimental setup and depicts the common understanding of root structure and water transport processes at the soil – vegetation interface.

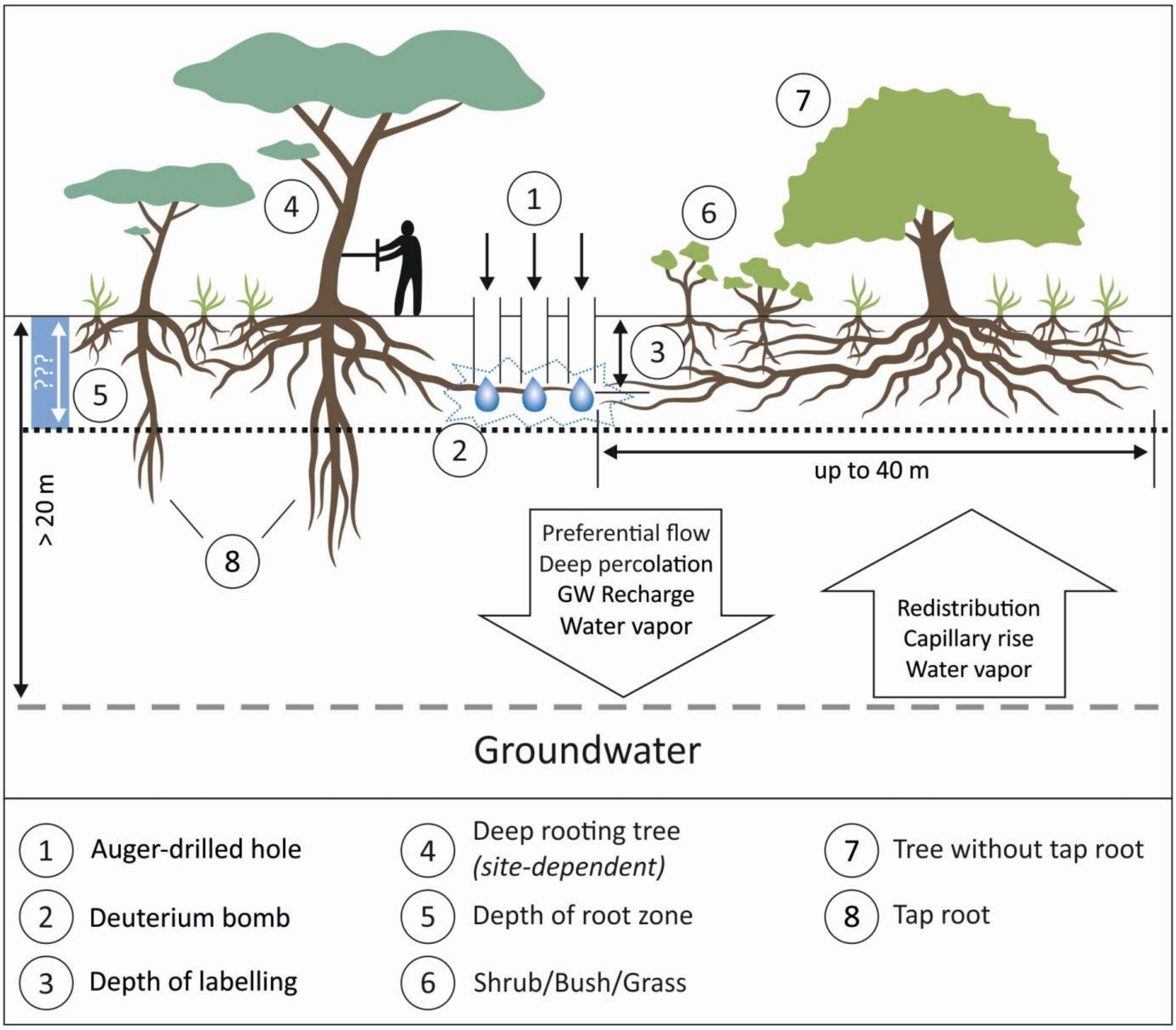


Figure 4.3: Schematic visualization of the tracer application via the auger-drilled holes and the typical composition of different functional groups (grasses, shrubs, trees) typically present in semi-arid environments. Notes: **Deep penetrating tap roots are common in dry environments, but species-, soil- and climate dependent and not necessarily present at the study site. Grasses were not present at study site.**

Starting two days before the injection of ^2H_2O, plant samples were taken at the established plots as well as throughout the study site in order to obtain background isotopic concentrations. During the experiment control samples were collected from all species under investigation at non-labeled locations at different times every day. We used both xylem and transpired water samples for the analysis. Xylem sampling took place only once per day to avoid harm to the trees under investigation, using an increment borer, whereas bags for collecting transpired water (Calder et al., 1986, 1992a; 1992b; Edwin et al., 2014; Lambs and Saenger, 2011; Luvall and Murphy, 1982) were used at least twice per day. The xylem samples were taken at chest height and only suberized stems were sampled (Dawson and Ehleringer, 1993). In comparison to xylem, which has to be vacuum-extracted in the laboratory, the transpiration samples can be measured directly. Fractionation, however, becomes relevant and has to be accounted for when using the stable isotopes of water as an environmental tracer. For our study using very high concentrations of ^2H_2O this was not relevant: if a plant takes up deuterium one would be easily able to distinguish between fractionation and artificial ^2H_2O because of the high input concentration of the tracer (35 % ^2H_2O); hence the sampling with transpiration bags is useful. Following the assumption of xylem flow rates of 1-5 m d^{-1} (Fravolini et al., 2005; Meinzer et al., 2006) we assigned a sampling period of 5 days to assure that potential uptake even in the deepest of the drilled holes can be detected. In total, 162 plant samples were collected. Xylem cores were split into three replicates and extracted separately in order to improve the measurement accuracy. Additionally, the upper 50 cm of the soil at each plot was sampled for 2H concentrations 7 days after the experiment to examine if hydraulic redistribution took place. These soil samples were collected at a vertical resolution of 10 cm with an *Eijkelkamp* hand auger. For a long-term investigation of upward water transport within the soil, deep soil profiles were taken after the dry season within the carefully marked (using GPS and local markers) plot extent. In total, 109 soil samples were collected throughout the two campaigns.

Due to the small amount of tracer necessary, this method can be regarded being cost-effective. The price of 70 % ^2H_2O is currently 200 € per kg. For the experiment at the six plots approximately 3 kg were used (500 ml 70% ^2H_2O plus 500 ml tap water per hole). Sample analysis at BGR (*Federal Institute for Geosciences and Natural Resources, Hanover, Germany*) is currently 20 € per sample, but with increasing popularity of using stable isotopes the prices constantly decrease. For 162 plant and 109 soil samples this equals to around 5500 €. This results in an overall cost of such an experiment far below 7000 € (and the sample amount, especially for soil samples, can be minimized in future studies). As alternative tracer, only tritium or oxygen-18 could be used (because they will equally be taken up by plants). Oxygen-18 is about 100 times more expensive than deuterium (Speakman, 1997). Tritium is, due to its toxic character, not allowed anymore in most countries. As stated, at present other methods in the unsaturated zone are not available at present other than manual excavation.

Gravimetric water content of the soil samples was determined after drying the samples for 24 h at 105°C. Grain size distribution was derived by dynamic image analysis. For fine soils the grain size distribution smaller than 63 µm was analyzed by sieving and sedimentation (Altuhafi et al., 2013). Soil hydraulic properties and saturated conductivity were obtained in the laboratory using the evaporation method (Schindler et al., 2010). Saturated conductivity was additionally examined in the field using a double ring infiltrometer.

The transpired water, xylem and soil samples were stored in headspace glass vials and sealed with a crimping device. Transpired water samples were measured maximum two weeks after collection in the laboratory. For the extraction of water from xylem and soil samples cryogenic vacuum distillation was used, which is described in detail by West et al. (2006) and was modified for higher throughput by Koeniger et al. (2011). We slightly modified the method again by using a custom-made aluminum block as heating device in order to achieve higher and more stable temperatures within the vials. Despite recent developments of measuring stable isotopes in-situ (Gaj et al., 2016; Volkmann and Weiler, 2013), cryogenic vacuum extraction remains the most commonly used method and applied for soil, xylem, and plant water (Hangen et al., 2005; Koeniger et al., 2011; West et al., 2006). We used extraction times of 120 min for xylem samples and increased the extraction temperature to 180°C because pre-investigations showed signs of incomplete extraction of water when using lower temperatures.

The extracted water samples were analyzed for ^{2}H concentrations using a Picarro L2120-i cavity – ringdown (CRD) water vapor analyzer after vaporization. Isotope values are expressed in δ-notation in per mill [‰] following the definition of Coplen (2011) given in equation 4.1 (Coplen, 2011):

$$\delta\ ^{2}H/^{18}O = \left[\frac{(R_{Sample})}{(R_{Standard})} - 1\right] \cdot 1000 \quad \text{(eq. 4.1)}$$

where R_{Sample} is the ratio ($^{2}H/^{1}H$ or $^{18}O/^{16}O$) of the less abundant to the more abundant isotope in the sample and $R_{Standard}$ the ratio ($^{2}H/^{1}H$ or $^{18}O/^{16}O$) in a standard solution, respectively. The analytical long-term precision for a quality standard (non-labeled sample) is 0.1‰ for ^{18}O and 0.8‰ for ^{2}H, respectively. For highly elevated concentrations of ^{2}H the standard deviation can be up to 5 times higher. The samples were corrected for drift and memory using the procedure described in van Geldern and Barth (2013). The software *ChemCorrect*™ (*Picarro Inc., Santa Clara, CA, USA*) was used to check whether organic contamination was an issue. Contaminated samples should be ignored for further analysis; however, this was not an issue in any of the taken samples.

The deuterium excess (*d*) is a measure of fractionation (or, isotopic enrichment) of individual samples and can was calculated using the relationship proposed by Dansgaard (1964):

$$d = \delta^2H - 8\delta^{18}O \qquad \text{(eq. 4.2)}$$

The lower *d*, the more evaporation occurred. The deuterium excess therefore is an important measure for the degree of fractionation a sample was exposed to. It can also be used as a quality check for the cryogenic vacuum extraction (i.e. if *d* is unreasonably high, it could indicate incomplete extraction).

In order to identify whether tracer was present in a sample we use an adaptation of the criteria proposed by Kulmatiski et al. (2010). If a sample had a ^2H – concentration with at least four standard deviations (*std*) higher than the background value (control samples), tracer was assumed to be present (Kulmatiski et al., 2010 used two *std*). We therefore applied a linear regression to all samples belonging to one type of sampling (T – transpiration bag or X – xylem) containing no artificial ^2H (which is the control or background samples) and then defined a four-*std*-line for each. This resulted in a robust criterion for an objective evaluation of the samples and takes into account contingently occurring differences in isotopic ratios in particular for the samples collected in transpiration bags.

4.4 RESULTS

4.4.1 EVALUATION OF ISOTOPIC SIGNATURES

In Figure 4.4 the dual-isotope plot for δ^2H and δ^{18}O is presented.

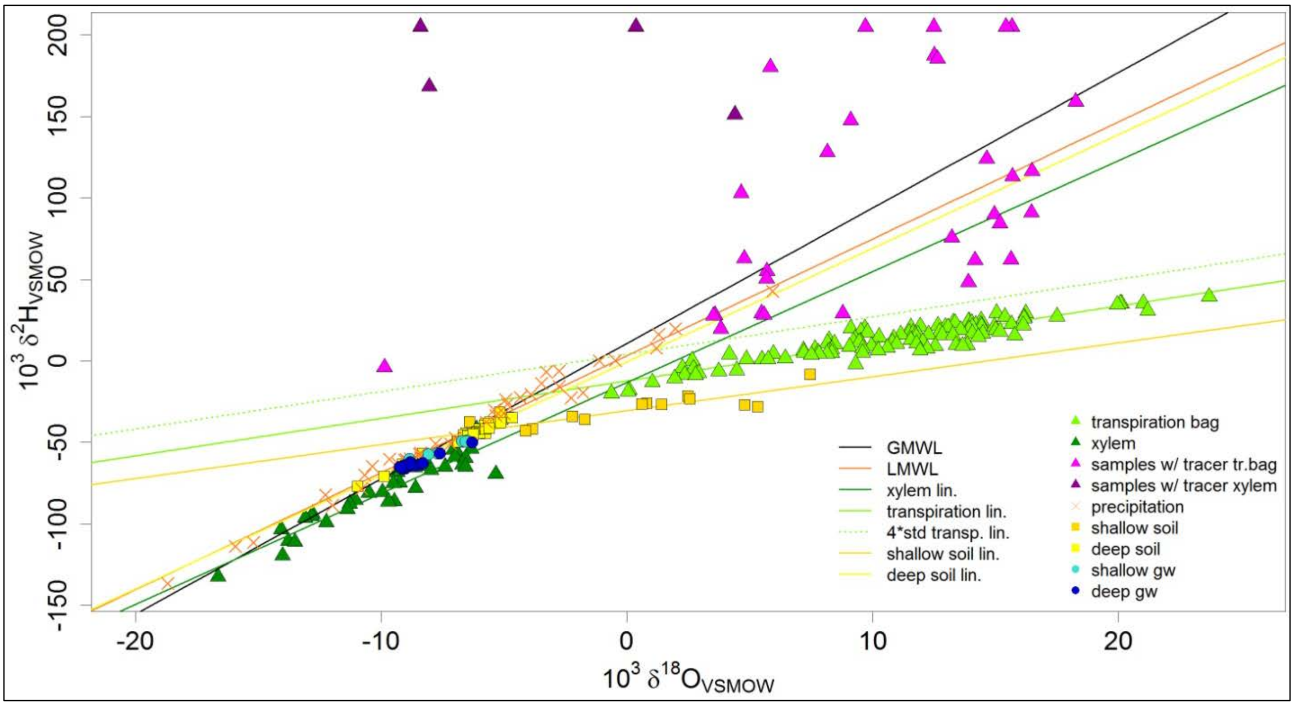


Figure 4.4: Dual-isotope plot of all samples collected and analyzed throughout the field campaigns. All plant samples taken are indicated by triangles. Violet symbols represent samples clearly containing artificial ^{2}H. The equations of the regression lines are compiled in Table 4.2.

The graphic displays the isotopic compositions of local precipitation, soil water, groundwater (shallow and deep) and plants (xylem and transpired water). Precipitation and groundwater data was obtained during previous campaigns using a recently developed cumulative rain sampler (Gröning et al., 2012) and groundwater pumping at observation wells, respectively. Figure 4.4 further shows the global (GWML) and local (LWML) meteorologic water lines as well as a transpiration line and the four-*std*-line for the objective decision whether a sample contains artificial ^{2}H or not.

Of the 162 plant samples collected, 31 clearly contained artificial ^{2}H. Separated by sample type, 4 of 48 xylem and 27 of 114 transpiration samples, respectively, displayed highly elevated values for ^{2}H concentrations (displayed in violet colors in Figure 4.4). The highest measured concentration was slightly above 2000‰ and found in a xylem sample of a tall individual of *B.*

plurijuga. The maximum encountered concentration in transpiration samples was 825‰, encountered for the same species. Further statistics of the experiment are compiled in Table 4.1.

Table 4.1: Summary of the experiments related to rooting depth and water uptake dynamics at the six plots.

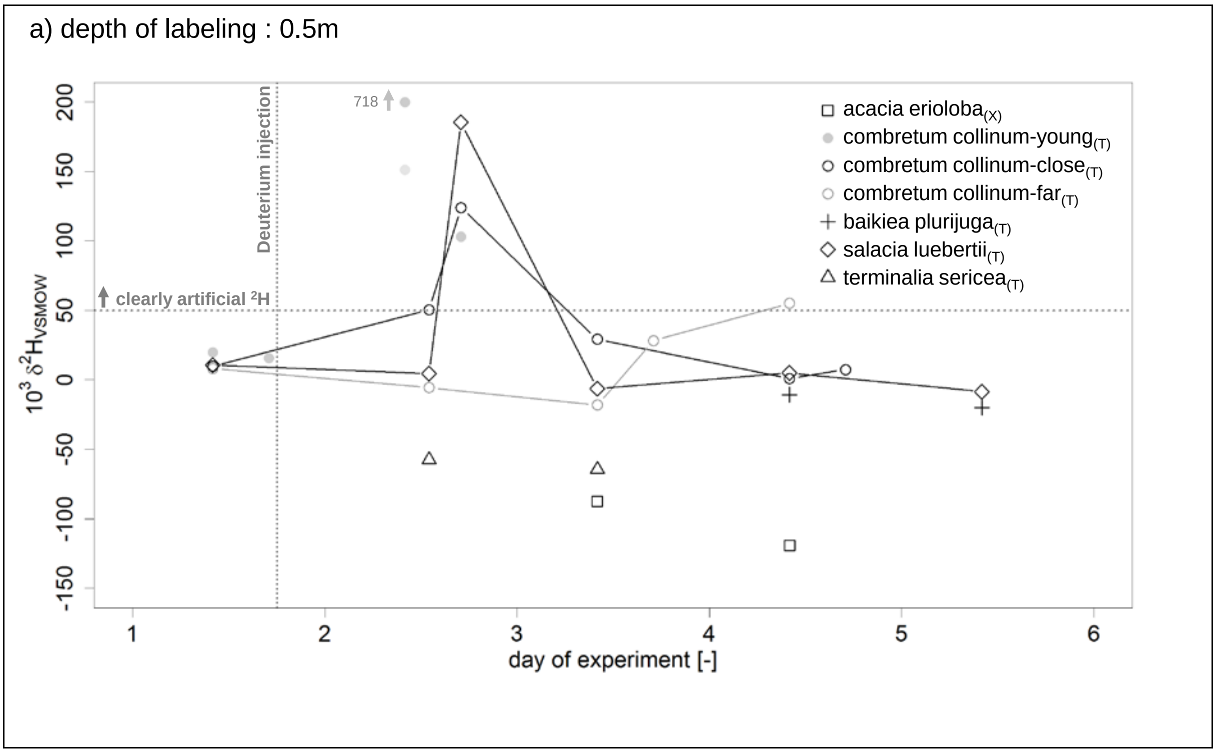
Vegetation type	Kalahari woodland/forest	
Dominant plant species (main focus of investigation)	*Baikiea plurijuga (Zambezi Teak); Acacia erioloba (Camelthorn); Salacia luebertii (Wild mango)*	
Other plant species investigated	*Baikiea plurijuga (Zambezi Teak); Acacia erioloba (Camelthorn); Combretum collinum (Kalahari Bushwillow);Salacia luebertii (Wild mango); Terminalia sericea (Silver cluster leaf); Erythrophleum africanum(Ordeal tree); Ochna pulchra (Mermaid tree)*	
mean isotopic composition of background samples	**$\delta^{18}O$ / $\delta^{2}H$ / d-excess [‰]**	
	xylem samples	**transpiration bag samples**
▪ all samples	-8.9 / -72.1 / -1	8.9 / 7.3 / -64
▪ *Baikiea plurijuga*	-7.4 / -60.4 / -1	12.3 / 16.3 / -82
▪ *Acacia erioloba*	-10.1 / -82.0 / -1	10.9 / 11.5 / -7
▪ *Combretum collinum*	-9.8 / - 73.6 / 5	7.8 / 5.4 / -57
▪ *Salacia luebertii*	-8.7 / -75.3 / -6	10.7 / 14.6 / -71
▪ *Terminalia sericea*	-7.5 / -60.9 / -1	-
▪ *Erythrophleum africanum*	-10.0 / -80.4 / -1	5.0 / -7.8 / -48
samples containing ^{2}H	**no. of samples with $^{2}H_2O$ (total no. of samples)**	
▪ total	31 (162)	
▪ depth of labeling: 0.5 m	10 (29)	
▪ depth of labeling: 1 m	9 (37)	
▪ depth of labeling: 2 m	10 (28)	
▪ depth of labeling: 2.5 m	0 (17)	
▪ depth of labeling: 4 m	0 (29)	
▪ depth of labeling: 4 m near stem	2 (22)	
farthest species with ^{2}H found [species / lateral distance to labeling]	*Combretum collinum* / 6 m	
deepest uptake [species / vertical distance to labeling]	*Salacia luebertii* / 4 m	
highest concentration of ^{2}H encountered for xylem samples [species / concentration]	*Baikiea plurijuga* / 2015‰	
highest concentration of ^{2}H encountered for transpiration samples [species / concentration]	*Baikiea plurijuga* / 825‰	
regression coefficients & coefficient of determination (R^2)	**$\delta D = sl\ \delta^{18}O + b$**	
▪ xylem samples	sl = 6.80; b = -13.17; R^2 = 0.90	
▪ transpiration samples	sl = 2.29; b = -12.17; R^2 = 0.86	
▪ precipitation samples (LMWL)	sl = 7.31; b = 5.38 ; R^2 = 0.97	
▪ shallow (< 0.5 m) soil water samples	sl = 2.08; b = -30.42; R^2 = 0.79	
▪ deep (> 0.5 m) soil water samples	sl = 6.96; b = -0.50; R^2 = 0.97	

From the samples not containing artificial deuterium, a clear separation of the xylem and transpiration samples due to fractionation during the latter process can be identified (light and darker green symbols in Figure 4.4, respectively).

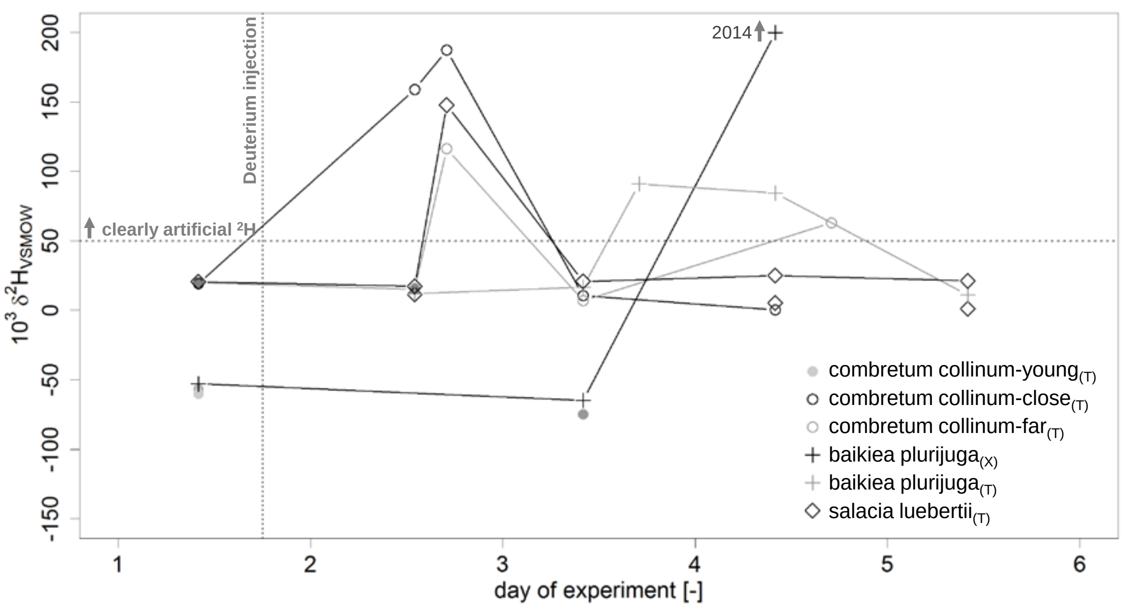
The mean of the deuterium excess over all background samples, – 1 for xylem and – 64 for transpiration bag samples, respectively, emphasizes the high influence of the latter method of sample collection on fractionation. Non-artificially-enriched samples for both sampling types fall on a distinct line each. The transpiration line has a slope (*sl*) of 2.3 with a coefficient of determination (R^2) of 0.86 and is displaced from the LMWL (*sl* = 7.3, R^2=0.96). The transpiration line falls on an approximate parallel to the regression line of shallow soil water isotopes (depth < 0.5 m; *sl* = 2.1, R^2=0.79). Deep soil water (depth > 0.5 m) plots mainly in the range of isotopic values for precipitation and groundwater and shows very little enrichment (*sl* = 7.0, R^2=0.97). Analysis of the xylem samples yielded in values of 6.8 for *sl* and 0.9 for R^2, indicating no (or negligible) influence of evaporation on the source water. A number of xylem samples plot in the same area on the plot as the analyzed groundwater samples (both shallow and deep). Almost half of the taken non-artificially-enriched xylem samples show isotopic ratios depleted in heavy isotopes which coincide with those measured in precipitation.

4.4.2 ROOTING DEPTH AND WATER UPTAKE DYNAMICS

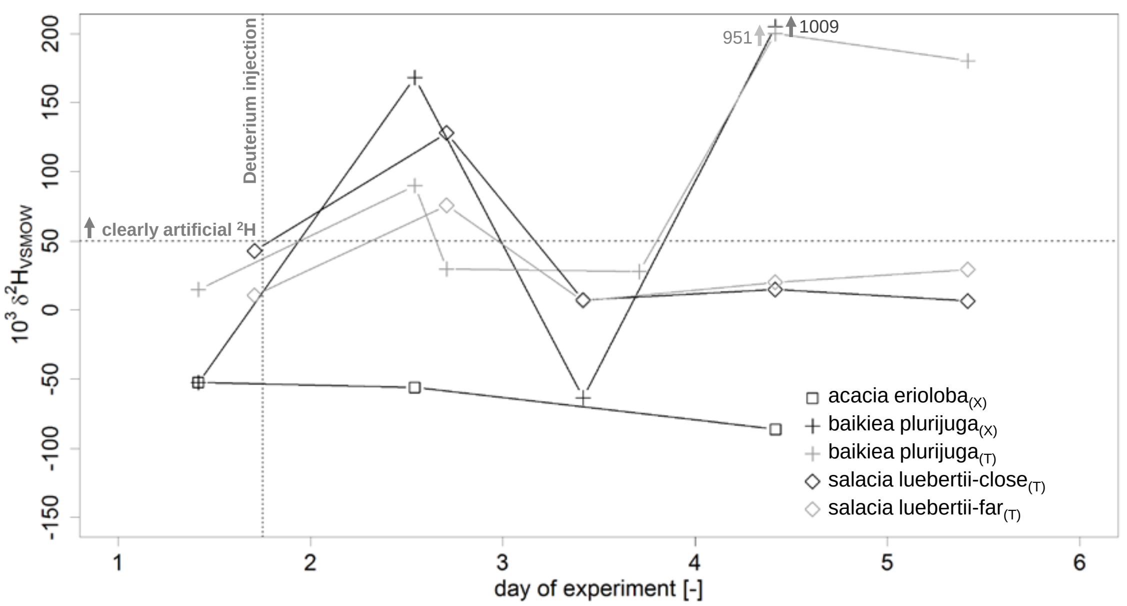
By evaluating the course of ^2H concentrations for each experimental plot over time an approximation of rooting depths for the species of interest and water uptake dynamics can be derived. The temporal evolution of isotope ratios for each plot is presented in Figure 4.5a–f. In the graphic, we use indicators for each plant (e.g. 'far', 'young', etc.) in accordance to Appendix A. For a differentiation of the sampling type the subscripts '(T)' and '(X)' are used for transpiration bag or xylem samples, respectively.



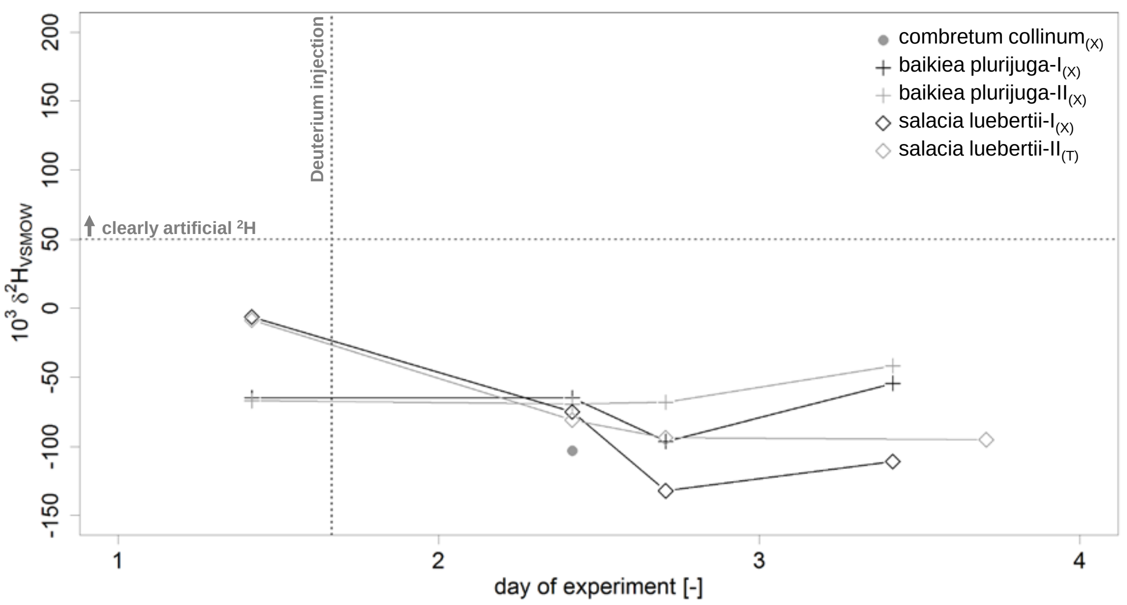
b) depth of labeling : 1m



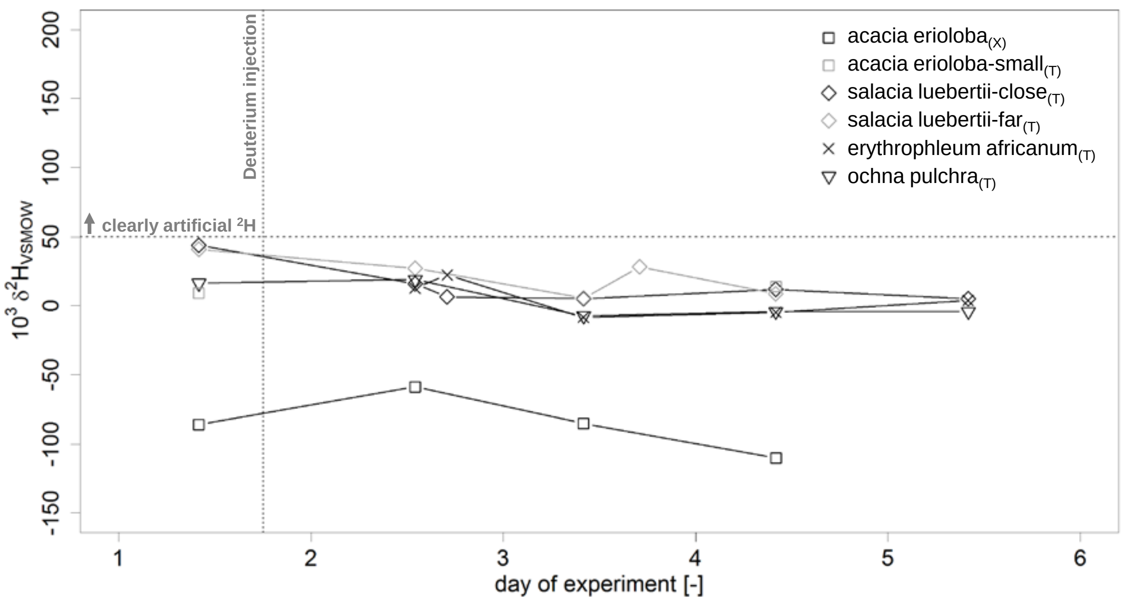
c) depth of labeling : 2m



d) depth of labeling : 2.5m



e) depth of labeling : 4m



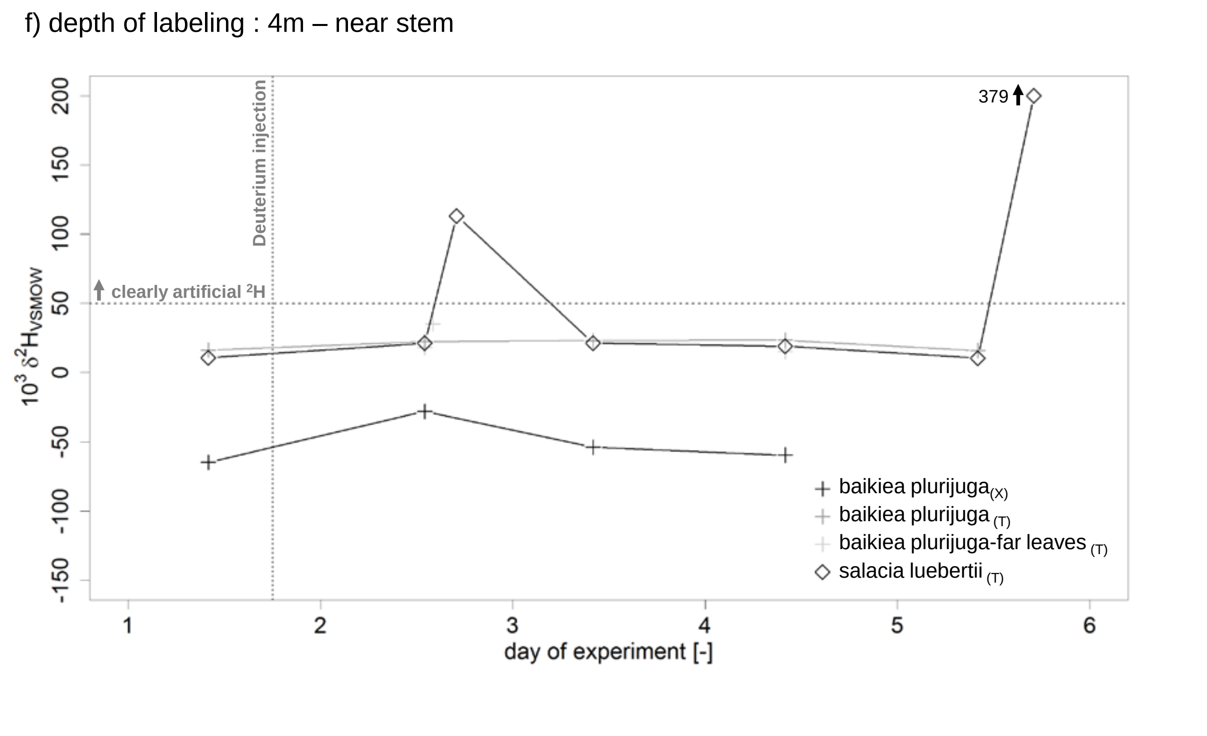


Figure 4.5: Dynamics of tracer uptake during the course of the experiment for labeling depths of a) 0.5 m, b) 1 m, c) 2 m, d) 2.5 m, e) 4 m and f) 4 m (near stem of B. plurijuga). In the graphic indicators for each plant (e.g. ‹far›, ‹young›, etc.) are employed in accordance to Appendix A. For a differentiation of the sampling type the subscripts '(T)' and '(X)' are used for transpiration bag or xylem samples, respectively. For simplification, a line was inserted above which samples are clearly artificially enriched in ^{2}H. Symbols not connected by lines represent additional (control) samples taken at the particular plot.

As can be seen in the figure, the dynamics of the uptake of ^{2}H by different plant species can be tracked to a depth of 2 m. At the deeper labeled plots, no artificial tracer was found besides two samples of the shrub species *S. luebertii* (refer to discussion section).

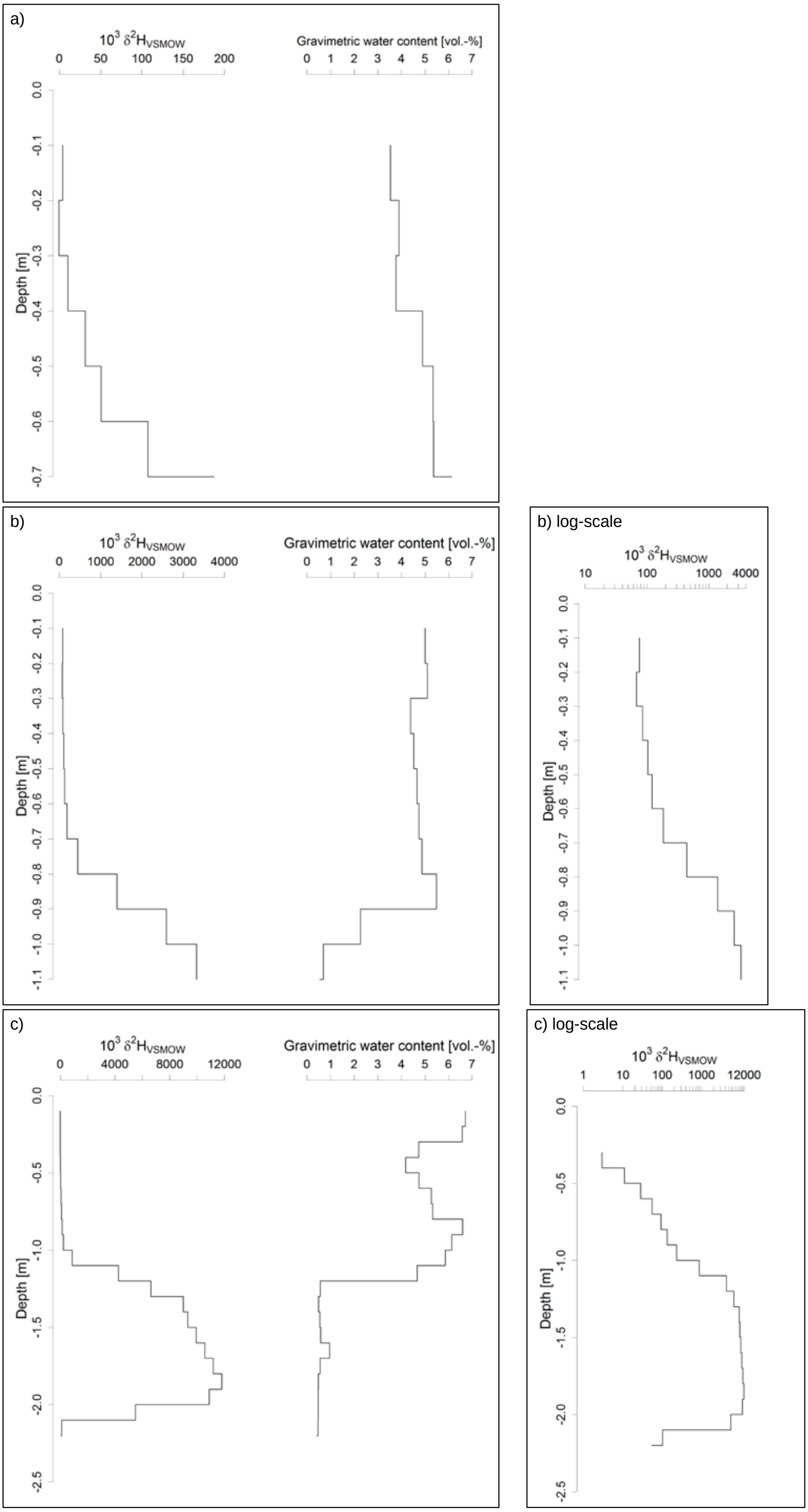
In the experimental plots where labeling occurred in 0.5, 1 and 2 m (Figure 4.5a–c), respectively, water becomes available for the plants immediately. This gets reflected in the elevated ^{2}H values for the samples taken one day after the injection characterizing those as clearly containing artificial tracer. At the 0.5 m labeling plot (Figure 4.5a) the concentration of artificial ^{2}H reaches its maximum for the afternoon sampling one day after the injection for the species close to the experimental plot (*C. collinum* and *S. luebertii*). In contrast, trees far from the plot show no artificial ^{2}H. During the third day of the experiment, concentrations of ^{2}H for the nearby plants return to background values. At the same time, uptake through one of the farther *C. collinum* occurs. In the larger trees (which were not sampled continuously at this plot), no artificial tracer was found. Small trees and shrubs dominate water uptake at this depth.

A similar situation can be observed for the plot labeled in 1 m depth. The sampled individuals of *S. luebertii* and *C. collinum* immediately react to the introduced ^{2}H with highest isotopic ratios one day after injection and then return to background concentration. At this plot, the young *C. collinum* under investigation had no access to the labeled water. However, an individual of the same species as far as 6 m from the application area could be associated with tracer uptake. In this *C. collinum*, artificial ^{2}H was found again in the afternoon of day four of the experiment. In contrast to the 0.5 m plot, ^{2}H was also encountered in the taller trees that were sampled. The *B. plurijuga* at the 1 m plot contained high concentrations of ^{2}H both in xylem and transpiration samples. The peak values were encountered almost two days later than in the smaller *C. collinum* and shrubs. For the 2 m labeling depth (Figure 4c) the pattern of ^{2}H uptake displays similar patterns. One day after labeling, artificial ^{2}H was found in both far and close individuals of *S. luebertii* as well as in the tall *B. plurijuga*. Whilst in the subsequent days no further uptake is registered in the shrubs, a clear tracer pulse was found in the *B. plurijuga* on day 4 of the experiment. No uptake of the labeled water was registered in the far *A. erioloba* tree throughout the whole sampling campaign.

In Figure 4.5d to f the temporal evolution of ^{2}H-concentrations for the plots labeled in 2.5 and 4 m are shown. With two exceptions, namely two samples of *S. luebertii* at the 4 m plot where the soil was labeled near the stem of *B. plurijuga* (Appendix A), no traces of ^{2}H were found. The uptake encountered in the two mentioned samples, however, needs to be examined in detail (refer to discussion section).

4.4.3 SOIL PROFILES AT THE END OF DRY SEASON AS INDICATORS FOR WATER VAPOR TRANSPORT

In order to investigate the possibility of up- or downward water or water vapor transport, the soil at the plots was sampled at the end of the field campaign (upper 50 cm) as well as six months later (up to 4.2 m depth; at the end of the dry season). No artificial deuterium was present in the profiles taken immediately after the campaign (i.e. 7 days after tracer injection; profiles not presented here) indicating no hydraulic redistribution of water to the upper soil layer within the experimental plots during the sampling campaign. The profiles taken after the dry season for four of the experimental plots are shown in Figure 4.6.


a)
$10^3\ \delta^2H_{VSMOW}$
Gravimetric water content [vol.-%]
Depth [m]
b)
$10^3\ \delta^2H_{VSMOW}$
Gravimetric water content [vol.-%]
Depth [m]
b) log-scale
$10^3\ \delta^2H_{VSMOW}$
Depth [m]
c)
$10^3\ \delta^2H_{VSMOW}$
Gravimetric water content [vol.-%]
Depth [m]
c) log-scale
$10^3\ \delta^2H_{VSMOW}$
Depth [m]

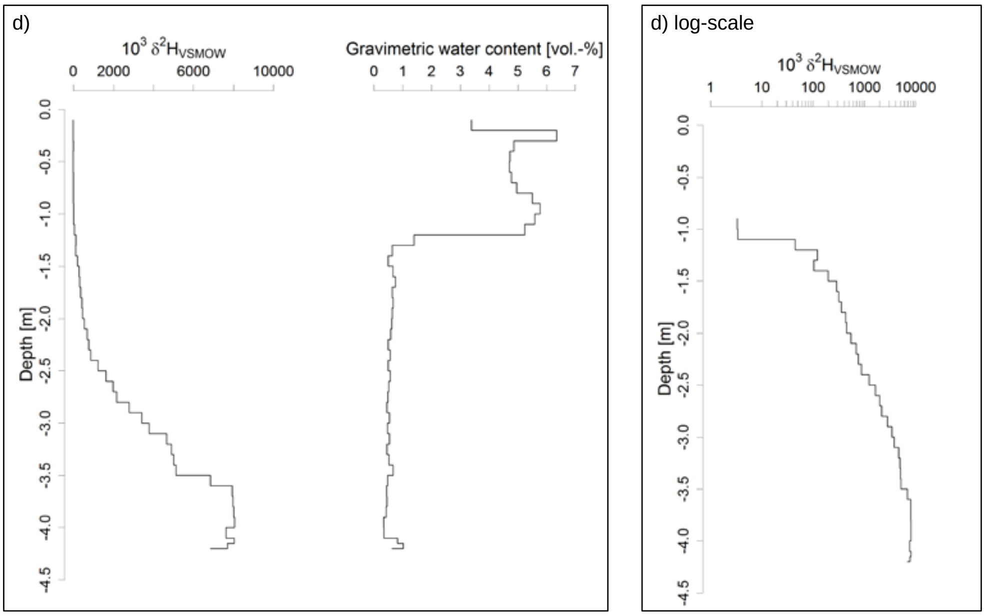


Figure 4.6: Figure 5: δ^2H and water content profiles after the dry season for labeling depths of a) 0.5 m, b) 1 m, c) 2 m and d) 4 m (near stem of *B. plurijuga*). A distinct signature of artificially injected δ^2H can be identified at all plots. Note that in log scale negative isotopic ratios cannot be displayed (i.e. the missing values close to the surface represent background concentration due to recent rain events).

At all sampled plots, elevated concentrations of ^{2}H can be observed not only at the depth of tracer application but also in both directions vertically. Upward tracer transport from depths as great as 4 m is clearly recognizable by δ^2H-ratios greater than 100‰ up to a depth of 1.2 m (Figure 4.6d). In the 4 m profile, the position of the introduced ^2H_2O prior to the dry season is still distinguishable by the elevated water content around this depth (Figure 4.6d). At both plots labeled deeper than 1 m the tracer peak coincides approximately with the targeted application depths. Rather than a sharp peak at the target depth, however, a plateau of peak concentration is present (Figure 4.6c and d). The decrease of tracer concentration towards the surface has an approximate exponential shape at all sampled plots (Fig. 4.6a–d). In contrast, Figure 5c clearly displays a rather steep decrease of ^{2}H concentrations towards the soil compartments deeper than the depth of label injection. In other words, more tracer was transported towards the soil surface (in upward direction) than downwards during the period of observation (i.e. the dry season). Hence; there exist indicators for a dominance of upward transport. The plots labeled at 0.5 and 1 m, respectively, are influenced by rainfall occurring prior to the sampling campaign after the dry season (compare the water contents at all plots; Fig. 4.6). As a result, the tracer at these plots is shifted downwards. It can further be seen that the deeper labeling occurred, the more tracer remained within the soil. This gets reflected by the higher deuterium concentrations found in the 2 and 4 m profiles compared to the surface near plots and clearly points out the influence of evaporation and transpiration to which the latter are exposed. Summarizing our findings, it can be stated that at all plots a pronounced transport of tracer towards the soil surface was observed (either purely diffusive or with an additional advective component). At the plot labeled in 2 m depth (Fig. 4.6c), a dominance of upward over downward transport could be shown.

4.5 DISCUSSION

4.5.1 ISOTOPIC SIGNATURES

The dual-isotope plot presented in Figure 4.4 provides an overview of the interaction of different processes at the soil-vegetation-atmosphere interface. The separation of xylem, transpiration bag samples and samples containing artificial ^2H can be clearly distinguished; thus, the chosen methodology proved to be suitable for the main purposes of this study. The use of four standard deviations for the objective decision on whether a sample contains artificial ^2H was beneficial, because the natural isotopic composition of transpired water is variable throughout the day and depending on how long the transpiration bag is left on the tree. In addition to the decision if artificial ^2H is present (or not), the dual-isotope plot allows an interpretation of plant-water-atmosphere interaction, which is presented in the following.

The non-tracer-containing transpiration bag samples plot on a line that is significantly displaced from the xylem samples. This displacement clearly shows the effect of fractionation at the leaf surface. In the regression lines this gets reflected by a lower slope of the transpiration line compared to the xylem line (compare Table 4.1). The intercepts, however, are comparable (–12.17‰ for transpiration bags and –13.17‰ for xylem, respectively), which might be coincidence. Cooper et al. (1991) discuss the role of the slope in the regression equation and state that the lower the slope in this equation, the larger the effect of kinetic fractionation (Cooper et al., 1991). The results we obtain for our regression lines of different types of water support this finding (Table 4.1). Remarkably, the regression lines for transpired water and shallow soil water are approximately parallel. This indicates that evaporative enrichment is similar in the upper soil and in the leaves.

However, Figure 4.4 reveals that the source water for the soil samples from the shallow unsaturated zone, transpired water and also xylem water is not the same. In regard to the different source water for soil and transpired water, the explanation could be that light rains (which are more enriched in heavy isotopes) might be taken up by plants immediately; thus, transpired water coincides with more enriched events at the LMWL. The same might hold true for rain events at the end of the rainy season (which are also more enriched): When rains slowly recede, evapotranspirative demand by plants is still high and water might be taken up immediately. In contrast, the source soil water might result from more intense rainfall events infiltrating slightly deeper into the soil.

In regard to the step-shift between xylem and transpired water, we believe that this is caused by the sampling method using transpiration bags and/or leaf-level effects causing this step-shift. In theory, the intersection of xylem and transpired water, respectively, should be in a similar range of δ-values. It would be worth studying this effect in greater detail (i.e. by sampling individual trees for both xylem and transpired water over a longer period of time) to reveal relations between the results of these two types of sampling.

The xylem samples (which are not subject to fractionation) plot predominantly in the range of isotopic compositions of precipitation, deep soil water and groundwater, respectively. Hence, the source water could be any of these, or a mixture; hence, a clear conclusion cannot be drawn. It is obvious, however, that none of the xylem samples coincides with shallow soil water (<0.5 m depth). This might be due to the fact that the upper soil was completely dry (< 1 vol.-%) and plants were not able to extract water from here anymore. Or, a small proportion is taken from there and the rest from deep soil water (>0.5 m depth) or groundwater.

4.5.2 ROOTING DEPTH AND TRACER UPTAKE DYNAMICS

A pronounced uptake of introduced tracer was observed in soil profiles labeled at 2 m or above, however, none of the sampled individuals took up water from profiles labeled at 2.5 m and deeper. Whether 2 m is the maximum depth lateral roots can reach is uncertain for three reasons: i) *A. erioloba* was not present at the 2.5 m plot and not all species present on the site were investigated; hence, a generalized conclusion cannot be drawn; ii) there is still a chance that no roots were present within the covered volume at any of the plots labeled deeper than 2 m, but somewhere else; and iii) heterogeneity of rooting depths (e.g. caused by tree age, height or soil heterogeneity) has to be recognized. Nevertheless, our study shows that the presented method is effective for approximating rooting depth on site and capable of capturing water uptake dynamics at different soil layers. In addition, the results are in agreement with the findings of

Beyer et al. (2015) who found a step – shift of soil water contents in profiles taken one month after the rainy season at a depth of 2.3–2.4 m at the same study site, indicating the end of the main lateral root zone at this depth. The authors further observed a change in the color of the sand towards a clear, almost white color, whereas organic contamination could be visually identified at shallower depths. In regard to ii) and iii) we state that the injection of ^2H_2O was designed in a way that a rather large volume of soil is labeled. With 0.14 m³ labeled soil volume, the area is much bigger than 0.005 m³ in the study of Kulmatiski et al. (2010). It can therefore be assumed that if a certain plant has lateral roots in the investigated depth, the labeled soil volume is sufficient to cover at least a portion of that root. The experimental plots were chosen carefully and at representative locations within the forest where root structure is undisturbed. Since we aimed on marking a bigger soil volume not only the horizontal, but also the vertical distance from the application that was labeled increased. Therefore, we had to sacrifice a more precise vertical labeling in a way that the peak concentration spreads over a vertical depth of ~30 cm, which is confirmed by the soil profiles (Figure 4.6 c and d). Heterogeneity of rooting depths caused by different sizes of trees, different soil properties or even locally varying precipitation amounts can only be tackled by establishing more (repetitive) plots. The same holds true for i). However, this issue is typical for point investigations; hence, final evidence might only be achievable with tremendous effort. The results imply that there is water available frequently at depths reaching ~2 m; otherwise, there would simply be no roots at these depths (in accordance with Schenk and Jackson, 2002b). Applying a previously proposed conceptual model relating mean annual precipitation to rooting depth (Schenk and Jackson, 2002b), predicted rooting depth would be around 1.5 m (less than the supposed rooting depth in the present study) using a mean precipitation of 500–600 mm for the area (Mendelsohn et al., 2013). In November 2015 we further excavated one exceptionally tall individual of *B. plurijuga*. The tree showed strong lateral roots which proceed almost horizontally at 2–2.2 m depth, but no tap root. An extensive rooting network of different trees and shrubs (*S. luebertii, Burkea africana, T. sericea*) was found up to 2 m. From this depth downwards, root density declined exponentially. At 2.5 m soil was without roots other than occasional fine roots of low density; the soil color changes to almost whitish sand at this depth. Even though no generalization can be drawn from excavating one tree, these observations coincide with what was found during the labeling experiment.

Water uptake dynamics

When examining the dynamics of plant water uptake, we speculate that there are indications that shrubs and smaller trees might dominate the upper root zone, while trees might have favorable access to water in deeper layers (Fig. 4.5a–c). For instance, at the 0.5 m and 1 m plots, an immediate reaction to the tracer injection by *S. luebertii* (height of shrubs ~1.5 m) and *C. collinum* (lower than 3 m in height) was observed. In contrast, no (at the 0.5 m plot) or delayed (1 m plot) uptake by the tall trees of *B. plurijuga* (8 m height), *T. sericea* (6 m height) and *A. erioloba* (8 m height) was found. At the 2 m plot the situation seems to turn around. Very high tracer concentrations and pulse-like uptake were measured in the tall individual of *B. plurijuga* (8 m height). However, this interpretation has to be examined in further studies aimed explicitly on evaluating partitioning of the root zone between different species.

The presence of tracer in *S. luebertii* at the plot labeled in 4 m depth near the stem of *B. plurijuga* (Fig. 4.5f) was rather unexpected. No clear evidence can be drawn from these results; hence further experiments will be beneficial. From our understanding, there are four possible explanations: i) During the injection, tracer accidently entered areas of the soil above the targeted labeling depth; ii) the roots of the investigated individuals of *S. luebertii* are exceptionally deep; or, hydraulic redistribution through iii) the tap root of *B. plurijuga* or iv) mycorrhizal fungi occurred. Option i) can be almost excluded, because if this would have happened, the tracer would have probably been present in other sampled species as well. Option ii) is also unlikely due to the fact that *S. luebertii* was also sampled at the 2.5 m and the second 4 m plot, respectively. At these, no uptake was registered. From our perspective, the most likely explanation is either iii) or iv). This would imply that the tap root of *B. plurijuga* was able to access the labeled water and distribute it to the upper soil layers or, a rapid transfer through the mycorrhizal tissue (e.g Allen, 2007; Duddridge et al., 1980; Plamboeck et al., 2007) took place, respectively. A shallow soil profile was taken at each of the plots indicating no hydraulic redistribution. However, this only holds true for the position where this profile was taken (which is within the area of the experimental plot). Therefore, redistribution to the soil elsewhere cannot be excluded. The latter aspect is far out of scope of our research; thus, it was not investigated if such fungi are present on site. We did not find tracer in this exceptionally tall individual of *B. plurijuga* (height approximately 20 m). An explanation for this might be that timing of xylem sampling was chosen in a way that we missed the tracer throughput. Similarly, it could be possible that the chosen branches for transpiration bag sampling were unfavorable, so that no tracer could be found. However, this hypothesis cannot be completely proven by our results and requires further examination.

The significance of tap roots

In our investigation we excluded the role of tap roots within the soil–vegetation–system. No evidence – both isotopically and based on drilling – was found that tap roots are present on site. As stated previously, the excavated individual of *B. plurijuga* did not have a tap root. Local farmers, elders and people who are responsible for well digging observed that the only local trees in this region capable of developing deep tap roots are *A. erioloba* and taller individuals of *C. collinum* (*personal communication during several interviews conducted in the last three years*). From a scientific perspective, a number of xylem samples coincide with shallow and deep groundwater. However, precipitation and deep soil water are also plotting in the same range; hence, no clear conclusions can be drawn from our results (Figure 4.4). Using the presented technique to investigate such roots at great depths is not possible with the current setup (drilling deeper than 10 m with a hand-auger is simply not feasible). The importance (in terms of quantitative estimates of uptake and their role on the overall water balance) of potentially present deep tap roots is yet not fully understood. Canadell (1996) state in their review that ‘we know of the potential of some species to have very deep roots at few sites, yet very little is known about how common the habit of deep rooting is across species and environments’ (Canadell, 1996). The authors further found that deep roots are mainly limited to sandy loose soils where mechanical impedance to root penetration is least’. Up to now it is known that certain trees and shrubs are occasionally – depending on the local climate and soil type – capable of supplying themselves with water during droughts by developing deep tap roots in the unsaturated zone with the ultimate goal of reaching the groundwater table and ‘pump’ water from there (Jennings, 1974; Lemmens et al., 2012; Moore and Attwell, 1999; Moustakas et al., 2006; Phillips, 1963; Schenk and Jackson, 2005; Seymour and Milton, 2003). Still, the occasional character of deep tap roots needs to be recognized. Ringrose et al. (2000), for example, drilled two individuals of *A. erioloba* trees to 60 m in Botswana. The authors found no evidence of roots appearing deeper than 6 m. In their study in the Etosha National Park, Hipondoka et al. (2003) discovered that roots of the species under investigation, *T. sericea*, displayed tap roots more often in the wetter part of the park than the ones in the drier (Hipondoka et al., 2003).

Thus, we state that at the studied site deep tap roots are likely but if this is really the case remains uncertain. Nevertheless, the potential of deep tap roots needs to be recognized because they seem to be very efficient in the acquisition of water (Canadell, 1996; Reicosky et al., 1964).

Future research should focus on the distribution and number of deep rooting trees and species and the quantification of water uptake through the tap root in order to incorporate such effects. For example, the deuterium tracing method proposed by Calder (Calder et al., 1986, 1992; Calder, 1992) could be used for this.

4.5.3 UPWARD WATER VAPOR TRANSPORT AND IMPORTANCE FOR ESTIMATIONS OF GROUNDWATER RECHARGE

The occurrence of ^{2}H in the upper soil layers of all profiles that were sampled after the dry season (i.e. 6 months after injection) was unanticipated. The clear sign of tracer transport from the 4 m plot towards the surface was particularly unexpected. We interpret this in accordance to findings of Phillips et al. (1988), Scanlon (1992) and Walvoord et al. (2002a, 2002b) as follows: During the dry season water movement in regions where the groundwater table is far from the surface is mainly limited to vapor transport resulting from temperature gradients within the soil. These gradients change from day to night, i.e. they are diurnal. In the upper soil layer, temperature gradient is steepest but downward vapor flux during the day is small because of steep water potential gradients introduced by evaporation. In the night, when the upper soil layer cools down rapidly, the thermal gradient changes and upward water vapor transport occurs. For desert soils, Scanlon (1992) found that 'below 1 m soil depth downward vapor flux in summer is balanced by upward vapor flux in winter; net vapor flux on an annual basis should be negligible.' Extending this concept to semi-arid environments including the occurrence of a rainy season and plant cover, one could say that the downward water vapor transport during the days in the dry season is very small due to very low water potentials (very dry soils) throughout the whole root zone. In contrast, the overall upward transport during the night will be greater than in deserts due to the availability of water in deeper soil layers (introduced by rainfall in the rainy season), but also due to the very low water potentials in the lower part of the root zone. As a consequence, there would be a net upward water vapor flux during the dry season which results in the tracer profiles presented in Figure 4.6. This theory is supported by the findings of Seyfried et al. (2005) who state that plants are amongst the main determinants for the control of deep drainage in semi-arid regions (Seyfried et al., 2005). The authors found that due to very low water potentials at the end of the root zone, a constant upward water vapor flux can develop even from deep soil layers or groundwater tables as deep as 50 m (Seyfried et al., 2005). At the study site groundwater is approximately 30 m deep (Lindenmaier et al., 2014). The concept of vapor phase diffusion is also supported by the study of DePaolo et al. (2004). On a strictly porous-media-property standpoint, the theoretical depth at which diffuse water vapor transport is initiated (Stage I evaporation), can be calculated by applying the concepts published by Lehmann et al. (2008):

$$L_G = \frac{2\sigma}{\rho g}\left(\frac{1}{r_1} - \frac{1}{r_2}\right) = \frac{1}{\alpha(n-1)}\left(\frac{2n-1}{n}\right)^{(2n-1)/n}\left(\frac{n-1}{n}\right)^{(1-n)/n} \quad \text{(eq. 4.3)}$$

where L_G [m] is the gravity characteristic length or length associated with stage I evaporation, σ [Nm^{-1}] surface tension, ρ [kgm^{-3}] the liquid density, g [ms^{-2}] the gravity acceleration, r_1 and r_2 [m] the radii of the small and large capillaries, respectively and α [1/m] and n [-] the shape parameters of the van Genuchten model. The calculation can be performed either with the pore size distribution (first part of the equation) or, if available, the fitted parameters from the van Genuchten model.

Shokri et al. (2009) (summarized in Or et al., 2013) presented an equation to estimate diffusive water vapor transport from a vaporization plane at a certain depth (Stage II evaporation):

$$e_{II}(t) = D_S \frac{C_{sat} - C_\infty}{L_{dried}(t)} = \frac{\theta_a}{\phi} D_0 \frac{C_{sat} - C_\infty}{L_{dried}(t)} \quad \text{(eq. 4.4)}$$

where $e_{II}(t)$ is the diffusive flux as a function of time, D_S [m²s^{-1}] the vapor diffusion coefficient through (nearly) dry sand which is approximated using the model of Moldrup et al. (1997) for intact soils, C_{sat} [gm^{-3}] saturated water vapor density, C_∞ water vapor density at surface [gm^{-3}], $L_{dried}(t)$ the time-dependent depth of the vaporization plane [m], θ_a volumetric air content [-],ϕ porosity [-] of the soil and D_0 [m²s^{-1}] the vapor diffusion coefficient in free air.

In order to obtain an estimate of the length associated with stage I evaporation (in isotope hydrology it is also referred to as the zero flux plane), we applied equations 3 and 4 to our data assuming i) a dry soil (θ = 0.01, which has been observed on site; Beyer et al., 2015), ii) a temperature of 25 °C, iii) a water vapor density at surface ranging from 5 to 10 gm^{-3} (taken from estimations by the International Telecommunication Union, http://www.itu.int/) in June/July/August and iv) a vaporization plane at a constant depth. The results, together with soil hydraulic characteristics of the soil on site, are summarized in Table 4.2.

Table 4.2: Soil hydraulic properties of the soil at the study site and derived parameters from i) soil cores, ii) pore size distribution (parameters estimated using the software Rosetta (Schaap et al., 2001); and iii) calibration (based on data published in Beyer et al., 2015) using the SVAT model DAISY (Abrahamsen and Hansen, 2000). Based on these parameter sets, the depth associated with stage I evaporation and diffusive flux over the dry season (stage II evaporation) were calculated.

Parameter	Soil cores (mean)	Pore size distribution	Calibrated	Sources/Method
Bulk density	[1]1.59 g cm^{-3}	-	1.53 g cm^{-3}	-
Porosity		0.4		-
Van Genuchten parameters Alpha *n* Residual water content Saturated water content Saturated hydraulic conductivity	[1]0.025 [1]5.819 1/cm [1]0.033 [1]0.35 [1]2491 cm d^{-1}	[2]0.033 [2]3.881 [2]0.05 [2]0.38 [2]1057 cm d^{-1}	[3]0.125 [3]2.200 [3]0.005 [3]0.36 [3]2500 cm d^{-1}	[1]Schindler et al. (2010) [2]Schaap et al. (2001) [3]Abrahamsen and Hansen (2000)
Saturated hydraulic conductivity (field)		2304 cm d^{-1}		Double ring infiltrometer
Stage I evaporation – associated depth (L_G)	32.0 cm	21.2 cm	22.2 cm	Lehmann et al. (2008)
a) Stage II diffusive flux with vaporization plane = 4 m (tracer application depth) **c_∞ = 10 gm^{-3}** **whole dry season (165 d)** **c_∞ = 5 gm^{-3}** **whole dry season (165 d)**		1.79 x 10^{-3} mm d^{-1} **0.30 mm** 2.44 x 10^{-3} mm d^{-1} **0.40 mm**		Shokri et al. (2009) Or et al. (2013)
b) Stage II diffusive flux with vaporization plane = 2.5 m (supposed end of root zone) **C_∞= 10 gm^{-3}** **whole dry season (165 d)** **C_∞= 5 gm^{-3}** **whole dry season (165 d)**		2.87 x 10^{-3} mm d^{-1} **0.47 mm** 3.91 x 10^{-3} mm d^{-1} **0.65 mm**		Shokri et al. (2009) Or et al. (2013)
grain size distribution 0 – 100 cm 100 cm >>		**% sand / % silt+ clay** sand (97.7 / 2.3) sand (97.3 / 2.7)		Dynamic image analysis
total rainfall 2013/14		660 mm y^{-1}		Beyer et al. (2015)
potential recharge 2013/14		45 mm y^{-1}		
percent of precipitation		~7 %		
mean groundwater recharge		2 – 20 mm y^{-1}		Struckmeier & Richts (2008)

We used data derived from soil cores, pore size distribution and fitted model parameters from a labeling experiment conducted by Beyer et al. (2015) for comparison. Based on the fitted model (which is believed to be the best-estimate), a characteristic depth of ~22 cm (based on the calibrated parameters) is associated with Stage I evaporation. This means that below this depth upward water transport takes place in the vapor phase. The diffuse water loss from a saturated layer of water at 4 m depth (i.e. the depth where the tracer solution was applied) results in a total of 0.4 mm over the whole dry season. Assuming the vaporization plane immediately underneath the root zone (i.e. 2.5 m; this would be the approximate depth based on the results where water surpassing the root zone is located after the rainy season) the diffuse loss of water increases to ~0.7 mm. For very wet rainy seasons (e.g. 2013/14) this is negligible because potential recharge in such is fairly high (Beyer et al., 2015). However, the mean recharge rates in this part of the CEB are estimated as ranging between 2 – 20 mm (Struckmeier and Richts, 2008). Therefore the diffusive loss has to be accounted for, especially for the lower end of this spectrum. In addition, water vapor fluxes caused by thermal gradients (as explained above) can be much higher than purely diffusive (Hendrickx et al., 2005). In order to quantify these, however, further experiments and subsequent numerical modeling is crucial. Practically, this requires injecting exactly predetermined amounts and concentrations of ^{2}H at a certain depth and detailed monitoring of tracer distribution, soil temperatures and meteorological variables. Especially the prior is challenging, but might be possible soon with recent developments of measuring soil water stable isotopes in situ (Gaj et al., 2015; Volkmann and Weiler, 2013). This comprises great potential for future studies. For example, diurnal cycles of stable isotopes and water vapor transport could be investigated contributing to an enhanced understanding of this important process.

In essence, the existence of a net upward water flux affects estimation of groundwater recharge through the unsaturated zone which is commonly referred to as water infiltrating underneath the root zone. In humid environments this might be true since groundwater tables are usually close to the surface. In semi-arid and arid climates, however, the unsaturated zone can be very thick and the time from infiltration of water underneath the root zone to the groundwater can be long. If in such cases the effect of upward vapor transport is present, it has to be accounted for in the form of a negative component – or loss term – in the water balance. While there might be a significant amount of water surpassing the root zone on site due to generally favorable conditions for infiltration during the rainy season (e.g. Beyer et al., 2015), this same water (or a fraction of it) might be lost in the subsequent dry season due to water vapor transport. If there was a water table at that depth, loss would be from there. Quantification of such effects requires numerical modeling on which future research should focus. Similarly, if present, uptake of deeper soil water through the tap root of certain species might have to be considered and be accounted for. Having these concepts in mind, it is crucial in dry environments to distinct between potential groundwater recharge (equal to deep drainage) and actual groundwater recharge (water arriving at the groundwater table).

Actual groundwater recharge is then to be determined as follows:

$$R_A = D_D - V_u - UP_D \qquad \text{(eq. 4.5)}$$

where R_A [L] is actual groundwater recharge. D_D [L] represents deep drainage, Vu [L] upward water vapor transport and UP_D [L] uptake of deep soil water through the tap root of certain species. Nevertheless, until now, the quantification of the latter two components remains very difficult (Hendrickx et al., 2005) and has to be investigated further, as stated previously. Quantification of UP_D becomes possible by applying a known amount and concentration of ^2H_2O in the unsaturated zone of a bare soil and subsequently monitoring tracer movement, moisture, matrix potential and soil temperature. Numerical models can then be fitted to the data and water vapor transport might be quantified. The role of deeper-penetrating tap roots is labor intensive and appropriate methods are yet not available.

Since previous studies show that year-to-year change of soil water storage within the root zone is zero (Seyfried et al., 2005), precipitation or water input P [L] must exceed the storage capacity C [L] of a soil in a given period of time (i.e. the rainy season) in order to create deep drainage D_D [L] (Seyfried et al., 2005):

$$C = P_S * D * A_W \qquad \text{(eq. 4.6)}$$

where P_S [-] represents the soil porosity, D [L] the effective rooting depth and A_W the water available to the plants [-]. For the presented study site, C calculates as 73 mm for a rooting depth of 2 m and 91 mm for a rooting depth of 2.5 m. This means, that a period where P is exceeding 73 or 91 mm, respectively, is necessary in order to create groundwater recharge. This fairly low storage capacity indicates favorable conditions for the creation of deep drainage (not taking into account the unknown negative terms defined in equation 4.5). However, as stated previously, this does not necessarily coincide with high actual groundwater recharge. Nevertheless, such estimations can provide an initial assessment of an investigated site.

Ecohydrological separation?

We conclude this chapter with a brief discussion on how the presented research fits into the presented concepts of recent studies on ecohydrological separation (Brooks, 2015; Brooks et al., 2010; Evaristo et al., 2015; Goldsmith et al., 2012; Good et al., 2015; McDonnell, 2014; Phillips, 2010). Related to this ecohydrological separation (or, the '*two water worlds – hypothesis*') we interpret our findings as follows: In the dual-isotope plot (Fig. 4.4), xylem samples plots in the same range as groundwater, precipitation and deep soil water (> 0.5 m). Shallow soil water (< 0.5 m), on the other hand, does not coincide with any of the xylem samples. In the authors' opinion, this simply is due to the fact that the upper soil dries out very fast after the rainy season or individual rain events and at a certain point plants are not able to extract anymore water from there. Water contents in the upper soil layer during the time of data collection were less than 0.5 vol.-% (data not shown herein). If water in deeper zones of the soil or groundwater is accessible by plants we suppose that the local vegetation would utilize it. Thus, based on the data presented in Fig. 4.4, we do not see in our case that 'plants are using soil water that does itself not contribute to groundwater recharge or streamflow' (Evaristo et al., 2015). Rather than that, the mechanism in our case could be explained as follows: In deep unsaturated zones (such as our study site) water needs many years to reach the groundwater table. Eventually, only extreme events or very wet seasons create recharge (Beyer et al., 2016b; Evaristo et al., 2015; Taylor et al., 2012). This water, once reaching the groundwater, could be isotopically different from water present in the upper unsaturated zone (refer to Fig. 4.4). Small rain events will be completely consumed from the upper part of the soil by plants and evaporation. It seems obvious that these events do not contribute to groundwater recharge. Hence; if water supply to plants is from the upper soil – which is the case mainly during the rainy season – the reservoir used by plants is different than the water recharging the ground, but this is mainly due to the nature of rainfall events (extreme events and long wet spells). In the dry season, on the other hand, plants use deeper soil water (and/or potentially groundwater), because the upper soil simply is too dry and this is what Figure 4.4 reflects. We believe that this concept mainly applies to arid and semi-arid environments, but needs to be considered when investigating ecohydrological separation.

4.6 CONCLUSION

A field methodology for the investigation of rooting depths (or, maximum depth of water uptake), water uptake dynamics and water transport through soils using the stable water isotope deuterium as artificial tracer has been developed. The use of ^2H_2O was proven to be appropriate for minimum-invasive investigations in the unsaturated zone of semi-arid environments. The technique can be used to investigate root activity, which proposes a major benefit for future application.

We conclude that in order to potentially create groundwater recharge, single (extreme) rain events or wet spells have to reach depths of at least 2.5 m. Even if this is the case, processes such as upward water vapor transport and potential uptake of groundwater through the tap root of certain tree species have to be accounted for. We therefore propose incorporating such processes into groundwater recharge estimations in arid and semi-arid environments. The proposed methodology enables studying water uptake dynamics and partitioning of water between different plant species in certain areas of the root zone. The application of the proposed methodology can support the parameterization of SVAT – models, where rooting depth is one of the main parameters related to plant water uptake but also one that is generally treated as unknown. The study also showed that upward water vapor transport through the unsaturated zone during the dry season at the investigated site is present. The diffusive component of this effect was approximated in this study, but the overall contribution of this process (diffusive and thermal) transport of water vapor needs to be investigated further. Using a known concentration of tracer, monitoring in higher spatiotemporal resolution and the application of SVAT models which are able to simulate vapor phase transport processes might enable a quantification of this effect. ^2H_2O has been shown to have a great potential for studies at the soil–vegetation–atmosphere interface. Small amounts of tracer are necessary; hence, field experiments become increasingly economically feasible. Furthermore, the use of ^2H_2O enables quantitative studies of water fluxes. Future research should focus on incorporating the complete range of processes within the unsaturated zone of dry environments important for the water balance. As a first step, the magnitude of effects such as groundwater uptake through trees or, as proven to be of importance in the presented study, upward water vapor transport, should be determined. Tracer methods and, in particular ^2H_2O, are valuable and necessary tools for such applications.

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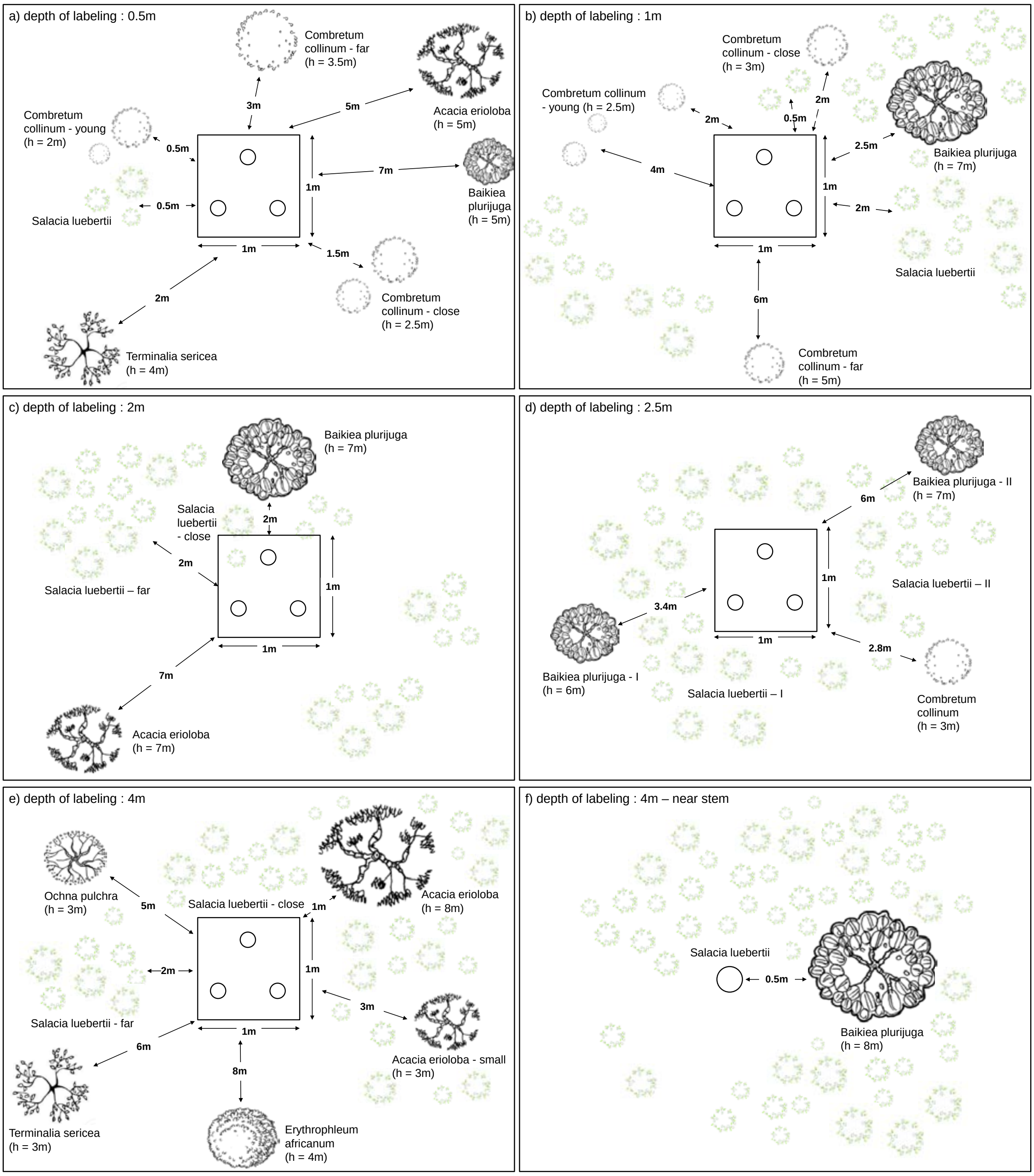
Appendix A: Plant distribution at the labeled plots, height of plants (in brackets) and tracer application area. Indicators used in the scheme (e.g. 'young', 'far', etc.) are in accordance to Figure 4.5.



5 SYNTHESIS

5.1 SUMMARY AND CONCLUSIONS

The goal of this work was to develop different methods for the investigation of critical processes along the soil–vegetation–atmosphere interface in WLE. In such environments, data scarcity often is the main issue. Yet, understanding of the hydrological cycle and quantification of processes such as groundwater recharge or agricultural yields are inevitable. Here, three different approaches, at the meso- and point-scale, respectively, were established:

i) A framework based on open access data, modeling and artificial neural networks for evaluating the impact of rainfall characteristics on rain-fed farming;
ii) A deuterium-based labeling strategy for the estimation of groundwater recharge through the unsaturated zone; and
iii) A deuterium-based labeling strategy for the investigation of rooting depths, water uptake dynamics and unsaturated zone water (vapor) transport.

Each of these papers presents a novel approach or method related to the subject investigated. As for i), the main innovation is a combined framework of remotely sensed data, SVAT modeling, a criteria-driven analysis of rainfall characteristics and a multivariate approach based on an artificial neural network (*SOM*).

In study ii), an existing method (peak-displacement) is used, but tritium (^{3}H) the tracer mainly used in the past (Koeniger et al., 2016) is replaced by deuterium (^{2}H). This tracer, when used as applied tracer, is more difficult to handle and no previous study in semi-arid environments with the purpose of groundwater recharge estimation exists, to the author's knowledge. Therefore, the study comprises a valuable insight and starting point for related applications.

In study iii) a novel technique for investigating rooting depths on the point scale is presented, which has otherwise been costly and much more work-intensive up to now. This enables closing a gap in the parameterization of unsaturated zone models. In addition, the experimental setup allowed an investigation of temporal and depth-dependent water uptake dynamics and an identification of the main direction of water vapor transport.

All three studies show that even in data scarce environments, cost-efficient methodologies (refer to Chapter 4) can be developed in order to investigate crucial processes of the ecohydrological cycle. This enables – if applied consequently – to inform decision-makers, help to parameterize SVAT models and assist predictions for future climatic developments. The results emphasize how important it is to approach soil–vegetation–atmosphere studies from an interdisciplinary point of view. Rainfall and soil characteristics determine the depth and frequency of infiltrating water; plants, on the other hand, adapt to this regime and develop strategies to supply themselves with sufficient water. These adaptations in turn affect groundwater recharge. As for study i), the results and methodologies developed in this thesis can be used as hands-on information for famers and rural planners as well as a basis for further, detailed research including locally important characteristics as well. It is further useful for planning of areas where additional irrigation might be necessary in order to obtain better outcomes from farming. The studies using stable water isotopes are aiming at local scale; hence, applying the developed techniques might become useful for rural planning (e.g. water availability from shallow resources such as hand-dug wells), e.g. at particular villages. They further contribute to improve understanding of the interaction between climate, soils and vegetation in dry environments. The use of ^2H_2O as artificial tracers enables - rather than being purely qualitative – a quantification of components of the water–balance and therefore overcomes a criticism that has been associated with the application of stable water isotopes in the unsaturated zone previously (Healy, 2010).

5.2 IMPROVEMENTS AND ONGOING RESEARCH BASED ON THE FINDINGS

This chapter mainly focuses on improvements of the field methodologies presented in the chapters three and four. The improvements for the investigation presented in chapter two can briefly be summarized as: i) a more accurate or spatiotemporally higher resolute data input; ii) incorporating additional rainfall characteristics, and iii) include nutrient cycles into the analysis.

5.2.1 GROUNDWATER RECHARGE ESTIMATION USING PEAK DISPLACEMENT

Despite being straightforward, the peak displacement method applied in its original form comprises a number of shortcomings (refer to chapter 3.6.3), both in its theoretical as well as practical considerations. After applying the method for the first time in the rainy season 2013/14, several improvements were implemented in the following rainy season. These are summarized in Table 5.1 and commented subsequently.

Table 5.1: Shortcomings of applying peak – displacement in its original form (Leibundgut et al., 2009; Zimmermann et al., 1966) and ideas for improvement

Criticism/ Shortcoming of the original method	Ideas for improvement	Comments
Irrigation introduces additional water to the profile which might affect water movement	Pointwise application of tracer via 'deuterium balloons'	Developed originally for investigating of rooting depth (refer to chapter 4), Figure 4.3
Does not account for site-specific heterogeneity	Labeling of multiple plots	Choose different characteristics, e.g. with/without litter cover, next to big trees, next to shrubs, non-vegetated
Disturbance of plot	Use angle when drilling holes for 'deuterium balloons'	Difficult for very dry conditions, because auger hole can collapse
Application of tracer underneath root zone difficult when using irrigation	Pointwise application of tracer via 'deuterium balloons'	Developed originally for investigating of rooting depth (refer to chapter 4)
Investigation of preferential flow is not possible	Sampling of multiple profiles within one plot	Applied in rainy season 2014/15
Theoretical equation does not account for immobile water	Modification of equation 3.5	Refer to equation 5.1; residual water content needs to be known
Does water infiltrating underneath the lateral root zone really become actual recharge?	Quantification of the impact of water vapor transport/ uptake via deep tap roots	Strong relation to results of chapter 4; use of the term 'potential recharge' recommended

The foremost aspect that needs to be included into a quantification of groundwater recharge via peak displacement is the incorporation of the residual water content of the particular soil into equation 3.5. After application of the original method as described in chapter 3, equation 3.5 was modified in order to account for this water, which is per definition 'immobile' and thus, does not take part in water transport (and, subsequently, recharge). The modified equation can be written as

$$R = \frac{\int_{z_0}^{z_n} [\theta(z) - \theta_r(z)] \cdot dz}{T}, \qquad \text{(eq. 5.1)}$$

where R represents recharge [L]; z_0 and z_n [L] are the soil depths of the tracer peak after injection of the tracer and after a certain time period T (i.e. one rainy season). $\theta(z)$ and $\theta_r(z)$ [-] are the water contents at layer z [L] and the residual water content of the soil, respectively. This raises the question 'How is residual water content defined'? There are several definitions, but the one that is most appropriate for semi-arid environments is the definition that for field soils, the residual water content equals the lowest observed water content over a sufficient period of time (Nitao and Bear, 1996; Walvoord and Scanlon, 2004). Only if no further information is available or decreasing the number of calibration parameters for models and increase their numerical stability, θ_r might be set zero (Fredlund et al., 2012; Pfletschinger et al., 2014). This is assumed in equation 3.5; however, not incorporating θ_r in the calculation of recharge results in a large overestimation of R especially for low recharge rates. The soil hydraulic parameters determined in the laboratory and listed in Table 3.1 certainly represent only an approximation of their real values; hence, they need to be fitted to represent field conditions. For the application of equation 5.1 the observed water contents from the monitoring stations (several soil moisture monitoring stations were equipped with continuous TDR probes and pF meters) and several hundred laboratory-determined water content samples were analyzed. Based on these, a value of ~ 0.5 vol. –% was assigned to θ_r.

The resulting groundwater recharge through the unsaturated zone over the rainy season 2013/14 yields in 29 mm. This is significantly less than the initial estimate of 45 mm.

These 29 mm should be seen as 'potential' recharge rate, given the possibility of water loss during the dry season via water vapor transport (refer to chapter 4). The remaining aspects listed in Table 5.1 are self-explaining and will not be discussed here in detail. Through the incorporation of these improvements the uncertainty of the method – which is difficult to quantify but found to be ranging in between 1 and 20 percent (Cook et al., 1994; Gvirtzman and Magaritz, 1986; Munnich, 1983; Rangarajan and Athavale, 2000) – can be reduced and more accurate recharge estimates derived.

In the framework of SASSCAL these methods are continued to be applied. For the subsequent rainy season (2014/15), which was a notably dry year, no potential recharge was recorded (i.e. the position of the tracer peak did not move downwards). This emphasizes the vast inter–annual variability semi-arid areas are often exposed to. In addition, the long term mean recharge was approximated for the same site by the chloride mass balance method (CMB) and was found to be in the range between 8–19 mm y^{-1}. Larger scale studies have been carried out by BGR (Struckmeier and Richts, 2008) and Shehu (2014, Master thesis, unpublished) who found mean recharge rates of approximately 20 mm $y^{-1}$for the CEB. In comparison to these numbers the estimates from the present work seem reasonable.

5.2.2 INVESTIGATION OF ROOTING DEPTHS

The methodology presented in chapter 4 has – to the authors' knowledge – never been applied before[1] and is an alternative, non-destructive and minimum-invasive technique for investigating rooting or water uptake depths at a particular site. The setup and sampling protocol of the presented experiment not only allows to investigate the rooting depth at a site, but also to potentially identify the partitioning of the root zone between shrub and tree species and the temporal dynamics of water uptake of certain individuals or species. Through the repeated sampling of soil after the dry season, inferring the existence of water transport in its vapor form was possible. Indices were found that the direction of this transport is preferentially pointing upward, i.e. a loss from the water that infiltrated underneath the root zone during the rainy season can be expected. One criticism associated to the results of the presented publication might be that such an experiment needs to be repeated at a different time of the year and at more plots in order to decrease the probability of a tracer application at an unfavorable position. Furthermore, one sample at the plot labeled at 4m depth was positive. These – justified – criticisms are currently addressed by a repetition of the experiment with a strict sampling protocol and a focus on labeling the deeper unsaturated zone (> 2 m). Related to the 'outlier' identified in the first experiment, there were again samples found where the small shrub species *S. luebertii* displayed elevated concentrations of deuterium. No other tree or shrub that was sampled showed elevated deuterium when labeling deeper than 2 m, which confirms the overall results found in Beyer et al. (2015). *S. luebertii*, however, seems to be able to acquire water from depths as great as 4 m (and potentially deeper). Either there are still roots present at this depth or the species is capable of taking up water vapor that eventually diffused upwards during the course of the experiment. A list of possible improvements of the methods and assumptions of the experiment described in chapter 4 are compiled in Table 5.2. Table 5.2 further contains ideas of further improvements of the developed technique, of which several are currently implemented.

[1] However, one study was found where groundwater was labeled with the toxic tracer lithium chloride (refer to Haase et al., 1996)

Table 5.2: Shortcomings of the deuterium-based labeling technique presented in chapter 4 (Beyer et al., 2016a) and ideas for improvement

Criticism / Shortcoming of the method	Ideas for Improvement	Comments
Repetition necessary and more plots to assure results are distinct	Repetition with focus on deeper labeled plots	Ongoing analysis (three additional plots established in November 2015 with plots at 2m, 3m, 4m) within SASSCAL
Depth of deep tap roots cannot be investigated	Combination with sap flow measurements; use of natural isotopes when groundwater samples are available	Two of the species present on site are known to be capable of developing deep tap roots
One positive 'outlier' at plot labeled at 4m depth	Further investigation in repetition experiment	Further positive samples found for the same species at plots labeled in 2m, 3m, 4m; *S. luebertii* has access to deep soil water either through deep roots or uptake of water vapor
The root zone of plants is not stationary	Repetition in intervals	Even though the statement is true, this depends on long term climatic conditions, which are unlikely to change rapidly
Not only diffusive, but also advective component of water vapor transport needs to be quantified in order to evaluate the overall importance of vapor phase transport	Injection of known tracer concentration via 'deuterium balloon' and subsequent monitoring of deuterium distribution in all directions and subsequent parameterization of a model allows quantification	Ongoing work within SASSCAL
Water uptake dynamics could be misinterpreted, if tracer throughput was missed (relevant for xylem samples)	High-resolute *in-situ* monitoring of deuterium	Field instrument developed within SASSCAL (Gaj et al., 2016)

5.3 FUTURE RESEARCH

The methodologies and results presented in this thesis provide multiple opportunities for future research. One general aspect that is important for future studies is an intensified effort on the establishment of monitoring stations. For climatic variables, a great number of stations were installed within SASSCAL and this data is freely available for the public (www.sasscal.org). In terms of monitoring of soil moisture there is currently no network and stations from a diverse range of projects are widely spread. In order to improve the analysis of rainfall characteristics, any additional data would improve the satellite datasets and, hence; result in a reduced uncertainty and better estimations of agricultural yields. The same holds true for more or at least more accessible information on yields from rain-fed agriculture. If such data would be available, the framework presented in the first study could easily be adapted and more detailed aspects could be investigated. An extended examination of the connection between the studied rainfall characteristics (i.e. how does an early/late onset of rains affect the remaining indicators?), an analysis over different stages of maize growth as well as scenario studies with other varieties or even crops are only a few possibilities for future applications. Especially investigating the effect of rainfall characteristics on phenological aspects, such as the sensitivity of maize (and/or other crops) in its different development stages is worth examining further. With improved future predictions from global or regional circulation models, an evaluation of future rainfall characteristics could be done. This would aid in finding adaptation strategies and assist planning of irrigation. In addition, there is a need for intensified studies on rainfall characteristics not only in regard to agriculture, but also for studying flood creation and groundwater recharge. An ultimate goal for the future is to predict probable rainy season onset dates, which remains difficult due to the vast variability. Yet, there is a pressing need for such predictions that should further be accessible by local small-scale farmers (Reason et al. 2006). Using neural network approaches such as *SOM*, which are capable of identifying relationships in highly complex and large datasets with a high number of parameters might allow advancing in this regard (as shown by Rivera et al. (2011) in their study in central Chile). Connecting the spatial patterns of rainy season characteristics with synoptic patterns might provide a basis for the development of a forecasting system.

As shown, the presented studies using stable isotopes as applied tracer in the unsaturated zone can be further improved (compare chapter 5.2) and used to parameterize SVAT models. This will lead to a more precise representation of water movement in the unsaturated zone and thus, improved estimates on groundwater recharge for longer time periods. The uncertainty of the presented methods needs to be addressed in greater detail in future investigations. Before this can be assessed, the question ‘Does all water infiltrating underneath the primary root zone really become groundwater recharge?’ needs to be examined further. This includes the quantification of water uptake through deep tap roots which are present in many (semi-) arid environments and a quantification of water vapor transport from (or to) the deep unsaturated zone. In this thesis, only the diffusive part could be addressed. These aspects remain to be the most difficult to quantify (Scanlon, 1992; Scanlon et al., 1997; Walvoord and Scanlon, 2004). However, the use of $^{2}H_2O$, combined with other tools (compare chapter 5.2) offers great potential for advancing in this regard. It is further possible to combine the two presented methodologies using $^{2}H_2O$ as artificial tracer in order to investigate a wide variety of processes simultaneously. With recently developed *in-situ* measurement techniques for stable isotopes (Gaj et al., 2016;

Volkmann and Weiler, 2013) efforts in the laboratory can be reduced significantly. This in turn enables to increase the spatial and temporal scale, which is a major step forward.

Finally, the presented methods can be effectively combined, for example to derive empirical relationships between groundwater recharge and certain rainfall characteristics. This would be beneficial for local water management. Such efforts, however, require a continuous application of the proposed field methodologies over a longer period of time and a subsequent parameterization of a SVAT model.

In essence, the methods and techniques developed in this thesis can be seen as a starting point for further investigations aiming on an improved understanding of processes along the soil–vegetation–atmosphere continuum of semi-arid environments. The main determinants for the water balance of such climates have been pointed out (equation 4.5), yet, a precise quantification over longer time periods is missing. By using stable water isotopes as applied tracer and multivariate techniques based on artificial neural networks these main determinants can be quantitatively investigated. The presented thesis points out ways forward and can constitute a baseline for further quantitative investigations of unsaturated zone processes in semi-arid environments, which are urgently needed for a sound management of water resources. In Namibia, the current dry period emphasizes how important a sound management of water resources is and how important the capability of aquifers to ‘buffer’ the impact of droughts is.

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