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Measurements and modelling of energy and greenhouse gas fluxes from complex cropland ecosystems

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Chapter 1

Introduction

1.1 Background

1.1.1 Crop demand and planetary boundaries

At the moment, agricultural crops cover 12% of the (ice free) land (Ciais et al., 2013; Foley et al., 2011). With a growing human population from 7 billion (Bloom, 2011) to 9 billion in 2050 (Roberts, 2011) and growing meat consumption due to increased wealth (Godfray et al., 2010), the demand for agricultural crops will further increase (Fritz et al., 2015; Godfray et al., 2010).

By now, industrial agriculture feeds most humans on planet Earth. Mainly the enhanced N-fertilisation made possible by industrial synthesis of ammonia (Erisman et al., 2008; Haber and van Oordt, 1905) led to this success. However the other side of this coin is not so attractive. There is a long list of problems that arise as humans influence the Earth-System. Summaries can be found for example in Rockstrom et al. (2009) or Vitousek et al. (1997). The main problems are: biodiversity loss, atmospheric aerosol loading, chemical pollution, climate change, stratospheric ozone depletion, overload of biogeochemical nutrient cycles (nitrogen and phosphorus), global freshwater use and change in land use.

Some, as climate change, are already in a state where the risk of reaching so called tipping points is enhanced (Rockstrom et al., 2009). Tipping points are moments when elements of our earth system can change to new stable states (Lenton et al., 2008; Steffen et al., 2015). A change in the earth system is for example the weakening of the Gulf Stream (Bryden et al., 2005). This weakening is both presented by Thornalley et al. (2018) and Caesar et al. (2018) and estimated to be 15% since 1850. Due to the global consequences of climate change, Steffen et al. (2015) state that it is seen as one of the core environmental problems that damages the earth system more than other. A further problem that damages

the Earth-System more than any others is seen in the loss of biodiversity (Steffen et al., 2015).

1.1.2 Regional climate change at the study site from 1936-2015

The regional climate change at the study area is illustrated by a temperature and precipitation plot from 1936 to 2015 (see Fig. 1.1 a, b). The blue line in subfigure a) represents a 24-years temperature time series measured at the research station Scheyern, which is completed with temperature measurements in the proximity of the research farm Scheyern (Wetterdienst, 2016a,b). In subfigure a) the additional temperature time series are shown by the black and the red line. The difference in the average annual means during the overlapping time series are small. The highest annual mean temperature value is 10.1 °C in 2015. The lowest annual temperature value in the study area is 6.0 °C in Hüll in 1940. To show the trend in the study area a 10-year moving average was calculated. The 10-year-trend of Hüll is shown with the left brown line and the 10-year-trend of Altomünster is shown with the right brown line.

Comparing the 10-year averages, the highest warming rates appear after 1980. This behaviour is known as a global phenomenon (Smith et al., 2015). Jones et al. (1999) showed the period between 1979 and 1997 to be one of two periods with the greatest warming in the 20th century. The other period with a great warming rate was from 1925 to 1944. This time period however is only partially shown in the graph.

To quantify climatic temperature changes in a study area, climate normal periods of 30 years are recommended (Trewin, 2007). The average temperature from 1961-1990 in the study area was 7.5°C. According to the preliminary climatic mean in Scheyern 1991-2015, the next average will most probably lie around 8.5°C, which is 1.0°C higher than the former average. The measurements agree well with the literature published about the study area (KLIWA, 2005a).

Fig. 1.1 b) shows precipitation measured at the monastery Scheyern from 1936 to 2015 (Wetterdienst, 2017). A trend in the precipitation is almost not visible. This is in agreement with other studies that did not find a significant change in the precipitation sums over whole Bavaria (KLIWA, 2005b), however they found a significant change in the temporal distribution of precipitation within the years in Bavaria. According to the study of (KLIWA, 2005b), the number of dry days is increasing as well as the number of days with heavy precipitation is increasing, however the number of extreme precipitation is not increasing.

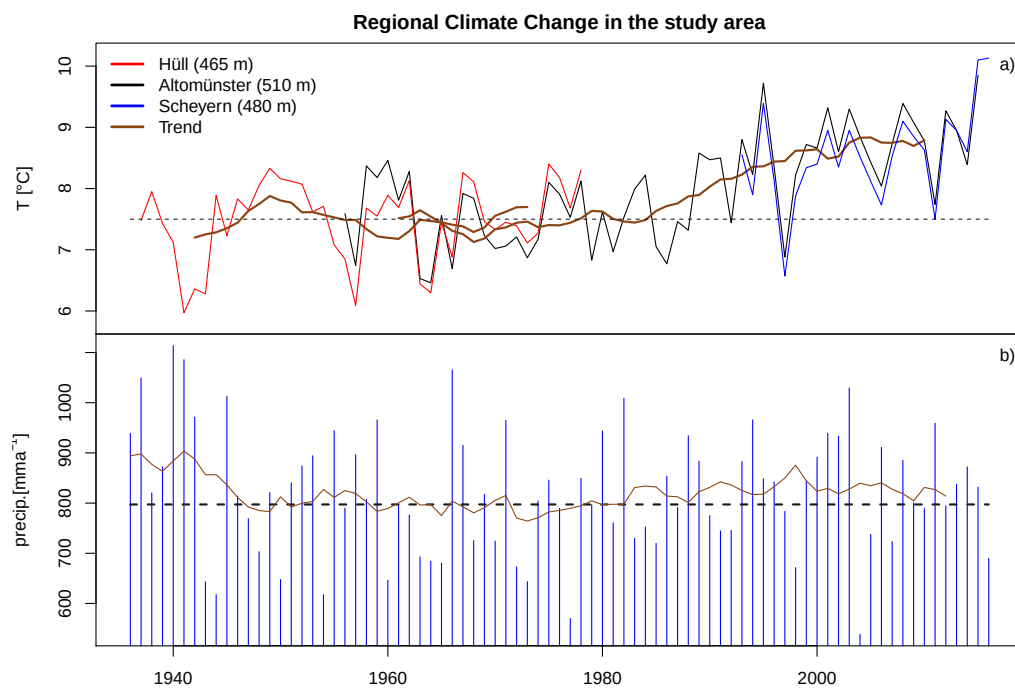


Fig. 1.1 Depicted is the trend of annual temperature and precipitation in the study area since 1936 (Wetterdienst, 2017). In the upper panel (a), the data in blue is collected in Scheyern (2012 to 2015 own data collection, 1991 FAM database). The red and black line represent temperature measurements by the Gerclman weather service in the proximity of Scheyern (Wetterdienst, 2016a,b) . In the lower panel (b) precipitation is depicted. The precipitation measurements were conducted directly at the monastery Scheyern. The complete time series starts at 1881 (Wetterdienst, 2017).

1.1.3 Fluxes in croplands and climate-land coupling

Croplands are open systems, where stocks of energy or matter are connected and can flow across compartment borders (e.g. atmosphere, hydrosphere, pedosphere, biosphere). Compartment borders are crossed, when nutrients from soils (pedosphere) are washed out into the groundwater (hydrosphere) or when they are converted to gaseous species (e.g. N_2O , NO , CH_4 , N_2) that exit the soil into the atmosphere. Compartment borders are also crossed when solar irradiance is converted into heat at the earth's surface.

Fluxes determine the time rate of change in the reservoirs of ecosystems. Measuring fluxes in croplands gives us the information whether the measured cropland is a source or a sink for any parameter exchanged between land and atmosphere.

Numerous studies have shown the crucial role of terrestrial land surface, notably the biosphere, as regulators of climate and atmospheric composition (Arora, 2002; Eltahir, 1998; Seneviratne et al., 2006; Suni et al., 2015; Teuling et al., 2010; Wiß et al., 2017). Fig. 1.2 shows a modified version of a schematic picture by Stocker et al. (2013) with relevant contributors to global warming from the land use. The causal chain goes from changed land use to a changed land surface, which results in changed albedo and changed greenhouse gas fluxes. When greenhouse gas fluxes change, the mixing ratios of greenhouse gases in the atmosphere change. This again changes the radiative forcing on planet earth. With a changed radiative forcing, energy in the atmosphere changes. As a consequence of that other meteorological parameters such as temperature, wind speeds, precipitation, etc. change. Relationships between greenhouse gases and surface temperature on Earth are already mentioned by Arrhenius (1896). Besides changed greenhouse fluxes, land use also leads to changed albedo and changed surface energy fluxes.

When atmospheric parameters change within a few decades, this again influences biological, chemical and physical processes at the land surface (Fig. 1.2, brown arrow). The feedbacks on planet Earth are partly obvious and common sense, like the shrinking of pole and glacier ice or the rising sea water levels. Less obvious and investigated are the feedbacks of global warming on biogeochemical cycles in soils.

To quantify the fluxes that affect the global climate, the ultimate goal of researchers throughout the world is to obtain information about every relevant ecosystem flux, everywhere and anytime around the world (Baldocchi, 2014). To achieve this aim measurement networks like EUROFLUX (Valentini et al., 2000), AMERIFLUX or the worldwide FLUXNET with more than 650 measurement sites have been established (Baldocchi et al., 2001).

In 2008, TERENO, a terrestrial network of environmental observatories, was launched in Germany. The goal of TERENO is assessing the effects and feedbacks of climate change on

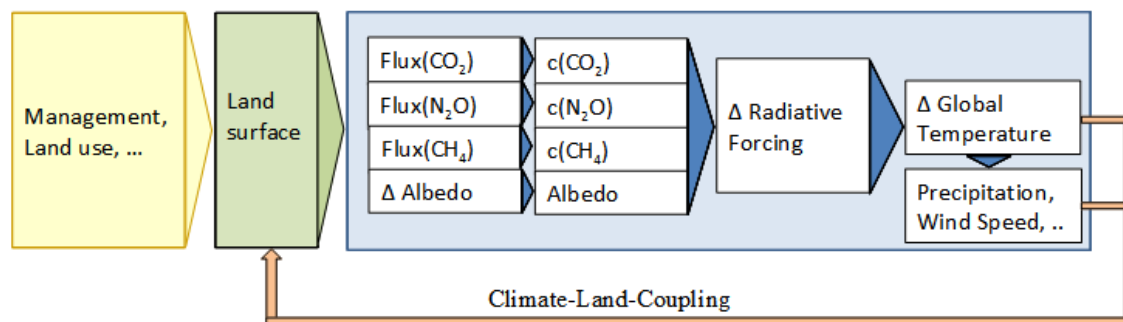


Fig. 1.2 Schematic interaction of human land use and climate: Fluxes of relevant greenhouse gases and albedo changes lead to an altered radiative forcing in the first place. Subsequently, changed temperature alters further atmospheric parameters. The brown arrow in the schematic picture depicts that both climate and land surface are coupled.

ecosystems (Mauder and Foken, 2011; Zacharias et al., 2011).

However, measurement networks will always have temporal and spatial gaps. Hence global estimations of surface and greenhouse gases fluxes are not possible by measurements alone. In order to transfer local measurements to global estimates, the multi- and inter-annual measurements have to be combined with remote sensing and modelling techniques (Baldocchi et al., 2001; Griebel et al., 2016; Krinner et al., 2005; Luo et al., 2012; Running et al., 1999).

1.1.4 N₂O-fluxes from agricultural soils

N₂O is the most important ozone depleting substance (Crutzen, 1970; Ravishankara et al., 2009) and the third most important anthropogenic greenhouse gas. N₂O contributes with about 6-7% to the anthropogenic greenhouse effect in total (Montzka et al., 2011), whereby N₂O only due to agricultural managed soils contributes about 4% (Herzog, 2009). In other words: mitigation of N₂O is mostly mitigation of N₂O-fluxes from agricultural managed soils, i.e. croplands and pastures.

In order to mitigate N₂O-fluxes, research about the underlying processes of N₂O-formation was conducted since the 1970ies. We know today that N₂O-production and consumption in soils is observed from microorganisms of all domains in biology such as eukaryotes (Bollag and Tung, 1972), archaea (Stieglmeier et al., 2014) and bacteria (Colliver and Stephenson, 2000). The processes how N₂O can be formed are manifold (Butterbach-Bahl et al., 2013). To our current knowlegde N₂O is mostly formed as a by-product of three microbial processes namely nitrification, denitrification (Davidson et al., 2000; Firestone and Davidson, 1989)

and nitrifier-denitrification (Kool et al., 2011; Wrage et al., 2001).

The ecological niches of the involved microorganisms can be defined by the response to abiotic steering parameters (Wrage et al., 2001). A major control is i) partial pressure of oxygen in the soil, which is controlled by changes in water filled pore space (WFPS) or rapid changes in carbon content, soil moisture changes with rainfall or groundwater fluctuations. Soil carbon changes for example after soil management, when residues are incorporated into the soil. The niche for nitrification goes along with a high oxygen partial pressure. The niche for denitrification is under low oxygen partial pressure. Nitrifier-denitrification takes place under sub-oxic conditions. Further constraints are ii) temperature, as the kinetics of enzymatic reactions strongly respond to temperature and iii) substrate supply. Microorganisms use C and N sources to gain energy in redox-reactions. Without low reactive nitrogen loads on agricultural fields N_2O -fluxes are diminished. A crucial biotic steering parameter, which is hard to estimate is iv) the microbial activity of microbial communities in soils.

The interaction of the above mentioned steering factors lead to the typical behaviour of N_2O -fluxes. Most of the time, when one factor is limiting, N_2O fluxes are very low. The values are around minimal uptake or minimal emission. Temperature for example is mostly a limiting factor during winter, with the exception of frost-thaw peaks (see chapter 1.2.5). When conditions are suitable, and many factors are favouring relevant pathways, fluxes can be very high. Due to the temporal and spatial heterogeneity of abiotic steering factors, heterogeneous flux pattern exists both in space and time. High emissions related to a certain location are called hot spots. High emissions in time are called hot moments.

From our current understanding, there are three important hot moments in agroecosystems: First, the so called frost-thaw-events (Risk et al., 2013) that represent ideal conditions for denitrification after freezing and thawing of the soil (see also 1.2.5). Second, fertilization events, which are triggered by high substrate loads of reactive nitrogen and third, rewetting events that are triggered by anoxic condition due to rain in summer after dry periods (Beare et al., 2009).

The published (annual) fluxes in review studies vary within a broad range. In a review study conducted by Meurer et al. (2016), yearly emissions were found between -0.07 to $4.26 \text{ kg-N ha}^{-1} \text{ a}^{-1}$ for fertilized soils in Brasil. This range is comparable to a study of Rees et al. (2013), where 6 European sites vary from 0.04 to $21.21 \text{ kg-N ha}^{-1} \text{ a}^{-1}$. For arable soils in Germany emissions between $0.53 \text{ kg-N ha}^{-1} \text{ a}^{-1}$ and $16.78 \text{ kg-N ha}^{-1} \text{ a}^{-1}$ are reported by Kaiser and Ruser (2000). Interestingly the highest value was reported from Scheyern, which is the study site of this work. In contrast to mostly positive fluxes, relevant negative fluxes of N_2O are still under scientific debate (Chapuis-Lardy et al., 2007).

Due to many uncertainties, the worldwide estimates, lie between $8.1\text{--}30.7 \text{ Tg N}_2\text{O} - \text{N}$

(Shurpali et al., 2016). The global estimates from agriculture are more stable and lie between 4.2 and 7.1 Tg N₂O-N year⁻¹ (Reay et al., 2012).

1.1.5 Statistical models, process-based models and machine learning algorithms

Statistical models (Freibauer and Kaltschmitt, 2003; Regina et al., 2013) and process-based models are up to date the two fundamentally different ways to predict N₂O-fluxes (Gabrielle et al., 2006). Statistical models are useful, as they provide estimates based on simple assumptions. In Albanito et al. (2017) these models are summarized as multiple linear regression models, linear mixed-effects models, or fixed regression parameter models. An example for a statistical scenario until 2050 is that N₂O emissions increase until 2050 compared to the last century, which is an interesting insight. However the quantitative accuracy of these estimates is low and the model uncertainty is -40% to +70% (Bouwman et al., 2013).

To understand the multi-causal and non linear relationships between controls and the fluxes of N₂O, process-based models are regarded as useful tools. Meanwhile many process based models, which simulate N₂O-formation in soils on basis of soil biology and soil physics exist (Blagodatsky and Smith, 2012): ECOSYS (Grant et al., 1993), DNDC-family (Gillespie et al., 2014; Kiese et al., 2005; Li et al., 1992), DAYCENT (Parton and Rasmussen, 1994), PASIM (Calanca et al., 2007), COUP (Jansson, 2012), Langefeld and Lefelaar (Lefelaar, 1988), Expert-N (Klein, 2018; Priesack, 2006), PASTIS + CANTIS (Condom et al., 2001), TOUGHREACT-N (Maggi et al., 2008) and ANIMO (Renaud et al., 2005; Rijtema et al., 1999).

Relevant input parameters and algorithms that trigger the formation of N₂O-processes differ. N₂O-flux can be triggered for example by a threshold value of water filled pore space (DNDC, Expert-N) or a threshold value of rainfall (APSIM) (Vogeler et al., 2013).

Despite all efforts a model which is transferable to different sites and simulates N₂O emissions reliable has not been developed yet (Butterbach-Bahl et al., 2013). Brilli et al. (2017) showed in a review paper between 9 different process based models that the associated errors of process based models calculating greenhouse gas fluxes are often because of a misrepresentation of the pedoclimate, incomplete management or the multiplicity of scales. Further methods to predict biogeochemical fluxes are neural networks as they have the ability to capture non-linear relationships. A neuronal network was until this work not applied for N₂O-fluxes, but for CH₄-fluxes instead (Dengel et al., 2013). Neural networks are not only used for predictions, but also for pattern recognition.

1.2 Research Aims

The overall aim of this work was to establish an eddy covariance (EC) station to measure surface energy fluxes of latent and sensible heat (Q_E , Q_H) and greenhouse gas fluxes of carbon dioxide and nitrous oxide (CO_2 , N_2O) between two agricultural fields. An inherent question of this setup was the applicability of this approach for the above mentioned gases in a landscape that is complex in terms of landuse (see Fig. 2.3).

Furthermore unpublished nitrous oxide measurements over 7 years with the automated chamber method that were conducted at the institute of soil ecology on the Helmholtz Center Munich, allow to put the new findings with the EC method in 2015 into a broader context. Both methods were compared, fluxes were investigated according to their drivers and modeled with the ecosystem model Expert-N and a neural network.

1.2.1 Multiannual measurements of surface fluxes in an assembly of hilly croplands with the eddy covariance method at the complex site

Measurements are needed as ground truth to constrain models that are used to achieve regional and global budgets (see chapter 1.1.3). The standard method to measure ecosystem fluxes is the eddy covariance method (Baldocchi et al., 2001; Foken, 2016).

Historically, eddy covariance measurements were conducted in so called ideal sites that were thought to fulfil the prerequisites for eddy covariance. The most prominent example for these kinds of experiments are the KANSAS experiments (Izumi, 1971). However it has been shown in several studies, even when the terrain is very flat and homogeneous, terrain-induced problems remain and ideal sites might not be as ideal as they seem (Aubinet et al., 1999; Oncley et al., 2007). With the increasing number of eddy covariance sites, studying heterogeneous land surface within ecosystems became more popular. Examples are mountainous terrain (Hammerle et al., 2007; Wohlfahrt et al., 2016), heterogeneous forest ecosystem (Foken, 2017; Rebmann et al., 2005) or complex agroecosystems (Zhao et al., 2010). Rarely covariance stations between two land use types are used (Biermann et al., 2014; Kirschbaum et al., 2015).

A known problem of the eddy covariance method is the unclosed energy balance (Foken, 2008; Twine et al., 2000). This means that the available energy (R_n) at the land surface cannot be completely received in its resulting terms of sensible heat flux Q_H , latent heat flux Q_E , ground heat flux Q_G and the storage terms Q_S that occur e.g. in plant canopies. In

order to achieve more realistic measurements, the so called "residuum" (energy gap between available energy and measured heat fluxes) is added to Q_H and Q_E using different approaches (Charuchittipan et al., 2014; Ingwersen et al., 2011; Kracher et al., 2009). The cause for the problem of the unclosed energy balance is regarded as a matter of scale. While the eddy covariance method captures micro scale fluxes, additionally meso-scale fluxes exist that are not captured (Foken, 2016).

Another experimental challenge is related to the fact that the measurement values represent an underlying area which changes with atmospheric parameters. On behalf of the research question: what does the instrument see?, Schmid (1994, 2002) developed a mathematical model to characterize the source area of an eddy covariance measurement. The area described by the mathematical model is called footprint. Meanwhile various footprint models have been developed (Heidbach et al., 2017; Kljun et al., 2003; Kormann and Meixner, 2001). Footprint models are especially needed when the underlying area (see also Fig. 2.8) of the measurement is not homogeneous but complex (Schmid, 2002). Knowledge of the source area of the flux in a complex ecosystem is needed, because most probably source strengths of the fluxes are distributed in complex patterns instead of a heterogeneous distribution. If measurement or model studies are conducted at complex sites, omitting footprint analysis may lead to a misinterpretation of the results. In other words: one runs into the problem of comparing "apples and oranges". Two measurements with two different footprints have most probably two different source strengths in complex terrain (see also Fig. 2.8).

In Bavaria the average field size is 1.8 ha and 70 % of all fields are smaller than 5 ha (Zenger and Friebe, 2015). If one compares the field sizes in Scheyern one sees that the biggest fields have a size of 6 ha. All other fields are smaller. This leads to highly heterogeneous land surface and makes Scheyern a representative study site for Bavaria and small structured agricultural systems in general (see 2.2). Small structured agriculture is of concern in many countries and continents such as India, Africa, or South America (Fritz et al., 2015).

The approach to place an eddy covariance station between two fields was so far not conducted in croplands and also not applied to fluxes for such a long time period. Measurements of net ecosystem exchange of CO_2 (NEE), Q_E and Q_H were conducted over almost three years.

Main research questions are:

- (Micro)meteorological analysis of the special measurement location (between two fields): What are the meteorologic conditions that drive fluxes from 2013 to 2015? Which wind component dominates? To what extent does each field contribute to the measured flux?

- Does a simple sorting approach of the measured fluxes according to footprint origin lead to consistent results? What are the limitations of the sorting scheme?
- Is there a significant difference in the energy balance closure of both fields? Are there differences in the energy closure at different phenological growth stages?
- Can input data and evaluation data be provided for an ecosystem model study in heterogeneous terrain (Klein, 2018) and acquisition of Q_E -flux-data to evaluate a new evaporation model (Heinlein, 2018)?

1.2.2 N₂O-measurements with the eddy covariance method

The progress in quantifying sources and sinks of energy and different matter fluxes is not equal. While the understanding of surface energy fluxes and net ecosystem exchange (NEE) across terrestrial and aquatic ecosystems is growing, high frequent information on non-CO₂ greenhouse gases like N₂O and CH₄ are still sparse (Merbold et al., 2015). This is due to a less challenging sensor technique in case of temperature, water, and CO₂ than for CH₄ and especially N₂O. Main challenges are the low concentrations and episodic fluxes due to the reasons described in chapter 1.1.4. In the present situation few sites gather eddy covariance fluxes of CH₄ or even N₂O. Flux networks, e.g. iLEAPS, for non-CO₂ greenhouse gases are only about to develop (Suni et al., 2015). The main literature on N₂O and CH₄ fluxes is still based on chamber measurements, which have several shortcomings (see 2.3.5).

Kroon et al. (2007) showed that measuring N₂O-fluxes using the eddy covariance method (see chapter 2.2) is possible with quantum cascade lasers (QCL). Initially the experimental challenges were high but the measurement instruments which were unstable under field conditions in first experiments, could be improved. Over the last decade, Allan Variance, a measure of instrument performance (Werle, 2010), improved significantly. While Kroon et al. (2007) and Neftel et al. (2010) reported Allan Variances of 0.5 and 0.7 ppb respectively for the first QCL-Aerodyne Lasers used under field conditions, Wang et al. (2016) reported already 0.26 ppb, and Huang et al. (2014) reported 0.02 ppb for the same integration time (1s) of the measurement instrument.

The first short time studies of N₂O with the eddy covariance technique were published in various ecosystems since 2005 (Eugster et al., 2007; Mammarella et al., 2010; Pihlatie et al., 2005). However the experimental and financial effort for this method is still high. There are few QCL eddy covariance studies in the literature that cover a whole vegetation period. Merbold et al. (2014) and Kroon et al. (2010b) cover a vegetation period of grasslands. Cowan et al. (2016) and Huang et al. (2014) cover a vegetation period of croplands. More QCL-measurements in agricultural systems would be highly valuable, because the eddy

covariance method bears several advantages over conventional chamber measurements. The measurements are area averaged, not disturbed and permanent measurement is principally possible (see chapter 1.2.3).

High frequent N_2O -fluxes obtained by the eddy covariance have to be gap filled with a adequate gap-filling method. Therefore look-up tables (Merbald et al., 2014; Reichstein et al., 2005) with flux data of comparable field conditions to fill the gaps and generalized linear models (Cowan et al., 2016) are used until now.

These advantages are highly valuable for a proper process understanding and can therefore contribute to the improvement of process based modelling. To the authors knowledge, a study of N_2O -EC measurements was published for pasture but not for crops.

In this work, a comprehensive measurement station for greenhouse gases from croplands was set up to measure CO_2 , CH_4 , N_2O and H_2O). The purpose of this setup was to investigate a heterogeneous land surface in agroecosystems. The advantage of agroecosystems is that one knows the spatial distribution of at least crop species and varieties very well. We also have a rough overview (50m grid) over the soil properties at both fields. To the author's knowledge a setup between two fields for non- CO_2 greenhouse gases has been published only once (Cowan et al., 2016).

Experimental research questions:

- Can an eddy covariance station measuring CH_4 and N_2O be established between two fields?
- How accurate does the spectroscopy measure? Is there a -5/3 slope in the inertial subrange of the N_2O -spectrum, which is a sign for a sensible measurements?
- Does the range of measured N_2O -fluxes agree with first publications based on measurements using the eddy covariance technique?
- Do N_2O -fluxes and their controls behave differently to earlier studies in Scheyern?
- Can we see a diurnal pattern in the measured N_2O -fluxes?

Modelling aims/questions::

- How well can the N_2O -fluxes be modelled with the ecosystem model Expert-N?
- Can we fill the gaps in the annual N_2O -flux sum using a neural network approach?

1.2.3 Static chamber versus eddy covariance measurements

Automated chamber measurements and EC measurements are established methods to measure greenhouse gas fluxes between the land surface and the atmosphere. Both are used to derive greenhouse gas balances over ecosystems (Collier et al., 2014; Kroon et al., 2010a). While the flux measured with the chamber refers to a well defined area (see also chapter 2.3.5), the flux of the eddy covariance is related to an area at the field scale which varies with atmospheric parameters (see also chapter 2.2.6). For a similar representativeness at the field scale, multiple chambers have to be used in case of the static chamber method. In our case mostly four but never less than three different chambers were used.

Furthermore the EC measurement is an in-situ measurement, where the measurement devices are exposed to open air, while the static chamber measurement is decoupled from the atmosphere (see chapter 2.3.5). As ecosystem fluxes are coupled to atmospheric processes chamber fluxes differ from the real fluxes. Riederer et al. (2013) for example found systematic differences between chamber and EC measurements of NEE. These differences occurred during daytime, when chamber fluxes were higher in late afternoon. During night, chamber fluxes were more uniform than compared to EC fluxes. In a study about N₂O-fluxes with the chamber method, Denmead (2008) showed that the magnitude of the is correlated to the magnitude of chamber ventilation.

Comparisons of measured fluxes with the eddy covariance and the chamber method show different behaviours depending on the measured greenhouse gas flux. Podgrajsek et al. (2014) for example showed that CO₂-fluxes differ substantially with both methods. Fluxes of CH₄ measured with both methods showed at least measurements in the same range. The same holds true for measurements of N₂O-fluxes in a study, which was already examined in several investigations (Laville et al., 1999; Wang et al., 2013).

In this study, both eddy covariance and chamber measurement data exist over a continuous period of 6 months. The measurements were not conducted at the same field but at the research farm. Crop rotation, soil type, climate and weather were the same.

Experimental research question:

- To what extent agree the measured N₂O-fluxes and the half-yearly flux sums of field A17 EC-method and measurements of the the automated chamber site?

1.2.4 Modelling energy fluxes

The relevance of land use is reflected in land-surface modelling by consideration of albedo change due to land use and inclusion of dynamic vegetation growth models only in the recent

years (Arora, 2002; Casanova and Judge, 2008; Klein et al., 2018; Lei et al., 2010; Lokupitiya et al., 2009; Lu et al., 2015).

Under this aspect, it is not surprising that land surface models fail to simulate energy fluxes accurately. Lokupitiya et al. (2016) for example showed in a recent comparison of 20 models simulating Q_E and Q_H that most models overestimated Q_H and underestimated Q_E . This is in accordance with earlier findings (Krinner et al., 2005; Xing et al., 2008).

In particular Lokupitiya et al. (2016) proposes that too low Q_E is an overestimation of drought stress response for high bred plants in agroecosystems. In general, he stresses that models developed for natural systems fail in managed ecosystems, while models with plant specific parametrisation perform better. This is in agreement with other publications e.g., where the performance of Q_E improves with the implementation of a dynamic root distribution (Casanova and Judge, 2008).

As surface energy models with dynamic plant growth models are not excessively developed and evaluated yet, evaluation studies showing both intra-annual and inter-annual variations are sparse. Either they show sub-yearly time series of latent or sensible heat by displaying diurnal cycles (Casanova and Judge, 2008) or diurnal cycles are averaged on the monthly scale to show multi-annual variation (Krinner et al., 2005). The bowen ratio ($Bo = Q_H/Q_E$) is usually not used to evaluate the performance of energy fluxes, since Bo shows a very high variability when fluxes are small (e.g. early morning or late afternoon). However if one limits the data to a time window with high fluxes (during noon), this problem vanishes and dynamics of energy partitioning should be seen.

Research question:

- How well can the bowen ratio be simulated for a time series of almost 3 years?

1.2.5 Modelling long-term N_2O emissions with emphasis on snow cover and frost-thaw events

Frost-thaw is typical in tundra, boreal and temperate soils (Kurganova et al., 2007). It has been observed since the early 1990ies that high emission periods after the freezing and re-thawing of the soil exist and contribute an essential or even dominating part to the annual budget of N_2O -fluxes in agroecosystems (Röver et al., 1998; Skogland et al., 1988; Teepe and Ludwig, 2004).

According to a review of Risk et al. (2013), the current understanding of N_2O -formation consists of a sequence of processes: It starts with the die off of microbes or fine roots after rapid freezing and thawing. The dead substrate can then be used as C and N source for a

growing population of nitrifying and/or denitrifying bacteria (Smith et al., 2010). As anoxic conditions, intense temperature fluctuations and biological activity represent ideal conditions for denitrification, very high N_2O -fluxes occur during these periods. Additionally, duration of freezing, freezing temperature, water filled pore space during freezing or frequency of frost-thaw incidences influence the resulting N_2O fluxes (Risk et al., 2013).

However, these frost-thaw emissions are poorly quantified in ecosystems and mostly year-round measurements are not available (Wagner-Riddle et al., 2017). If year round measurements are available, they often have a low measurement frequency, which is a problem for the often short-lived pulses of N_2O (Wagner-Riddle et al., 2017). The longest modelling studies exist at the moment for the Höglwald (Luo et al., 2012) forest. The measurements last about one decade which is exceptional. A further problem is, that the time series are often only for very few vegetation periods. Ruan and Robertson (2017) state that a detection of trends on the annual scale is not possible with short time series due to a changed snow cover regime.

Process-based models (see chapter 1.1.5) can be used to investigate these frost-thaw interactions. de Bruijn et al. (2009) found indications for diffusion limitation by snow cover and deployment of microbial biomass by dying microorganisms. However, if model parameters that describe the processes of N_2O formation are only evaluated against short time series (e.g. one year) and constraints on the multi-annual scale are neglected, there is the risk that the model performs well over the time scale of one year but fails on the multi-annual scale. This is especially probable when multi-annual trends exist in the time series of N_2O -emissions. In this work, a permanent 7 years time series was used to evaluate the process-based ecosystem model Expert-N 5.0, which is capable of estimating N_2O -emissions (Klier et al., 2011) at sub-daily time scales (Klein, 2018).

Models with a sub-daily resolution are to the authors knowledge not available at all. As processes described above are known to happen at the sub-daily scale, sub-daily models are needed. In this study, N_2O -fluxes due to freezing and thawing of the soil are modelled over 7 years at the sub-daily scale (hourly).

Research question:

- How does the implementation of a simple snow model change soil freezing?
- Is the simple snow model correlated with better N_2O -simulations?

Chapter 2

Material and Methods

2.1 Research farm

2.1.1 History of the research farm Scheyern

The monastery Scheyern and its associated farm is located in southern Germany, 40 km north of Munich (N 48° 29.8', E 11° 26'). According to the Regula Benedicti "ora et labora et lege" (pray, work and read), the monks did not only fulfil church tasks, but also practiced farming and observed the environment. As a result of this, a very long precipitation time series exist (see chapter 1.1.2).

From 1990 on, about 100 ha coherent farmland around the monastery was rented and cultivated by the "FAM Research Network on agroecosystems" (Schröder et al., 2002). Since then the farm management was adapted to study the environmental impact of agricultural activities over multi-annual time scales at the landscape scale. The ultimate goal was, to establish a management form which combines environmental compatible land use, agricultural productivity and sustainability (Schröder et al., 2002). In order to gather information efficiently and comparable, a 41 x 43 raster grid with 50 m grid size was established. In addition, maps about soil physical parameters were gathered (Scheinost et al., 1997; Sinowski and Auerswald, 1999; Stenger et al., 1998). An example for such a map can be seen in Fig. 2.1. In many maps connections between different parameters can be seen (elevation and shading, field capacity and soil texture). Both research sites are marked by red dots. The EC station is located between the two largest fields. The chamber measurements are located in the north of the research station. The EC station is described in detail in chapter 2.2. The chamber site is described in detail in chapter 2.3.

A key focus according to environmental compatible land use was the measurement and understanding of the formation of greenhouse gases (Flessa et al., 1995, 2002; Ruser et al., 2001,

1998). Since 2008 the research farm Scheyern is part of the TERENO network (Zacharias et al., 2011), a network of terrestrial environmental observatories across Germany, which was funded by the Helmholtz association. Since then, the research platform is used to study long-term impacts of climate change on terrestrial ecosystems.

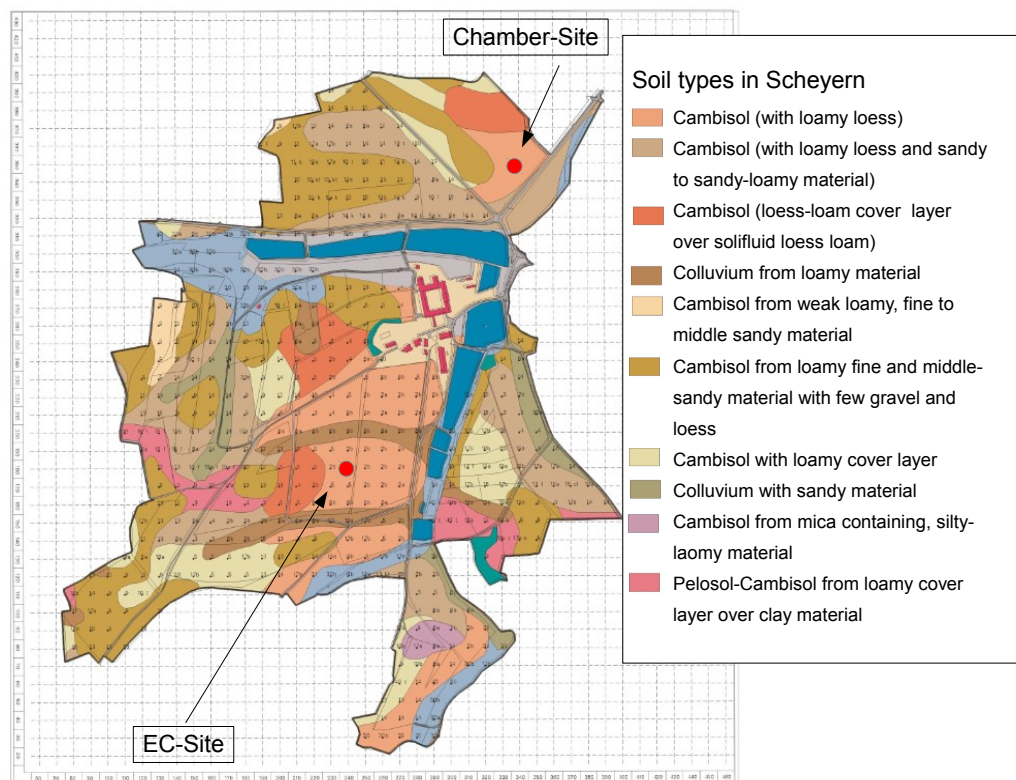


Fig. 2.1 Depicted are the soil types in Scheyern. The soils in the legend are transferred from the German classification into the the classification according to WRB (IUSS et al., 2014). The map is an unpublished map from the FAM database.

2.1.2 Climate, landscape and soils

The climate of Scheyern can be classified as Dfb, which stands for cold climate (D), without dry season (f) and warm summer (b). The classification was conducted according to the revised climate classification of Köppen and Geiger (Peel et al., 2007). Average temperature from 1992 to 2015 was 8.6°C and average precipitation was 778 mm a⁻¹ (Fig. 2.2). Frost days are typical during winter but their occurrence decreases in frequency. Three long-term averages from the measurement station Altomünster show this decrease from 113.4 (1961-1990) over 108.8 (1971-2000) to 104.4 (1981- 2010) frost days (Wetterdienst, 2018b,c,d).

The main vegetation period is between spring and autumn.

The landscape around the Research Farm is called Tertiary Hill Land. It consists of sedi-

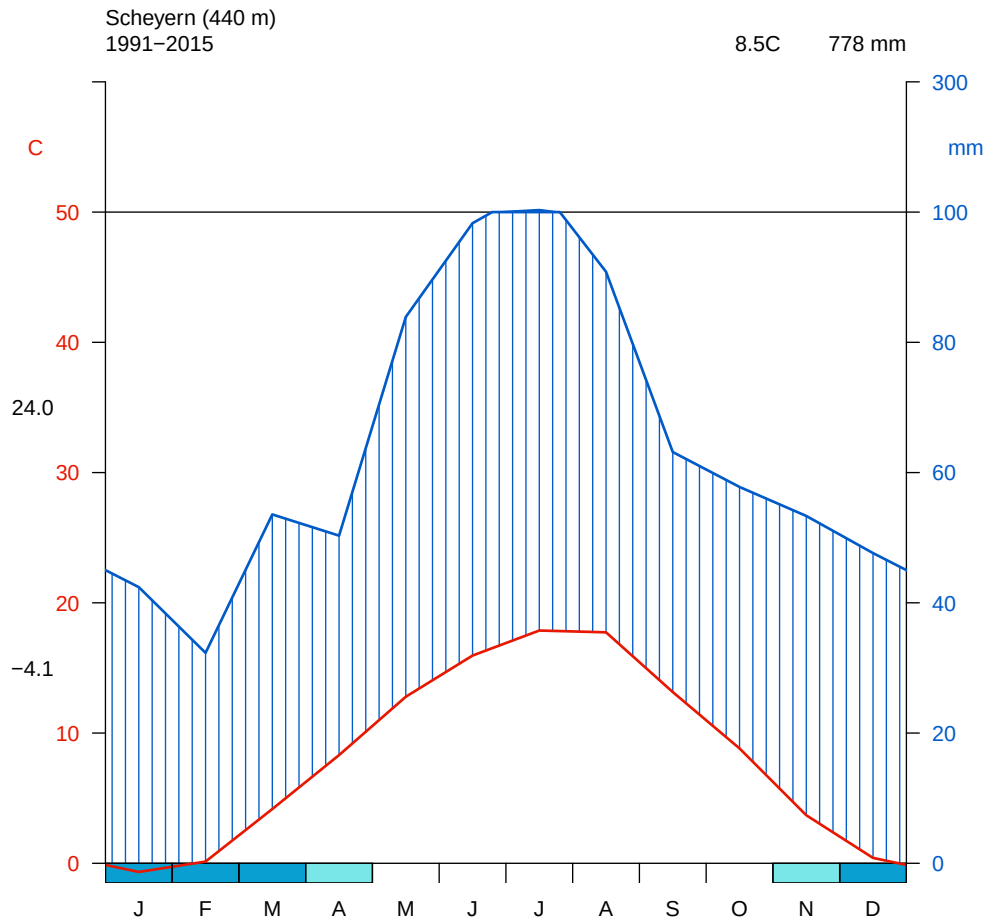


Fig. 2.2 Climate Diagram for Scheyern shows a fully humid climate, without dry season. As the average summer temperature is not warmer than 22 °C and the number of months with a higher average temperature than 10 °C is more than 4 (see months that are coloured in white at the x-axis), the climate can be classified as Dfb (Peel et al., 2007). The months at the x-axis with blue background are months with frost. The light blue colour are months with probable frost. 24.0°C is the warmest month within the period from 1991-2015. -4.1 is the coldest month within the observation period.

ments, transported from the Alps in the tertiary. In the Pleistocene, aeolian loess material was deposited on these sediments. These loess depositions are the basis for soil genesis of most soils in Scheyern that appear as upper soils (see Fig. 2.1). The soil types are, according to world reference base of soils, WRB (IUSS et al., 2014), primary Cambisols, Regosols and

Gleysols (Auerswald and Kainz, 1990). On the one side, soils from loess are increased in fertility and thus suitable for crop production, but on the other side, fine sediments in a hilly landscape make the agroecosystems vulnerable, due to an increased risk of soil erosion. In order to prevent erosion, the field sizes at the research farm Scheyern are small (Auerswald et al., 2006). From Fig. 2.1, we can see how complex soil types in landscapes are arranged. From Fig. 2.1, we can see, that both measurement locations have the same soil type, namely Cambisol.

2.2 Location and methods I: Eddy covariance

2.2.1 Complex site and landuse

The EC measurement station was placed in a complex landscape between two adjacent agricultural fields. The underlying idea of this setup was that, depending on the wind direction, either field A17, field A18 or a mixture of both fields is measured.

The fields A17 and A18, which surround the eddy covariance station, cover approximately 6 ha and 6.5 ha respectively (see Fig. 2.3). With an average slope of approximately 7° to the east, hill ridges from the south to the north and relatively small distances to the field borders (fewer than 200m), the site does not fulfil the ideal conditions for an eddy covariance site but represents many agricultural sites in Germany.

From measurements over the defined grid points of the FAM we know, that the soils at A17 and A18 are rich in nutrients. The usable field capacity is 160-180 mm and the cation exchange capacity is between 120 and 140 $\text{mmol}_c\text{kg}^{-1}$ (Scheinost et al., 1995). The dominating soil type at A17 and A18 is eutric Cambisol. Due to the slightly hilly landscape at the field site, two colluvia with loamy soil exist.

The adjacent fields will be subsequently referred to as A17 and A18. Both A17 and A18 follow the crop rotation wheat-potato-wheat-maize since about 20 years. Mostly, only one crop variety was planted on A17 and A18 (see also Fig. 2.3). A subdivision of both fields was only conducted when potato was planted (see Fig. 2.3 b and Fig. 2.3 c). The varieties grown in 2013 were Nicola (A17a), Cilena (A17b), Krone (A17c) and in 2014, Burana (A18a) and Krone (A18b). The different varieties are shown by different shades of grey. The potato plots are referred to as A17 a,b,c (1.5, 2.5, 1.8 ha) and A18 a,b (3.1 ha, 3.3 ha).

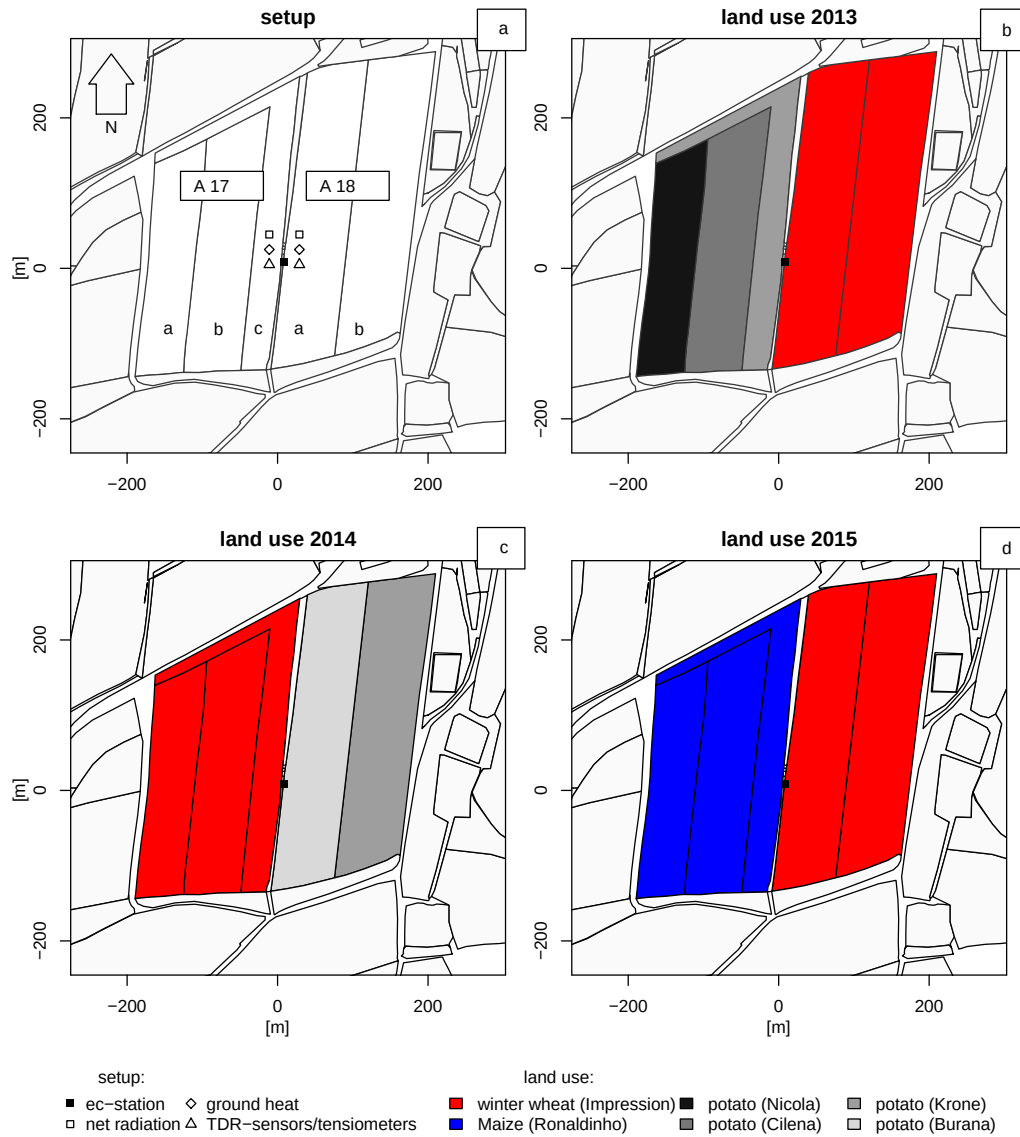


Fig. 2.3 Shown are the setup of measurement instruments (a) and the land use at the research farm Scheyern from 2012 until 2015 (b-d). The crop species and varieties are in accordance with the colour code of the legend. Land use in wintertime is mostly bare soil, except between winter wheat and maize mustard is planted.

2.2.2 Eddy covariance method

The eddy covariance method is the most direct measurement of the flux density across the atmosphere-ecosystem interface (Foken, 2013). Reynolds (1895) regarded flow quantities (X) to consist of a mean ($\bar{x}$) and a fluctuating (x') part (see equation: 2.1). The variable X in equation 2.1 describes any parameter of turbulent nature (e.g. water vapour content of air, temperature).

$$X = \bar{x} + x' \quad (2.1)$$

The Reynolds' averaging equations are then applied to momentum and scalar conservation equation (Foken et al., 2012). Some forces like coriolis force, pressure gradient, molecular viscous transport, and gravity are negligible for the turbulent transport between land and air in the atmospheric boundary layer. Under the assumption of horizontal homogeneity, coordinate rotation and steady state conditions the Navier-Stokes equations can be further simplified (Foken, 2006a).

In order to determine the covariance in the eddy covariance, Reynold's postulate about the mean of the product of two variables is used by the eddy covariance method (see equation 2.2). It is applied to vertical wind speed (w) and the entity of interest (X), which is transported by turbulent motion of the air. As the mean vertical wind ($\bar{w}$) can be considered to be zero, the whole first term of equation 2.2 is zero. Consequently the covariance is calculated directly from the second term ($\overline{w'X'}$) of the equation, which contains the turbulent information.

$$\overline{wX} = \underbrace{\overline{w\bar{X}}}_{=0} + \underbrace{\overline{w'X'}}_{\text{turbulent flux}} \quad (2.2)$$

The covariances of wind speed with temperature fluctuations, T' , humidity fluctuation, q' , or any mixing ratio, c' , are calculated as described in eq. 2.3, 2.4 or 2.5. Energy fluxes, i.e. sensible heat flux, Q_H , and latent heat flux, Q_E , are written in the unit Wm^{-2} . To obtain this unit, sensible heat in eq. 2.3 must be multiplied with the density of air ρ (kgm^{-3}) and the thermal conductivity of air c_p ($\text{Wm}^{-1}\text{K}^{-1}$). In eq. 2.4, the covariance must be multiplied with the density of air, ρ , and the enthalpy of evaporation, λ (J kg^{-1}). In case of 2.5, the covariance must be multiplied with the density of air, ρ (kgm^{-3}).

$$\frac{Q_H}{\rho c_p} = \overline{T'w'} \quad (2.3)$$

$$\frac{Q_E}{\rho \lambda} = \overline{q'w'} \quad (2.4)$$

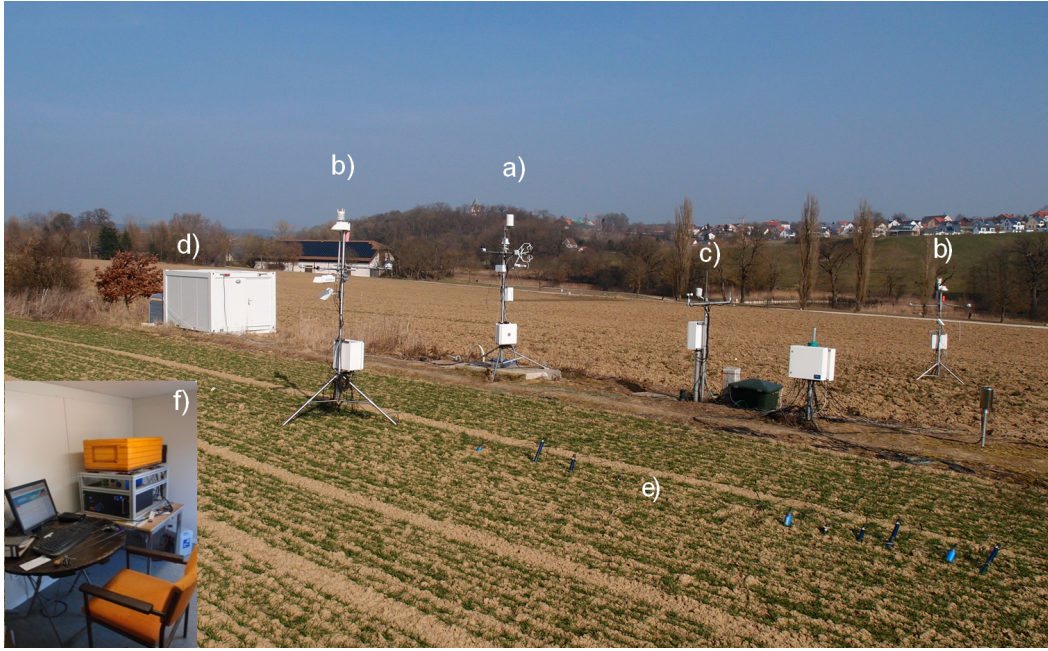


Fig. 2.4 Shows the setup of the eddy covariance station on a hill ridge between A17 and A18 at the TERENO-research station Scheyern. Between both fields the eddy covariance tower (a), a standard weather station (c) and a container for the QCL-TILDAS is placed (d). In both fields radiation stations (b) and soil measurement devices for water tension, temperature and water content are placed (e), (Photo: Christoph Thieme)

$$\frac{Q_c}{\rho} = \overline{c'w'} \quad (2.5)$$

Measurements with a temporal resolution of 10-20 Hz are necessary in order to measure turbulent fluxes. Otherwise flux information transported by small eddies at very small temporal scales cannot be captured. The advantages of eddy covariance are the investigation of surface fluxes with minimal disturbance and a spatial representativeness at the ecosystem scale as the point measurement stands for an underlying upwind area at the hectar scale.

In Fig. 2.4 one can see, that the prerequisites mentioned above are not fully satisfied. Neither is the site horizontally homogeneous in landuse nor is the terrain flat. The site is placed on a hill ridge with a slope to the east. Also from south to north the terrain is not flat. To account for the heterogeneities at the EC tower (see Fig. 2.4 a), measurement stations for a radiation balance (see Fig. 2.4 b) were set up in both field A17 and A18. Furthermore a measurement station for atmospheric standard parameters (wind speed, wind direction, temperature, humidity, see (Fig. 2.4 c), and measurement stations for soil physical parameters such as soil temperature, soil water tension, soil water content and ground heat flux (Q_G) are

placed in both fields (Fig. 2.4 e). A closed path absorption spectroscope for N_2O is placed in the container (Fig. 2.4 d) and is further described in chapter 2.2.3.

2.2.3 Instrumental setup for the eddy covariance measurements

EC-flux-measurements of Q_H , Q_E and CO_2

A crucial parameter which is needed to determine any flux with the eddy-covariance method is the vertical wind speed (w'). It is usually measured by 3-D sonic anemometers (see Fig. 2.5 a). 3-D anemometers can be also used to determine the high-frequent air temperature, which is needed for the calculation of Q_H (see equation 2.3). For the calculation of latent heat flux and CO_2 -flux (see equations 2.4 and 2.5), trace gas concentrations of water vapour and CO_2 need to be determined. Usually they are determined by IR-spectroscopy and open-path-sensors (see 2.5 b). Open-path means that the optical path of the instrument is exposed to the open environment.

In case of trace gases that occur in very low concentrations, closed path sensors with higher measurement accuracy must be employed. In this case the gas is sucked from the measurement point to a remote instrument. An example for such an instrument is the QCL-Laser described in the next chapter.

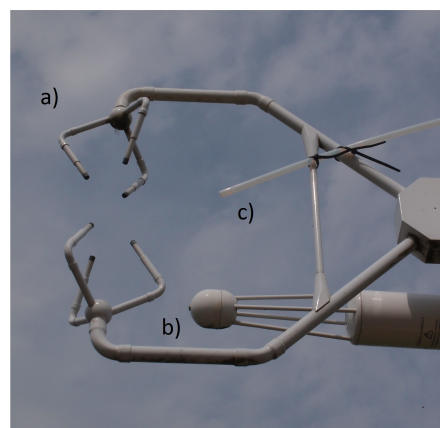


Fig. 2.5 Measurement devices for the EC-Method at the TERENO research farm Scheyern: 3-D anemometer for vertical wind speed (a), open path IR-spectroscope for CO_2 and H_2O (b) and a sampling-tube for a closed path spectroscope (c) (Photo: Christoph Thieme).

EC-flux-measurements of N_2O using a quantum cascade laser (QCL)

QCL-lasers are suitable tools for eddy covariance measurements of N_2O (Kroon et al., 2007). Therefore an additional measurement station for N_2O -fluxes was set up in this work. A scheme of the setup can be found in Fig. 2.6.

In a distance of 15 m north of the measurement station, a container for the QCL instrument was set up, as wind from the north hardly exists (1%) at the research site, which can be seen in the windrose in Fig. 3.2. Thus, flow distortion caused by obstacles (container, hedge) was held at a minimum. Temperature stabilization was found to be essential for the quality of the measurements by Kroon et al. (2007) for older Aerodyne Lasers. For newer generations of

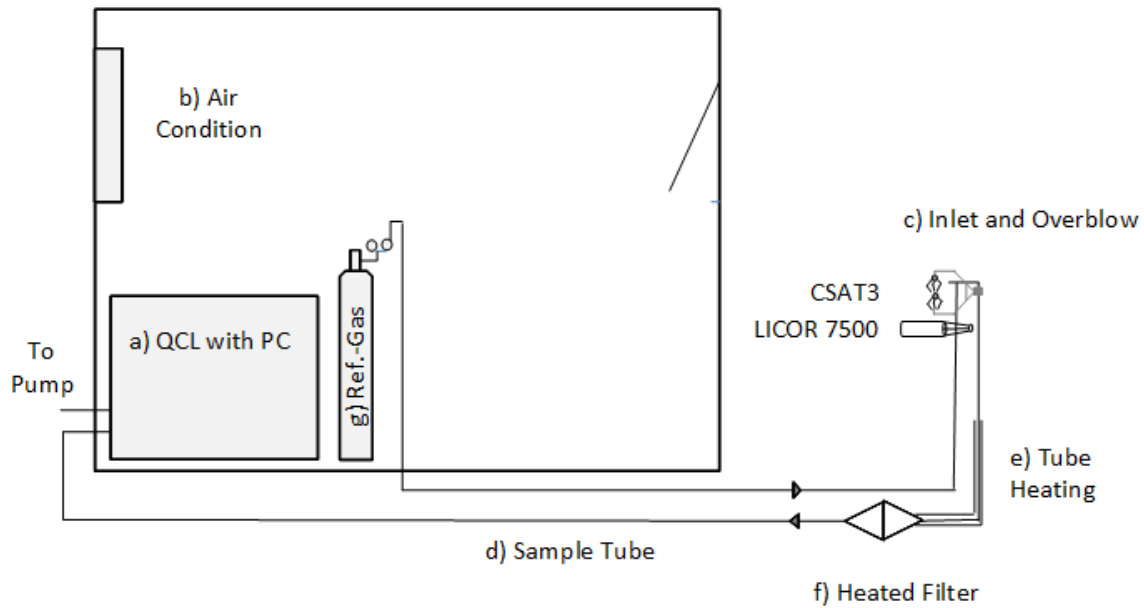


Fig. 2.6 Setup of QCL measurement system: The measurement instrument (a) was temperature stabilized by placing the instrument in a air conditioned room (b). In order to deliver the probe to the measurement instrument, the probe was sucked through a PTFE-tube (d) through the instrument (a). The inlet of the tube (c) was placed at the anemometer. In order to prevent condensation within the tube, both tube and filter were heated (e,f).

Aerodyne Lasers the problem is reported to be solved by a comparison study of Lebegue et al. (2016). However as we use an intermediate instrument from 2010, temperature stabilization was ensured as follows: 1) the ambient air in the container was held at a stable temperature (25 °C) by air condition/heating during the measurement period and 2) the optics box of the QCL was temperature stabilized at the bottom and at the top at 30 °C.

During the measurement process, the probe was sucked by a pump from the tube inlet (see also 2.5 c) through the QC-Laser, where the high-frequency measurement was conducted. Laminar flow was tried to be avoided by an exchange rate of the cell faster than 13 lmin^{-1} , as it would have reduced quality of the high-frequent measurement. and in order to exchange the measurement cell faster than sampling frequency (5 Hz). A flow rate of maximum 14 l/min was achieved. An inner tube diameter of 0.8 cm was chosen. Between the inlet and the instrument a filter (pore size $2 \mu\text{m}$) prevents the measurement cell of the instrument from pollution. Furthermore the pressure in the sampling cell was set to 30 hPa instead of 40 hPa to further increase the flow of the sample through the measurement instrument.

Tunable Quantum Cascade Laser

N_2O has two strong absorption bands in the near and mid infrared. They are located approximately at 2200 cm^{-1} and 1200 cm^{-1} . QCL are semiconductor lasers, which emit laser light in the range from the mid to the far infrared (Faist et al., 1994). So, they are suitable light sources for N_2O absorption spectroscopes.

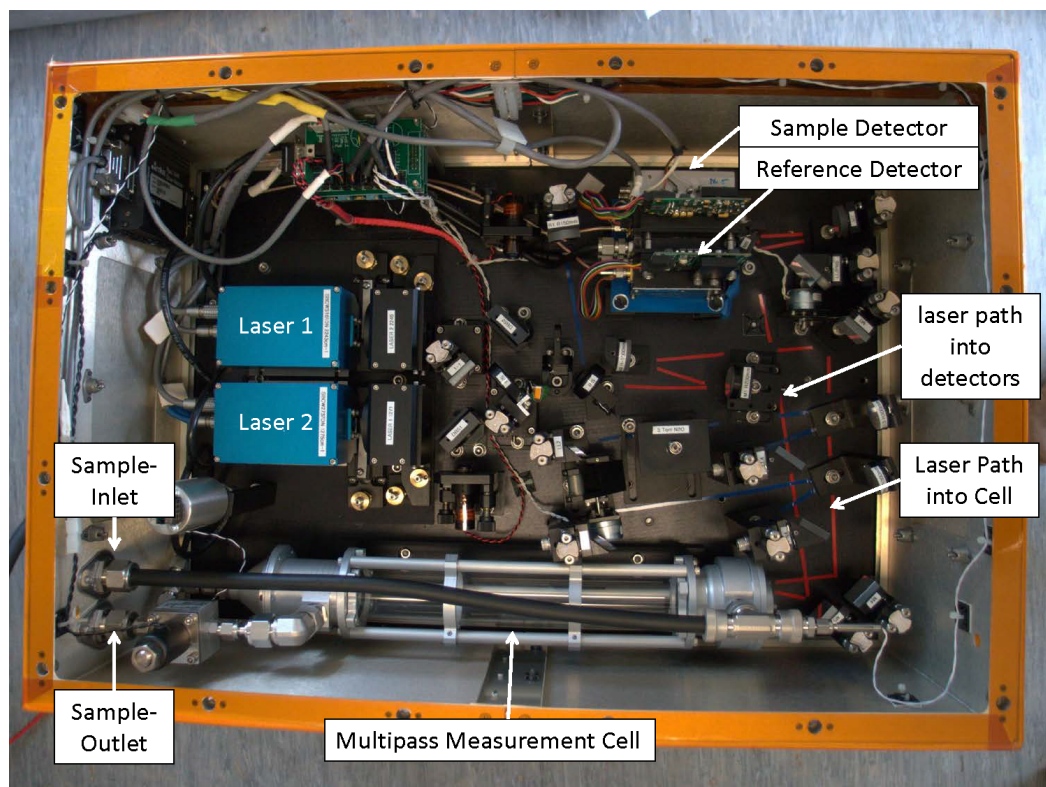


Fig. 2.7 Depicted is the optics box of the QCL instrument. The blue boxes are lasers of 2246 cm^{-1} and 1276 cm^{-1} wavelength, respectively. At the bottom of the optics box the way of the laser path is marked in red. The laser light is led by optical mirrors through the measurement instrument. The laser beam is split up, where one laser beam is passing the measurement cell (multipass cell) and the other beam is detected without passing a measurement cell (Photo: Christoph Thieme).

The band around 2200 cm^{-1} is stronger than the band at 1200 cm^{-1} . Additionally it has few interferences with other trace gases like H_2O , CO and CO_2 (Nikodem and Wysocki, 2012). Therefore the band at 2200 cm^{-1} is preferred to detect N_2O in the dual laser instruments of Aerodyne.

The generation of the laser light in QCL is based on a thin layered material (superlattice). Theoretically, it has been already shown in the 1970ies (Kazarinov and Suris, 1971) that the amplification and generation of electromagnetic waves is possible with this method.

The photon emission takes place in active regions (coupled quantum wells) of the layered material. The wavelength of the emitted light is determined by the structure of the layers. Tunable laser sweeps from spectral scans can be obtained by repetitively pulsing of the laser and simultaneously applying a sub threshold voltage ramp through a bias temperature (Faist et al., 1994). The laser excitation is typically repeated in the range of 1 MHz. A typical spectral sweep consists of 100-400 light pulses. This results in a spectral sweeping rate of 2.5-10 kHz. In case of the used instrument, these sweeps can be averaged to 5 Hz or 1 Hz measurement values.

The instrument used in this study was a tunable infrared laser differential absorption spectroscope (Dual QCL-TILDAS, Aerodyne Billerica) built in 2010. The electronic unit was updated in 2013. The basic components of the absorption spectroscope are light source (quantum cascade laser), measurement cell and detector. By using Lambert Beer's Law, the concentration of trace gas can be determined. In equation 2.6, P is the optical power of the light source after crossing the measurement cell and P_0 is the power of the laser light without interaction with the cell. The absorption of the light can be expressed as $(-\sigma(\nu)n_sL)$, where $\sigma(\nu)$ is the optical cross section and n_s is the gas concentration and L is the path length of the measurement cell (Faist et al., 1994).

$$P = P_0 \exp(-\sigma(\nu)n_sL) \quad (2.6)$$

The emitted light is lead by optical mirrors through the optics of the instrument (see Fig. 2.7). The laser path, which is depicted on the bottom of the instrument in red, leads from the two lasers into the measurement cell of 0.5 l volume. The cell has a length of 32.5 cm. At the beginning and at the end of the multipass cell, the laser beam is reflected 238 times by two mirrors (astigmatic herriott multipass cell). By this construction, a much higher measurement precision can be reached. Finally the beam exits the cell and is lead to the reference and the sample detector, where the signal is quantified.

Allan variance and Allan deviation

The Allan Variance, or two-sample variance, was originally proposed to measure oscillator stability (Allan, 1966). Werle found this statistical measure also a suitable tool to test QCL

stability (Werle, 2010). Equation 2.7 shows the computation of the Allan Variance $\sigma^2(\tau)$. The Variance is calculated from $\overline{y_{k+1}}$ and $\overline{y_k}$, which are both concentration averages adjacent in time. The variance changes with integration time (τ). Thus equation 2.7 is also a function of integration time. The concentration averages are calculated according equation 2.8, where $y(t)$ is the concentration measurement and τ is the time interval of the averaging process.

$$\sigma^2(\tau) = \frac{1}{2} \langle (\overline{y_{k+1}} - \overline{y_k})^2 \rangle \quad (2.7)$$

with

$$\overline{y_k}(\tau) = \frac{1}{\tau} \cdot \int_{t_k}^{t_k+\tau} y(t) dt \quad (2.8)$$

The Allan Deviation is the square root of the Allan Variance (Werle, 2010). The behaviour of Allan Deviation applied to QCL is that the Allan Deviation decreases with τ until a minimum is reached. This is the measurement interval where the measurement instrument measures most accurate. The rise of Allan Deviation with increasing integration time is due to an instrument drift. In this work Allan Deviation was computed and plotted with the R-Package "allanvar" (Carrio, 2015).

Power Spectrums and Cospectrums

In the measurement setup as depicted in Fig. 2.6, the 15 m long tube acts as a low-pass filter. This means that the high frequency fluctuations of N_2O , which carry information about the flux are dampened (Munger et al., 2012). This dampening can be caused by signal smearing, which occurs at too small Reynolds numbers in the sample tube leading towards the containers (see Fig. 2.6d) or a too small exchange rate within the measurement cell (see Fig. 2.7) of the instrument. Both problems occur, when the flow rate is too small.

To check the quality of the measurement, a power spectrum of the N_2O mixing ratio is used. Therefore a log-log graph of the frequency and the power spectrum of the N_2O signal can be plotted. According to Kolmogorov's findings about the energy cascade a slope of $-5/3$ in the inertial sub-range is an indicator for natural turbulence.

2.2.4 Additional measurements

Net Radiation and energy balance closure

For the quantification of energy balance closure, incoming short-wave radiation ($K\downarrow$), outgoing shortwave radiation ($K\uparrow$), incoming long-wave radiation ($I\downarrow$), outgoing longwave radiation ($I\uparrow$) is measured and balanced (see equation 2.9). Therefore a net radiometer (CNR1) is used.

$$R_n = K\downarrow - K\uparrow + I\downarrow - I\uparrow \quad (2.9)$$

The net radiation is the energy quantity that can be converted into other energy forms as for example latent heat (Q_E), sensible heat (Q_H), soil heat (Q_G) or other storage terms Q_s (see equation 2.10). For the determination of Q_G , three ground heat flux plates (HFP01) were installed in each field A17 and A18. The instruments were installed in 8 cm depth approximately 10 m away from the eddy covariance station. Further information can be looked up in table 2.2.

$$R_n = Q_H + Q_E + Q_G + Res \quad (2.10)$$

According to Aubinet et al. (1999) the energy balance closure (EBC) was calculated as the quotient of measured energy fluxes and available energy at the land surface, which is not converted into ground heat flux. The storage term was omitted in the calculation, as it can most often be mostly neglected in low crop canopies (Oncley et al., 2007).

$$EBC = \frac{Q_E + Q_H}{R_n - Q_G} \quad (2.11)$$

Knowledge about the degree of closure of the energy balance is required for modelling studies, since models have closed energy balances. As described above, energy flux measurements don't have closed energy balances. Hence, if one takes into account the residuum in model evaluations (Kracher et al., 2009), the comparability of model and measurement increases.

As the measuring non-closure of the energy balance is more meaningful during daytime, the energy balance calculations were conducted for the time window between 10 a.m. and 14 p.m.

Table 2.1 Measurement devices which are located between field A17 and A18. The measurement instruments are fixed to two measurement towers and the QCL-System is held at constant temperature in a container.

parameter	instruments type	analyser/producer	height
u,v,w	sonic anemometer	CSAT3 (Campbell Sci.)	2.5 m
CO ₂ , H ₂ O	infrared spectrometer	LICOR-7500 (LICOR)	2.5 m
T2	temperature sensor	rft2 (UMS)	2 m
RH [%]	humidity sensor	rft2 (UMS)	2 m
N ₂ O	infrared spectrometer	TILDAS (Aerodyne)	container

Table 2.2 Measurement devices which are located in both field A17 and A18. The distance to the eddy covariance tower is approximately 10m.

parameter	instrument type	analyser/producer	height
R _g	pyranometer	SPN1 (Delta-T Dev. Ltd)	2.5 m
Net radiation	net radiometer	CNR1 (Kipp & Zonen)	1.4 m
Soil heat flux	heat flux plate	HFP01 (Huxeflux)	-0.1/-0.3/-0.5 m
Water tension	tensiometer	TS1 (UMS)	-0.1/-0.3/-0.5 m
water content	TDR	Trime (UMS)	-0.1/-0.3/-0.5 m
Soil Temperature	temperature sensor	Temp107 (Campbell Sci.)	-5 cm
Logger		CR3000 (Campbell Sci.)	-
camera	webcam	Q24 (Mobotix)	3m

Standard meteorological, soil physical and plant measurements

Relative humidity, RH (%), temperature, T (° C), wind speed, WS (ms⁻¹) and wind direction, WD (°) were measured at a standard weather station, which was located between both fields. In both fields, tensiometers for soil water tension were installed. Aside the tensiometers, TDR-probes, measuring soil water content and soil temperature, were installed. For each above mentioned depth and parameter three repetitions were conducted. All in all 9 TDR probes and 9 tensiometers were installed at each of the two fields. Installation depth was 10 cm, 30 cm and 50 cm.

In 2015, plant measurements of LAI (leaf area index) and development stage were conducted. To determine LAI, a destructive measurement method was chosen. Three plants of maize and 10 plants of wheat were sampled at each measurement point per time. The leaves were cut from the stems, pressed, glued to DIN A4 paper and scanned. The different colours of the plant were then converted into either white or black with the software GIMP. From these two colours the share of leaf at the DIN A4 piece of paper could be determined. In case of maize the LAI of a single plant was multiplied with the plant density of 8 plants per m².

2.2.5 Processing of eddy covariance data

Processing of turbulence data and footprint calculation for energy fluxes in the years from 2013 to 2015

30 minute averages of energy fluxes were calculated from high frequency data (20 Hz) using the software package TK3 (Mauder and Foken, 2011). After despiking the raw data the measured time series this software applies necessary corrections to the flux calculations.

The used corrections are planar fit, which means that the x-axis of the measurement coordinate system is aligned into the mean wind. Moore-correction is used to account for high-spectral frequencies losses beyond the sampling frequency. The correction after Webb, Pearman and Leuning (WPL) takes into account density fluctuations of the air influencing the measurement of the mixing ratio of measured gas. The buoyancy flux correction converts the sonic temperature, measured by the sonic anemometer, into virtual temperature. Reviews of all corrections can be found in Foken and Wichura (1996) and Foken (2006b).

TK3 furthermore provides quality control schemes for turbulent fluxes. The determination of the data quality is based on tests for stationarity and integral turbulence characteristics (Arya, 2001; Stull, 2012; Tillman, 1972). In this work we chose the quality scheme according to the CarboEurope-IP Spoleto agreement, dividing fluxes in three quality categories. Best quality equals flag 0 (high quality), flag 1 (moderate data quality) can be used in longterm observations and flag 2 is low data quality which has to be discarded (Mauder et al., 2013). In this work, data of flag 0 and 1 are used.

Processing of turbulence data and footprint calculation for N₂O fluxes in 2015

30 min averages of energy fluxes were obtained from high frequency data. The measurement frequency was reduced to 5 Hz because of the available version of the Aerodyne Laser did not perform stable at 10 Hz. In order to process the high frequency data the software package TK3 was used. Due to the closed path absorption spectroscopy (see chapter 2.2.3) the software has to determine the tubing-time-lag (see Fig. 2.6). Therefore, the software performs a cross correlation between w' and $c'(N_2O)$. The time lag is found at the maximum of the cross correlation. All corrections except WPL correction are conducted as in the previous chapter.

The software provided sampling error according to Finkelstein and Sims (2001). This stochastic error measure is calculated as the variance of the EC measurement (Mauder et al., 2013). For a more detailed description see also chapter 2.7.

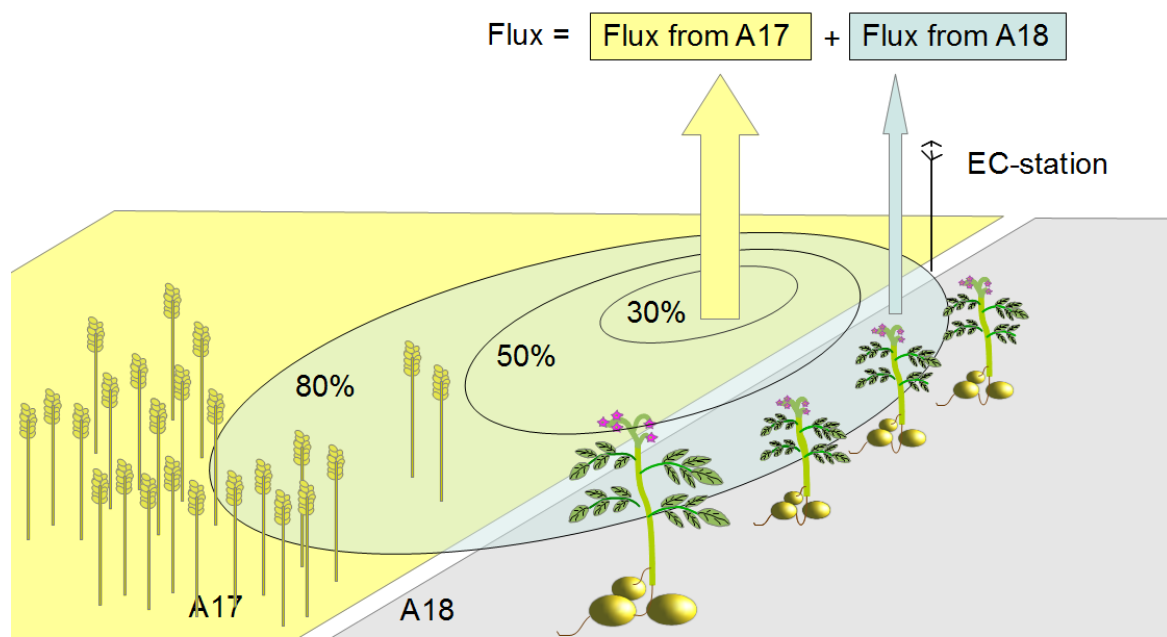


Fig. 2.8 Depicted is a schematic footprint which is drawn over a potato field and a wheat field. The picture illustrates that fluxes measured in complex ecosystems often consist of different land surfaces with different source strength, which is indicated by different arrow widths. The isolines surround the areas where 30%, 50%, or 80% of the flux footprint originates from. The footprint area is located both over field A17 and A18. The differing size of the yellow and the blue arrow shows the different magnitude of the flux due to the differing landuse and source area.

2.2.6 Analysis of EC-fluxes

Footprint analysis

Footprint analysis was performed to link flux observations to their underlying source area (Schmid, 1994). To obtain the footprints of all EC measurements, the TK3 software (Mauder and Foken, 2011) containing the Kormann-Meixner model (Meixner and Eugster, 1999) was used. As input for the calculation of the footprint in different parts of the complex landscape, micrometeorological measurements from the flux tower and geographic information about the measurement site in form of an ESRI compatible ASCII-grid were used (Mauder and Foken, 2011).

Using this input, the Kormann-Meixner model applies an approximation of atmospheric diffusion in order to estimate the spatial origin of the measured signal see e.g. (Horst and Weil, 1992).

In equation 2.12, $F(0,0,z_m)$ is the flux at the measurement height (z_m). $F(x,y,0)$ is the surface flux in the upwind direction and $\Phi(x,y,z_m)$ the so called flux footprint.

$$F(0,0,z_m) = \int_{-\infty}^{\infty} \int_0^{\infty} F(x,y,0) \Phi(x,y,z_m) dx dy \quad (2.12)$$

The assumptions of the analytical footprint model are i) horizontal homogeneous turbulence field over area of the footprint ii) no vertical advection, which can occur for example over sloping terrain iii) the Monin-Obukhov-Theory (Monin and Obukhov, 1954) applicable to the layer above the tower and iv) all eddy contributions are within one sampling period (Rannik et al., 2012).

A footprint evaluation study of Heidbach et al. (2017) showed reasonable results under all stability conditions for the Kormann-Meixner-Model (notably under neutral and stable stratification) and a study of Kljun et al. (2003) showed also reasonable results compared to a Lagrangian Footprint model.

The footprint model is applied to the site Scheyern although the requirements for an ideal site are not fulfilled (see site description 2.2). In this setup, the source area consists mostly of at least two different agricultural managed fields A17 and A18 in a hilly terrain.

Splitting of the time series into two time series (sorting scheme)

Due to its location in a complex landscape (see Fig. 2.3), the measured time series had to be sorted according to the underlying flux area.

According to Göckede et al. (2008) measurements from 80%-95% of the footprint within a target area can be seen as representative. Measurements with over 95% are regarded as homogeneous. Thus, fluxes were regarded from A17 when more than 80% of the footprint area lay inside the borders of A17. Vice versa fluxes were regarded to originate from A18, when more than 80% of the target area belonged to A18. Fluxes that did not fulfill one of the above mentioned criteria were not investigated in this work. This procedure was applied for fluxes of Q_H , Q_E , NEE , and N_2O .

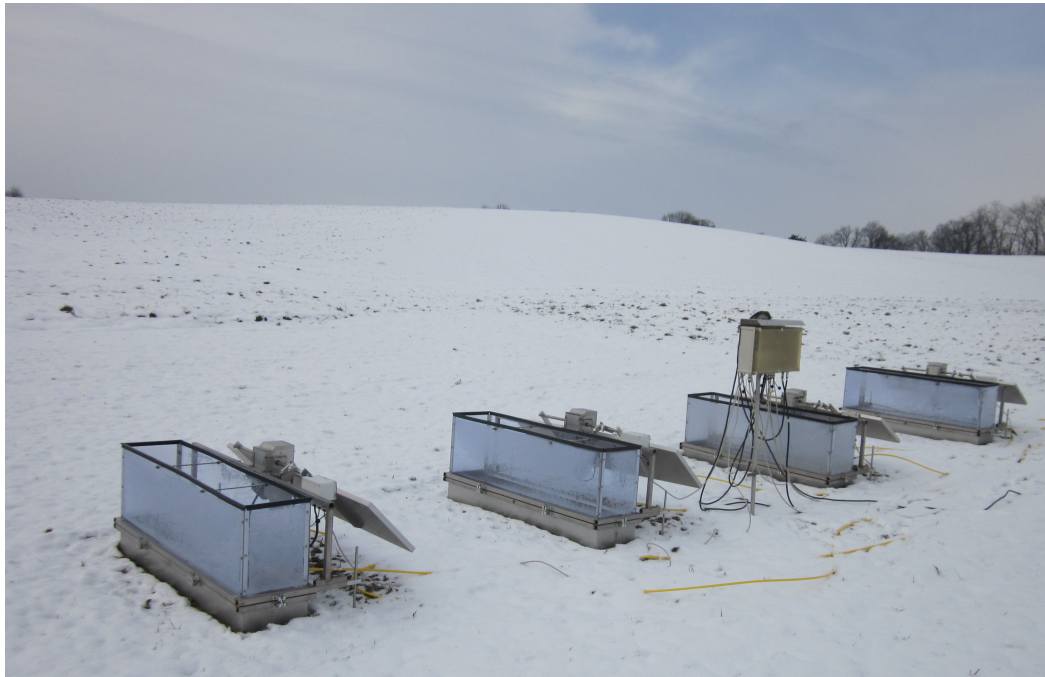


Fig. 2.9 Automated chambers in Scheyern during wintertime. Year-round measurements are needed to measure frost-thaw peaks (Photo: Christoph Thieme).

2.3 Location and methods II: Automated static chambers

2.3.1 Site description automated chamber site

The automated chamber system at the research farm was established in the year 1995 and measurements were carried out until the year 2015. It is located about 700 m north-west from the EC site on 445 m ASL. As the site is only a few hundred meters away from the EC site with comparable microclimate to the EC site, the climatic description is the same as given in chapter 2.1.1.

The crop rotation was the same crop rotation as on site A17 and A18 (see chapter 2.2), namely winter wheat - potato - winter wheat - maize, but without catch crops.

The management of the site is conventional (integrated) with high tillage (0-25 cm). All management procedures can be looked up in appendix F.2. The soil is a Cambisol (see also Fig. 2.1). The texture of the soil within the parcel next to the chamber can be looked up in table 2.8.

Table 2.3 The table shows the applied and the recommended fertilisation amounts for the crops planted in Scheyern at the automated chamber site. The fertilisation amounts are recommended for the yield level.

crop species	applied fertilisation [kg-N ha ⁻¹ a ⁻¹]	recommended fertilisation [kg-N ha ⁻¹ a ⁻¹]	expected yield level [dt/ha]
maize	135	190	90-109
winter wheat	180-185	240	70-79
potato	200	140-230	80-100

2.3.2 Fertilization at the automated chamber site

The fertilisation amounts are applied since the beginning of the 1990ies when the longterm trial was installed. The given amounts of nitrogen are shown in table 2.3. It can be seen, that the applied amounts lie beyond the recommended amounts of fertilizer.

The recommended fertilisation at the automated chamber site was estimated by the procedure after Wendland et al. (2012) at the study site. The estimations shown in table 2.3 use expected yield level and available soil mineral nitrogen before the fertilisation.

2.3.3 Yields at the automated chamber site

Tab. 2.4 shows the yields at the automated chamber site in Scheyern. In 2008, the measured dry masses for potato were 73.1 dt ha⁻¹, while four years later potato yield is only 68.0 dt ha⁻¹. For the three vegetation periods of winter wheat (WW), the amounts were between 55.4 dt ha⁻¹ and 60.3 dt ha⁻¹. Potato yields were highest during the first vegetation period, when potato was cropped in the observed time series (73.0 dt ha⁻¹). The second vegetation period of potato in 2012 the yield was only 68 dt ha⁻¹. Similarly maize was 99.3 dt ha⁻¹ in 2010 and 91.5 dt ha⁻¹ in 2014. The yield data were supplied by Phillip Koal and Georg Gerl (unpublished).

2.3.4 Snow heights at the automated chamber site

Measured snow heights were obtained from the climate data center of the German Weather Service (Wetterdienst, 2018a). Snow measurements are measured at the monastery Scheyern. The monastery is located only a few hundred meters away from the automated chamber site. Therefore the measurements are regarded to be representative for the automated chamber site.

Table 2.4 The table shows the yields measured at the research station Scheyern by Georg Gerl and Phillip Koal (unpublished) over the observed period. Dry masses are obtained by subtracting the water content of the weighted yield. The abbreviations of the crop species stand for potato (PT), winter wheat (WW), and maize (MZ).

year	yield (dt ha ⁻¹)	crop species	variety	water content (%)	dry mass (dt ha ⁻¹)
2008	430.8	PT	Nikola	83	73.1
2009	55.4	WW	Impression	14	47.6
2010	99.3	MZ	Lakta	14	85.4
2011	59.2	WW	Impression	14	51.0
2012	400.0	PT	Nikola	83	68.0
2013	60.3	WW	Impression	14	51.9
2014	91.5	MZ	Lakta	14	78.7

2.3.5 The automated chamber system

The used N₂O-flux measurements from 2008 to 2015 were conducted by Rolf Schilling. The measurements are an average of 3-4 almost simultaneous automated chamber measurements (+/-10min). Standard deviations per chamber measurement (see e.g. Fig. 3.31) and half-yearly coefficients of variation are calculated on basis of these measurements.

The measurement and flux calculation was conducted according to previous studies (Flessa et al., 1995; Loftfield et al., 1992). The procedure of the measurement and the flux calculation is as follows: The chamber was automatically closed for the measurement process for 80 minutes. The slope of the rising N₂O-concentration per time in the chamber head space, $dc(N_2O)/dt$, was determined by five successive concentration measurements. Therefore an on-field gas-chromatograph was used. In equation 2.13, T (K) is temperature in the chamber headspace, V is the chamber volume (m³) and A (m²) is the area that is covered by the measurement chamber. The constant k_{N_2O} is $1.25 \cdot 10^3 \text{ g N m}^{-3}$. The ground area of the chamber is 0.4 m² and the volume is 0.22 m³. Thus the flux, F_{N_2O} (g N₂O-N m⁻²d⁻¹), could be calculated (Flessa et al., 1995).

$$F_{N_2O} = k_{N_2O} 273 \frac{V}{T \cdot A} \frac{dc(N_2O)}{dt} \quad (2.13)$$

The theoretical measurement frequency for the field was 3 to 4 measurements per day. These measurements again consisted of 4 repetitions at 4 different places (see Fig. 2.9). If less than 3 measurements were available the measurement was dismissed.

2.3.6 Availability and variability of the measurements from 2008 to 2015

Winter and summer fluxes

For the evaluation of the chamber measurements the 7 years of chamber measurements were divided into a winter and a summer half-year.

The fluxes measured from November to April are called "winter fluxes". During this time nitrogen is limited and the freezing, thawing and snow cover occurs (see also Fig. 2.2). Fluxes from May to October are called "summer fluxes". During that time fertilisation events and rewetting events are regarded to be more important.

Number of measurements and coefficient of variation

The half-year with the least number of measured fluxes was in winter 2012/2013 (193 flux measurements). The half-year with the highest number of measured fluxes was summer 2008/2009 (418 flux measurements).

The coefficients of variation (CV) in Scheyern are smaller than 200%. This means that the fluxes measured in Scheyern can be classified (Barton et al., 2015) as moderate in cases of $CV < 100\%$ and high in case of $CV > 100\%$. Time periods of fluxes with extreme episodicity are missing. In contrast to CV values in the 1990ies, where average CV of 185% were measured, the episodicity during the last three years of the observed time frame is rather small (see table 2.5). The first three years resemble the episodicity of the measured CV values in the 1990ies.

Table 2.5 Numbers of measurements for winter and summer (N_{winter} , N_{summer}) and coefficients of variation [%] are shown for measurements of seven years. Numbers of observations are splitted up into summer and winter values.

year	2008/09	2009/10	2010/11	2011/12	2012/13	2013/14	2014/15
N_{winter}	316	308	306	226	193	234	300
N_{summer}	418	259	209	253	274	274	235
CV_{winter}	150	110	130	20	30	40	40
CV_{summer}	140	180	190	130	70	70	130

2.4 Ecosystem model description: Expert-N 5.0

2.4.1 The Expert-N ecosystem model framework

Expert-N is a process-based ecosystem model. The beginning of its development reaches back to the beginning of the 1990ies. The software is originally intended as a tool for agricultural consulting, mainly fertilization consulting. Thus, historically, the focus of the model was nitrate leaching to ground water at first. Due to the modular structure it could be extended with plant and atmosphere models during the last two decades. Expert-N is now used for a broad range of applications varying from the field to the regional scale.

Recently, the new version Expert-N 5.0 was developed. Due to its gridded structure the new model can also be used for regions consisting of patchy land use and land surface properties (Ewert et al., 2015). The model framework Expert-N 5.0 is based on its predecessors Expert-N 3.0 (Priesack, 2006), Expert-N 2.0 (Stenger et al., 1999), and Expert-N 1.0. In this study, the new version, Expert-N 5.0 was used. Characteristic for Expert-N is the modular structure, which allows the combination of different sub-models. In Fig 2.10, the "Model Options" are depicted. In this interface different model options for atmosphere, management, water, heat, plant and nitrogen can be chosen. In this specific example one can see, that all modules of the nitrogen turnover and transport model LEACH-N are used.

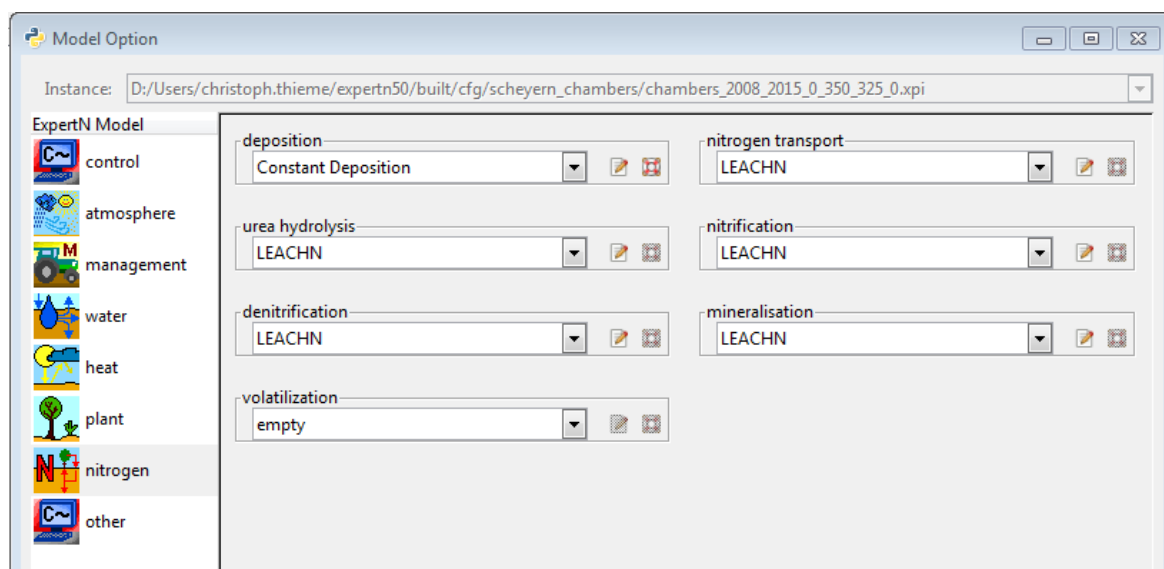


Fig. 2.10 Model Options in Expert-N 5.0: depicted. On the left side tabs of the figure the tab "nitrogen" is chosen. Under this tab sub-models simulating the nitrogen cycle can be configured. Further tabs e.g. plant contain sub-models for plant growth, etc.

In the course of the new development of Expert-N 5.0, the temporal resolution of the model was enhanced from former daily time steps to arbitrary small time steps (Klein, 2018).

2.4.2 Evaporation model: Expert-N-SPASS

In this work, actual evaporation is calculated on basis of potential evaporation at first. Then it is constrained by the SPASS model to actual evapotranspiration.

Penman-Monteith

Potential evapotranspiration is calculated after Penman-Monteith ASCE (American Society of Civil Engineers) for every hour (Irmak et al., 2006). The radiation term in equation 2.14 depends on net radiation, R_n ($\text{MJm}^{-2}\text{s}^{-1}$) minus ground heat flux, Q_G ($\text{MJm}^{-2}\text{s}^{-1}$). 24 is a conversion factor between day and hour (hd^{-1}), Δ is the slope of the water vapour saturation curve ($\text{kPa } ^\circ\text{C}$) and L_{evap} specific heat capacity of water ($\text{MJm}^{-2} \text{mm}^{-1}$). The ventilation term is mainly determined by the saturation deficit of the atmosphere, $e_s - e_d$ (kPa). Further parameters are wind speed, U_2 (ms^{-1}), the alfalfa reference surface, which is C_d (-) during day and C_n (-) during night, and the psychrometric constant, γ ($\text{kPa } ^\circ\text{C}$).

$$\lambda ET = 24 * \frac{\frac{1}{L_{\text{evap}}} \Delta (R_n - Q_G) + \gamma \frac{C_s}{T+273} U_2 (e_s - e_d)}{\delta + \gamma (1 + C_{d,n} U_2)} \quad (2.14)$$

Actual evapotranspiration

In order to further constrain the potential evapotranspiration to an actual evapotranspiration, LAI and soil water availability are used to derive an actual evapotranspiration from the potential evapotranspiration (Heinlein, 2018). Depending on LAI the calculated potential evapotranspiration is split into potential evaporation, E_{pot} , and potential transpiration, T_{pot} . Both rates are constrained by soil water availability to calculate the actual evaporation, E_{act} and actual transpiration T_{act} . In sum ($E_{\text{act}} + T_{\text{act}}$) the actual evapotranspiration, ET_{act} , is obtained.

2.4.3 Plant Model: Soil-Plant-Atmosphere System Simulation

Plant growth is simulated by the SPASS (Soil-Plant-Atmosphere System Simulation) model. Important processes for this study are phenological development, biomass growth, system

development, canopy system development, root senescence, water uptake and nitrogen uptake (Gayler et al., 2002; Wang, 1997). The simulated plant species in this study are winter wheat, potato and maize. A more detailed explanation can be found in Heinlein et al. (2017) or (Heinlein, 2018).

2.4.4 Nitrogen model: Leaching Estimation And Chemistry Model

LEACHN is the nitrogen module of LEACHM (Leaching Estimation And Chemistry Model). In Fig. 2.11, a simplified scheme of the nitrogen turnover dynamics in an arbitrary soil layer is depicted. This architecture allows exchange and transport between the layers and also the loss of nitrogen into other compartments such as the ground water or the atmosphere.

Soil organic nitrogen pools in the LeachN-Model (Engel et al., 1993) are Litter-N, Humus-N and Manure-N. These N-pools can be mineralized by microbial activity into either ammonium or nitrate. Immobilisation is the uptake of reactive nitrogen by a soil organic nitrogen pool. A more comprehensive model description can be found in Hutson and Wagenet (1992).

Reactive nitrogen species can be converted as follows in LEACHN. Urea is converted by

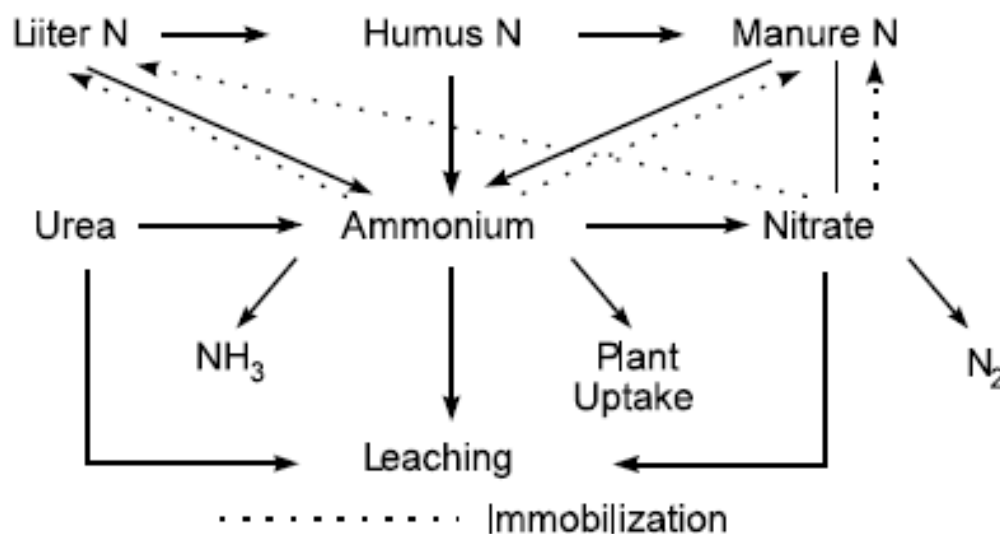


Fig. 2.11 The model LEACHN was proposed by Hutson and Wagenet (1992). The scheme of the matter flow shown with a picture according to Engel et al. (1993).

hydrolysis into ammonium. Ammonium can be converted to nitrate by nitrification. Gaseous losses, happen for example in the final stage of denitrification where nitrate is finally reduced to gaseous di-nitrogen N_2 or as a by-product during nitrification and denitrification (see Fig. 2.11, chapter 2.11).

Flux simulation of nitrous oxide

N_2O is modelled according to the "hole in the pipe model" of Davidson et al. (2000). N_2O is formed proportional to the nitrification and denitrification rate. The model formulation within Expert-N 5.0 is based on the principle of reduction functions as described in Johnsson et al. (1987). The simulation algorithm used here is a very simple approach to model N_2O -emissions.

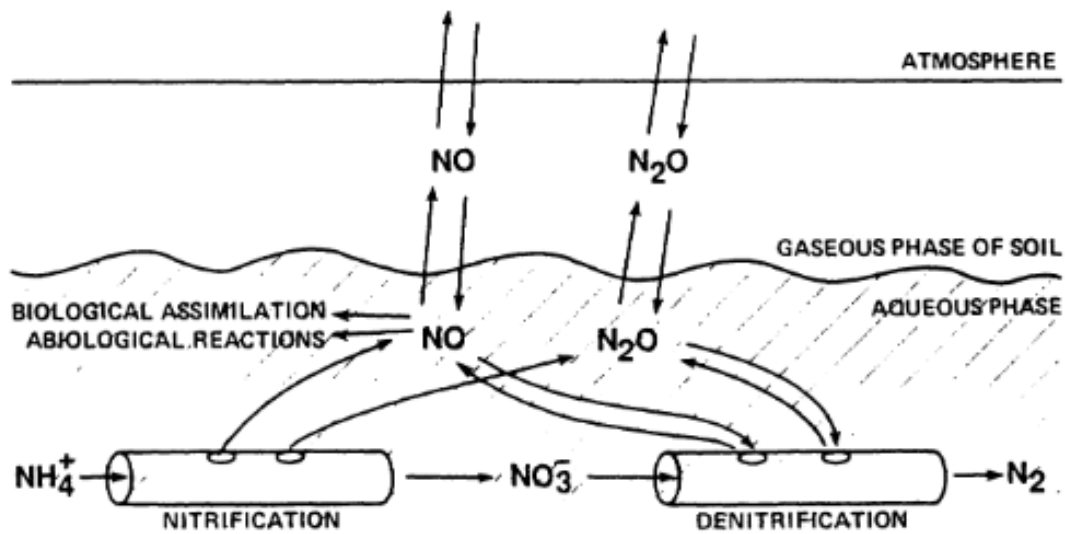


Fig. 2.12 Depicted is the hole-in-the-pipe model after Davidson Davidson (1993), where NO and N_2O are both byproducts during nitrification and denitrification. The formation of N_2O and NO occurs in the liquid phase. After their release, N_2O enters from where it is transported into the atmosphere

Simulation of N_2O -production during denitrification

In equation 2.15, $k_{den,\text{N}_2\text{O}}$ is the N_2O production rate during denitrification ($\text{mg m}^{-3} \text{h}^{-1}$). It is determined by both $k_{den,\text{N}_2\text{O},max}$, which is the maximum denitrification-rate and several reduction functions. The dimensionless reduction functions describe in schematic terms how microorganisms involved in N_2O production respond to their abiotic drivers, namely water, temperature and substrate supply.

$$k_{den,\text{N}_2\text{O}} = k_{den,\text{N}_2\text{O},max} \cdot f_\theta \cdot f_T \cdot f_{\text{NO}_3} \cdot f_{rew} \cdot f_{frost} \quad (2.15)$$

The reduction function for water (f_θ) depicts the rising anaerob microbial activity with rising volumetric water content θ ($\text{cm}^3 \text{cm}^{-3}$). In the used model of Johnsson et al. (1987)

denitrification only exists above a certain threshold of volumetric water content ($\theta_d = 0.5 * \theta_{sat}$) (eq: 2.16). Beyond this threshold f_θ rises with the exponent two and reaches its maximum at soil moisture saturation θ_{sat} ($\text{cm}^3 \text{cm}^{-3}$).

$$f_\theta = \left[\max\left(\frac{\theta - \theta_d}{\theta_{sat} - \theta_d}, 0\right) \right]^2 \quad (2.16)$$

The reduction function for temperature f_T (see eq: 2.17) represents the temperature sensitivity of microbial activity. In this model the exponent increases by 1 with the interval of 10 degree soil temperature (T) above a base temperature (T_B). The base is a given dimensionless Q_{10} -factor.

$$f_T = Q_{10}^{(T - T_B / 10)} \quad (2.17)$$

The reduction function for nitrate f_{NO_3} describes the N availability for denitrification eq: 2.18, by the half-saturation constant K_{NO_3} (mg cm^{-3})

$$f_{NO_3} = \frac{\theta_{CNO_3}}{\theta_{CNO_3} + K_{NO_3}} \quad (2.18)$$

Modelling of rewetting events

In order to simulate rewetting events (Davidson, 1992), the N_2O -Model contains a rewetting module implemented in Expert-N as described by Klier et al. (2011). It assumes that after at least 7 days of soil drying, rainfall events with more than 10 mm per day cause a rewetting event which increases N_2O emissions. The enhanced flux in the model is simulated by increasing the rewetting factor ($f_{rew,max}$).

First, the algorithm calculates a measure of soil drying (see equation 2.19), $F(t_j)$, which is the integrated difference between ET (mm) and N (mm) from t_j to t_{j-1} . The time of the actual rewetting event t_j and the time of the former last event t_{j-1} .

$$F(t_j) = \int_{t_{j-1}}^{t_j} ET(t) - N(t) dt \quad (2.19)$$

With the calculated measure of soil drying from equation 2.19, the maximal effectiveness factor of rewetting is calculated at time t_j . $F_{rew,max}$ in eq. 2.20 is a constant.

$$f_{rew,max}(t_j) = \min \left[\frac{F(t_j)}{F_{rew,max}}, 1 \right] \quad (2.20)$$

To account for observations in field measurements, where a delay of highest N₂O emissions after rewetting is observed (Klier et al., 2011), the maximal effectiveness factor from equation 2.20 is multiplied with equation 2.23. A restriction for a rewetting event is, that at least seven days have to pass for a rewetting event (see equation: 2.22).

$$f_{rew}(t) = g(t - t_j)f_{rew,max}(t_j) \quad (2.21)$$

for

$$t_j \leq t \leq t_j + 7 \quad (2.22)$$

$$g(x) = \begin{cases} x/2 & \text{for } 0 \leq x \leq 2 \\ 1 & \text{for } 2 \leq x \leq 3 \\ 1 - (x - 3)/4 & \text{for } 3 < x \leq 7 \end{cases} \quad (2.23)$$

Modelling frost-thaw events

A frost-thaw model is used to account for the hot moments during freezing and thawing. In equation 2.24 an enhanced frost factor, f_{frost} , is calculated during frost. This is realized by multiplying an amplification factor, C_{frost} , with the freezing rate, $\frac{\partial \theta_{ice}}{\partial t}$, in the soil.

$$f_{frost} = C_{frost} \max\left(\frac{\partial \theta_{ice}}{\partial t}, 0\right) + 1 \quad (2.24)$$

In case of freezing, i.e. $\frac{\partial \theta_{ice}}{\partial t} > 0$, the frost factor, f_{frost} , is going to be enhanced. The freezing-rate, which is used for the enhancement ($\frac{\partial \theta_{ice}}{\partial t}$) is calculated using the equations 5-37 in the documentation of the Daisy-Model (Hansen et al., 1991) for every soil layer. The implementation of these equations can be looked up from equation 313 to 317 in Priesack (2006).

$$\frac{\partial \theta_{ice}}{\partial t} = \frac{\rho_w}{p_{ice}} \left[\frac{\rho_w L_f}{T_f} C(\theta_{liq}) \frac{\partial T}{\partial t} + \frac{\partial \theta}{\partial t} \right] \quad (2.25)$$

In equation 2.25, the change of solid volumetric soil water content ($\frac{\partial \theta_{ice}}{\partial t}$) is dependent on the density of water (ρ_w), the pressure of ice p_{ice} (Pa), the latent heat at the phase transition from water to ice, L_f (Jkg⁻¹), the frost temperature, T_f , which is equal to 273.15°C, C_{liq} the differential water capacity (m⁻³), the soil temperature, T (°C) and θ , the volumetric water content of liquid water. For further information see Priesack (2006).

Table 2.6 Constants and variables that are used in the LEACHN-Model.

Abbreviation	Explanation	value	unit
θ_{sat}	water content at saturation	0.43	[kg kg ⁻¹]
θ_d/θ_{sat}	threshold water content	0.6	[-]
T_B	base temperature	0	°C
Q_{10}	reaction constant	2.0	[-]
K_{NO_3}	half saturation constant	5	kg Nha ⁻¹
$k_{den,N_2O,max}$	maximal N ₂ O production rate from denitr.	0.16	[mg cm ⁻³ d ⁻¹]
$k_{nit,NO_3}f$	nitrification rate		[mg dm ⁻³ d ⁻¹]
β	constant N ₂ O formation factor from nitrification	0.01	[-]
f_{frost}	frost factor	≥ 1	[-]
f_θ	reduction function for water	0-1	[-]
f_{NO_3}	reduction function for nitrate	0-1	[-]
f_T	reduction function for temperature	> 0	[-]
f_{rew}	rewetting factor	> 1	[-]

Simulation of N₂O-Production by Nitrification

Nitrification was simulated according to Johnsson et al. (1987). The model assumes that N₂O-production occurs proportional to nitrification (see equation 2.26). A constant factor β is applied to determine k_{nit,N_2O} from k_{nit,NO_3}

$$k_{nit,N_2O} = \beta k_{nit,NO_3} \quad (2.26)$$

Transport of N₂O out of the soil

The transport of N₂O from the soil into the atmosphere is realized by the "emit-all function". The formed N₂O is emitted from the soil, which is a simplified assumption neglecting physical processes that transport matter between soil and atmosphere. This implicates, that negative fluxes cannot be simulated with this model. Also atmospheric stability is not regarded.

2.4.5 Boundary conditions of Expert-N in case of snow

Default upper boundary condition (BC1)

By default, no snow model exists in Expert-N 5.0, which takes into account the effect of snow on the upper soil temperature. This leads to an unrealistic soil temperature regime. In order to take into account this shortcoming, boundary condition two (BC2) is formulated in the next sub-section.

Alternative upper boundary condition (BC2)

In case of snow cover the air temperature was set to 0°C. This in turn leads to the situation, that the upper soil layer in the model is exposed to 0°C (see equation 2.27). This was assumed to be reasonable since there is evidence in the literature, that snow cover is a strong controlling factor for the temperature of the upper soil layers (Yu et al., 2016).

The information on when snow cover appeared in the study area was extracted from on site cameras and snow heights were measured directly in at the monastery Scheyern by the German Weather Service and begin even in 1979 (Wetterdienst, 2017).

$$T_{surface} = \begin{cases} 0^{\circ}C, & h_{snow} > 0 \\ T_{air}, & h_{snow} = 0 \end{cases} \quad (2.27)$$

2.5 Model input and evaluation data

Weather data

26 years of weather data with hourly resolution were put together during this work. The data was partially measured during this work from 2012 to 2015, obtained from the FAM database from 1991 to 2012. In case of measurement gaps the weather stations Voglried, Altomünster and Hüll were used (see Fig. 1.1). For the simulation of the EC-fluxes meteorological driver data of 3 years was used. For the N₂O-flux measurements meteorological data of the last 7 years was used.

2.5.1 EC site

Management data and plant data

Management data consisted of management events concerning the plant and soil management (e.g. fertilization, tillage, sowing, harvesting) and quantitative information (e.g. amount of fertilizer or tillage depth). An overview over three years of plant management and additional plant data can be found in the appendix in table F.3 and F.4.

During the year 2015, several on site measurements of plant height and LAI were conducted. For further information see subsection 2.2.4.

Soil texture and hydraulic properties

The soil data were taken from the FAM database, which contains detailed soil descriptions in a gridded structure. The model was parametrized for 18 soil layers. Each numeric layer is 5 cm thick. The first four numeric layers (see Tab. 2.7) consist of have the same soil physical properties.

Table 2.7 Soil properties at the EC site site: The percentages of clay, silt and sand content are taken from FAM database) and parameters for soil moisture modelling (Campbell A, Campbell B and K_{sat}).

depth [cm]	clay [%]	silt [%]	sand [%]	Campb. A [Pa]	Campb. B [Pa]	K_{sat} [mm d^{-1}]
0-20	22 %	60 %	18 %	-0.85	7.48	3311.6
20-35	30 %	53 %	17 %	-0.17	11.54	2215.4
35-65	28 %	53 %	20 %	-1.05	12.37	952.3
65-90	29 %	49 %	22 %	-0.17	8.12	5925.6

2.5.2 Automated chamber site

In order to test the hypothesis that the change in winter emissions can be explained by changing weather conditions a simulation of nitrous oxide fluxes was conducted by using the nitrous-oxide formation model described in chapter 2.4.4. Simulations of 42 winter months and 42 summer months based on the 3790 measurements described in chapter 2.3.5 were performed.

Nitrogen and gravimetric water content measurements were measured by Phillip Koal (unpublished) in this study from 2012 on. Earlier measurements were conducted by the Institute of Soil Ecology (IBOE) at the Helmholtz Zentrum Munich. The measurements are gravimetric measurements, which are converted into volumetric water contents.

Table 2.8 Soil data: Texture (clay, silt and sand content, measured by Phillip Koal, unpublished) at the chamber site and parameters for soil moisture modelling (Campbell A, Campbell B and K_{sat}).

depth [cm]	clay [%]	silt [%]	sand [%]	Campb. A [Pa]	Campb. B [Pa]	K_{sat} [mm d^{-1}]
0-20	17.5	46.9	35.6	-0.85	7.48	2311.6
20-35	30.1	53.4	16.5	-0.17	11.54	1015.4
35-65	24.0	27.0	49.0	-1.05	12.34	152.3
65-90	19.0	15.0	66.0	-0.17	8.12	55.6

2.6 Description of the artificial neural network

In order to estimate missing values in the N_2O time series, an artificial neuronal network (ANN) was applied. In this work, the R-package "neuralnet" was used to fill the gaps of N_2O measurements. The package uses a back-propagation algorithm as described in Fritsch et al. (2016) and has been already used to estimate gaps of CH_4 -fluxes measured with the eddy covariance method (Dengel et al., 2013). An ANN has not been used yet to fill gaps in a time series of N_2O -flux data measured with the EC method, yet.

On the left side of Fig. 2.13 all independent or explaining variables are depicted. They were

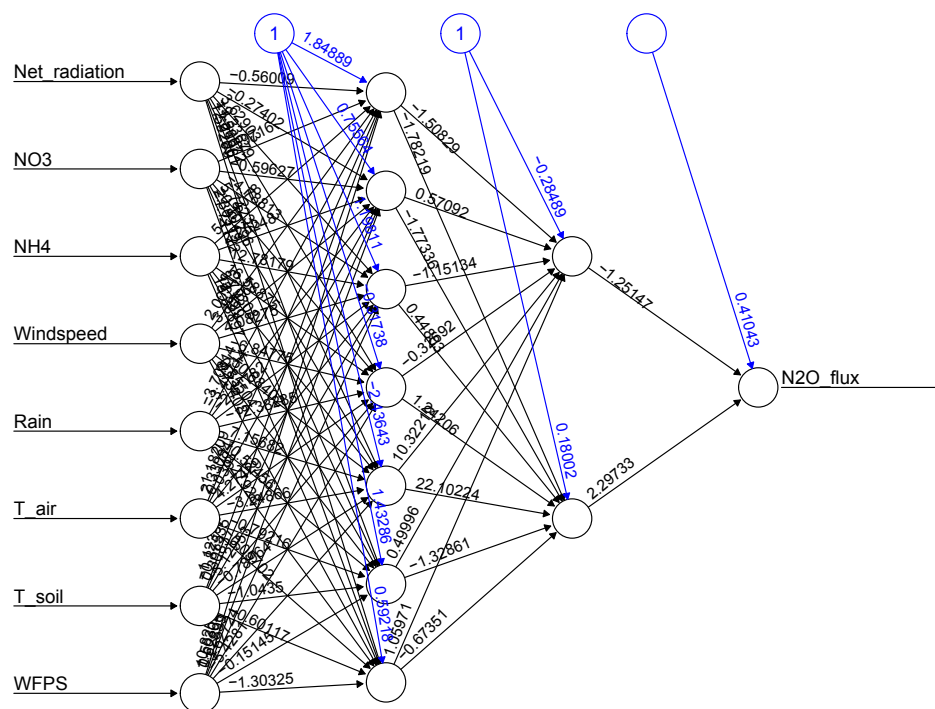


Fig. 2.13 Schematic picture of a artificial neuronal net. On the left side the explaining parameters are depicted. The neural net which was used in this work had two hidden layers with seven and two nodes respectively. The neuronal net was trained to estimate N_2O -fluxes. Therefore, the output of the neuronal net is N_2O -flux.

chosen as they are known or suspected drivers for N_2O -fluxes. The "neurons" of the input layer and the following layers are connected with black arrows in Fig. 2.13. The number on the arrow is the weight of the connection. Blue lines show the bias terms that are introduced in every step of the ANN (Günther and Fritsch, 2010). The two layers that lie between input and output are called hidden layers. The two hidden layers have 7 and 2 nodes, respectively.

To avoid the danger of over-parametrisation the number of hidden layers was held small. Hourly measurement data without gaps exist for T_{air} , T_{soil} , precipitation and wind speed (see Fig. 3.24 and Fig. 3.38). A mixture of simulated and measured data was used in case of WFPS and soil temperature (see Fig. 3.34). Only simulations were used for NO_3 and NH_4 (see Fig. 3.34).

The values of the single explaining and explained parameters were transformed by min/max-normalisation, which is not necessary for the functioning of ANN but recommended (Nawi et al., 2013). After the transformation the minimum value of each scaled parameter is 0 and the maximum is 1.

A sub-dataset from the N_2O measurements and their drivers was chosen in order to train the data set. In our case 75 % of the available measurements were taken to make the neuronal network learn the relationships between steering parameters and N_2O -flux. It is crucial, that the training dataset contains the whole span of observations. If this is not the case the chosen training-dataset is unlikely to be representative for the rest of the dataset. In order to evaluate, if the neuronal net gives reasonable estimates it is applied to a test data set, which consists of the 25% of the data that was not used to train the dataset.

After a successful testing of the estimated N_2O -values, the neuronal net can be applied to estimate the gaps in the dataset.

2.7 Statistics

2.7.1 Random error

For eddy covariance fluxes, the random error of the software package TK3 is used. It is calculated according to the strategy of Finkelstein and Sims (2001) and an algorithm described by Fuller (2009). The calculation of the random error ($\tau_{\text{cov}(x,y)}^{\text{stoch}}$) is described in Mauder et al. (2013) and shown in equation 2.28, where $\overline{xx'_p}$ and $\overline{yy'_p}$ are auto-covariances and $\overline{x'y'_p}$, $\overline{y'x'_p}$ are cross-covariances with time lag p. The number of measurements (N) is given as N and the summation bound is given as m.

$$\tau_{\text{cov}(x,y)}^{\text{stoch}} = \sqrt{\frac{1}{N} \sum_{p=-m}^m \overline{xx'_p} \cdot y'y'_p + \overline{x'y'_p} \cdot y'x'_p} \quad (2.28)$$

2.7.2 Daily standard deviation and yearly standard deviation

For the calculation of the standard deviation (μ) in equation 2.29, the "stats" package of the programming language R was used (R Core Team, 2018). Here x stands for any variable. The mean of this variable is $\bar{x}$. N is the number of observations.

$$\mu = \sqrt{\frac{\sum_{x=1}^N (x_i - \bar{X})^2}{N - 1}} \quad (2.29)$$

For the calculation of the standard deviation of the annual sums, the square root of the average variances of all measurements was taken.

2.7.3 Nash-Sutcliffe efficiency

The Nash-Sutcliffe Efficiency (NSE) or model efficiency is a standard measure to quantify the performance of a model simulation against observed data (Legates and McCabe, 1999). In equation 2.30, P are predicted values and O are observed values. $\bar{O}$ and $\bar{P}$ is the mean value of all predicted values or the mean value of all predicted values, respectively. N is the number of measurements.

$$NSE = \frac{\sum_{i=0}^N (O_i P_i)^2}{\sum_{i=0}^N (O_i - \bar{O})^2 - \sum_{i=1}^n (P - \bar{P})^2} \quad (2.30)$$

For the interpretation of the NSE following statements apply: 1) The lower the value of NSE, the worse the simulation according to this measure 2) If the NSE is zero the predictability is the same as the predictability of the observed dynamics with the mean value 3) The maximum value of the Nash-Sutcliffe Efficiency is 1, which stands for the agreement of the simulation with the observations.

2.7.4 Normalised root mean square error

The root mean square error is the square root of the variance of the measurements (RMSE). The normalised root mean square error (NRMSE) is divided by the standard deviation μ of the observations (R Core Team, 2013).

$$NRMSE = 100 \cdot \frac{\frac{1}{N} \sum_{i=1}^N (P_i - O_i)^2}{\mu} \quad (2.31)$$

2.7.5 Coefficient of determination

In equation 2.32, the calculation of the coefficient of determination is depicted. It is often referred to as the part of explained variance (SS_{tot}) by a linear regression, which explains the sample variance (SS_{reg}). SS_{tot} is calculated as the squared distance between $\hat{y}_i$, which is the y-value at the regression line and the y-value of the observation (Wooldridge, 2015).

$$R^2 = \frac{\sum (\hat{y}_i - \bar{y})^2}{\sum y_i - \bar{y}^2} = \frac{SS_{reg}}{SS_{tot}} \quad (2.32)$$

2.7.6 Coefficient of variation

The coefficient of variation is the standard deviation (μ) divided by the mean of a sample ($\bar{x}$). It is used in this work to characterize the variability of N_2O fluxes measured either by EC or the automated chamber method.

$$CV = \frac{\mu}{\bar{x}} \quad (2.33)$$

Chapter 3

Results and Discussion

3.1 Meteorological parameters from 2013 to 2015

Temperature (T), global radiation (R_g), saturation deficit (E-e) and precipitation (P_r) are shown as monthly averages in Fig. 3.1. The above mentioned state variables and fluxes are used in evapotranspiration models such as Penman-Monteith or rather simple methods as the Haude approach (Foken, 2016). Furthermore N_2O -models need temperature and precipitation as input (see chapter 1.1.5). Net ecosystem exchange models simulate photosynthesis and respiration by using global radiation, temperature and precipitation (Kirschbaum et al., 2015).

Temperature

Monthly averages of air temperature from 2013 to 2015 were calculated and depicted in Fig. 3.1 a). The monthly means in 2013 show a significant colder winter and a clearly warmer summer (annual mean = 8.6°C). In 2014, most enhanced temperatures against the multi-annual mean happen in January until April (+2.5/+3.2/+2.7/+2.1) and in October until December (+2.7/+1.9/+2.7 °C). In 2015, the summer months July and August showed an increase of +3.3 and 3.4°C against the multi-annual average from 1991-2015. Compared to the time series in Fig. 1.1 both years are the warmest years in the study area since the beginning of the time series in 1936 (annual mean = 10.1 °C).

The lowest of all average monthly temperatures was measured in March 2013 (-1.3 °C). The highest monthly average from 2013 to 2015 was measured in August 2015 (23.9°C). The exact values for monthly averages between 2013 and 2015 as well as multi-annual averages for each month from 1991 to 2015 can be found in Appendix A.

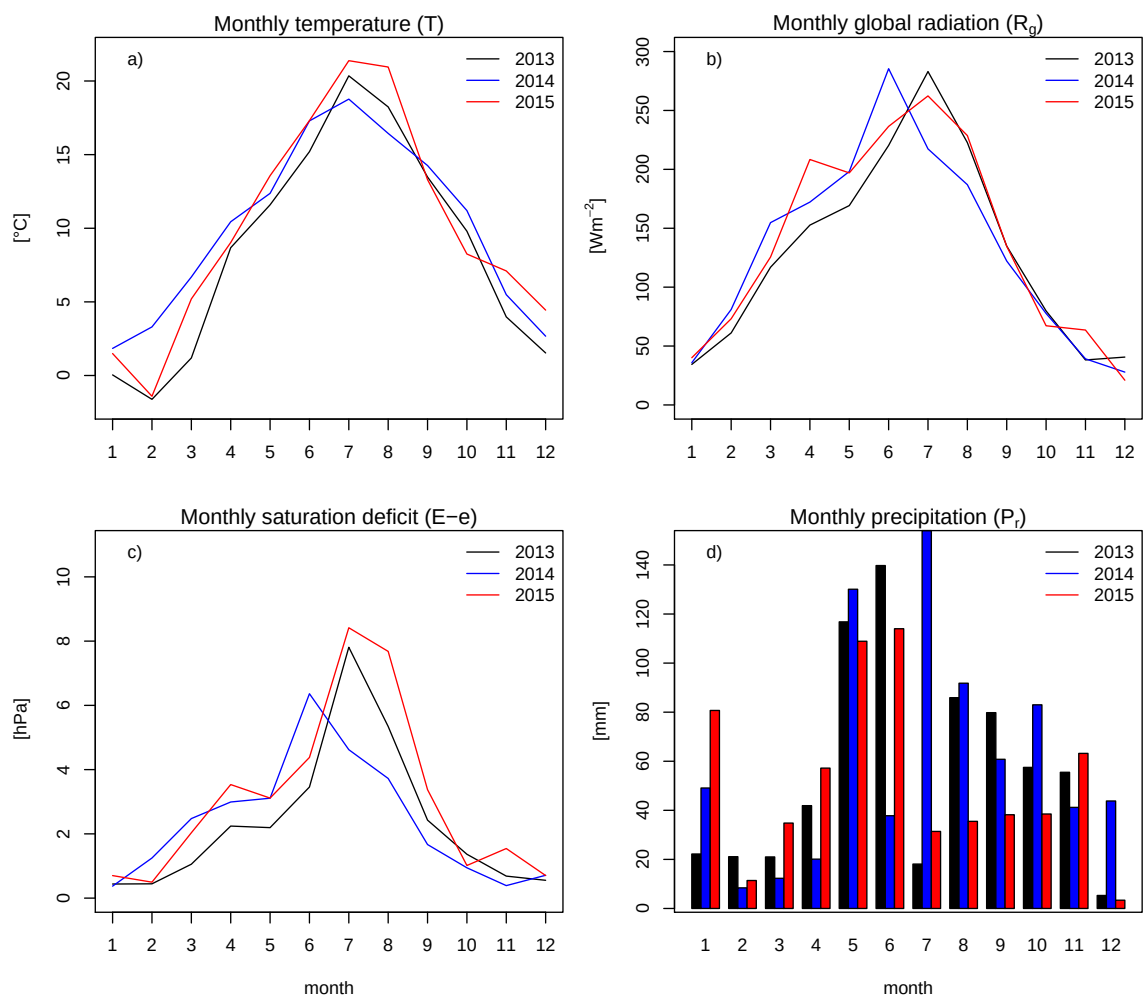


Fig. 3.1 Monthly averaged meteorological parameters from 2012 to 2015: Depicted in sub-figure a) is the monthly averaged temperature (T), in b) monthly averaged global radiation (R_g), in c) monthly averaged saturation deficit (E-e) and in d) monthly precipitation (P_r) during the observation period. The year 2013 is depicted in black, 2014 in blue and 2015 in red.

Global Radiation

Monthly averages of global radiation (see Fig. 3.1 b) differ throughout the three observed years. While in the year 2013 and 2015 the maximum average was measured in July, global radiation (R_g) had its average maximum value in June 2014. In summer 2015, R_g did not exceed the values of 2013 and 2014, however the temperatures did.

Saturation Deficit

The dynamics of the saturation deficit as the main driver for evapotranspiration depend strongly on global radiation (R_g), which can be seen if one compares the dynamics of the upper right panel to the dynamics of the lower left panel (see Fig. 3.1). Furthermore, the saturation deficit is dependent on the temperature as warm air can hold more water than cold air. Therefore the warm summers in 2013 and 2015 have higher saturation deficits than the rather cold summer in 2014.

Precipitation

Precipitation sums from 2013 to 2015 are all below the long-term precipitation average of 778 (2013: 665 mm, 2014: 732 mm and 2015: 617 mm). Depending on the time of the year, when the rain deficit is occurring, different negative impacts on the environment are observed. While during winter a lack of rain has e.g. negative effects on ground water recharge, during summer the optimal vegetation growth is affected.

A main result of this meteorologic observations is that 2014 and 2015 were extremely warm years on average but for different reasons. In 2014 the warm year was due to an extremely warm winter and in 2015 it was due to an extremely warm summer.

3.2 Source area analysis of fluxes

Averaged wind regime

The wind rose over one year is depicted in Fig. 3.2, showing the relative frequency of 12 wind directions (north = N, east = E, south = S, west = W) at the EC site. The highest frequency with 27% can be seen from the SWW. All wind directions with a western component (NNW, NWW, W, SWW, SSW) sum up to a relative frequency of 64%. All wind sectors with an

eastern component (NNE, NEE, E, SEE, SSE) sum up to about 27% wind frequency. Wind directly from the south happens in 7% of all cases. Wind from northern directions is rarely observed and under 1%.

At the explicit site, quantification of the wind pattern is important, because 1) of flow distortions in the north and 2) the special setup between two adjacent fields. The general result which can be drawn from this wind-rose is that the container in the north (see Fig. 2.4) does rarely disturb the turbulent flow of air to the EC station and measurements from the field A17 most likely prevail.

Beyond the information about the wind pattern, this wind rose offers information on the wind speeds of the different wind sectors. It is noteworthy that low wind speeds almost always come from the west. The most probable explanation for the systematic lower wind speeds from A17 are systematic lower wind speeds during due to terrain following catabatic winds. At open areas the land surface cools out due the lack of incoming long-wave radiation (Foken, 2006b). The air flows according to the terrain into the valleys like a viscous liquid, which can be observed at night in the hilly landscape in Scheyern. At the EC site, agreement of slope from west to east and average wind speed during night is observed. Better insights into the complex flow patterns might allow comparisons with assimilated wind data for the region, downscaled wind data from numerical weather simulations or large eddy simulations.

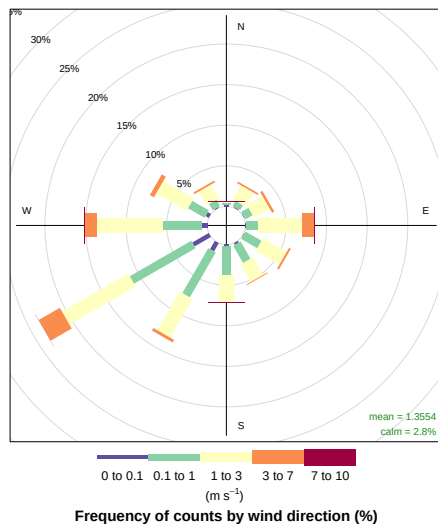


Fig. 3.2 Windrose over the time span of 1 year (1. August 2013 to 1. August 2014). Main wind directions at the EC-site are South west and East.

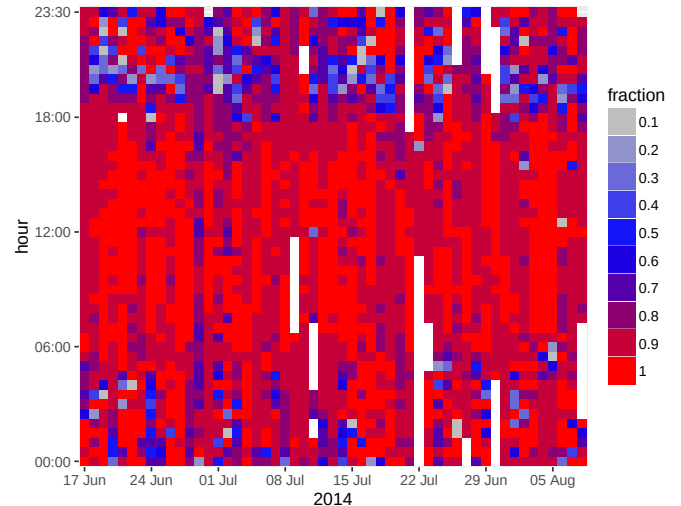


Fig. 3.3 Temporal dynamic of footprint fraction that lies within the fields A17 and A18 represented by colour code. White tiles represent missing data.

Halfhourly footprint fraction within both A17 and A18

To test the assumption that the source area from the measurements is mostly from A17 and A18 and not beyond the borders of both fields, footprint fractions within A17 and A18 were calculated with the the software TK3 (see Fig. 3.3). For location of the EC-station and the fields A17 and A18, see Fig. 2.3. The time period from 2014-06-16 to 2014-08-08 is shown. The colours in the heat map show the fraction of footprint that lies inside the two measured fields A17 and A18. On the x-axis days of the year can be depicted, the y-axis shows the daytime.

In Fig. 3.3 a strong diurnal pattern is visible. Grey colour indicates that between 0 % and 10% of the footprint lies within the two fields A17 and A18. Red indicates that between 90 % and 100 % of the footprint lies within the borders of the fields A17 and A18 (see chapter 2.2).

In the plot, during daytime, typical values for the footprint fraction are between 80% and 100%. After 6 p.m. the footprint fraction often drops to values between 0 % to 0.6 %, which is reasonable, as during night-time a stable nocturnal boundary layer evolves, where the footprints are bigger in size.

Footprint climatology under labile, neutral and stable stratification

In Fig. 3.4 results of a footprint analysis are given: subfigure a) shows the cumulative share of the cumulative footprint in all sub-fields. One can see in subfigure 3.4 a) that 55% (3% + 15% + 37%) of the footprint originates from field A17 and 21% (19% + 2%) from field A18. Thus 76 % of the cumulative footprint lies within both fields. Most of the footprint is located in the sub-fields close to the EC station. The sub-fields on the very left of A17 and very right of A18 contribute only little to the measurement.

In Fig. 3.4 b-d, footprint climatologies under labile, neutral and stable stratification can be seen (Amiro, 1998). The EC station is located on a hill ridge within the hilly landscape. During neutral and labile stratification most of the footprint lies over this hill ridge. The two colluvia which are mentioned in chapter 2.1.1 represent only a very small percentage of the footprint under any stratification. Furthermore Fig. 3.4 shows that the missing part of the footprint at night from Fig. 3.3 is located mostly beyond the south-eastern borders of the field A17. In a recent work by Klein (2018), knowledge about the cumulative and the half-hourly footprint from A17 and A18 could be used to improve the agreement between flux simulation and flux measurement over complex terrain.

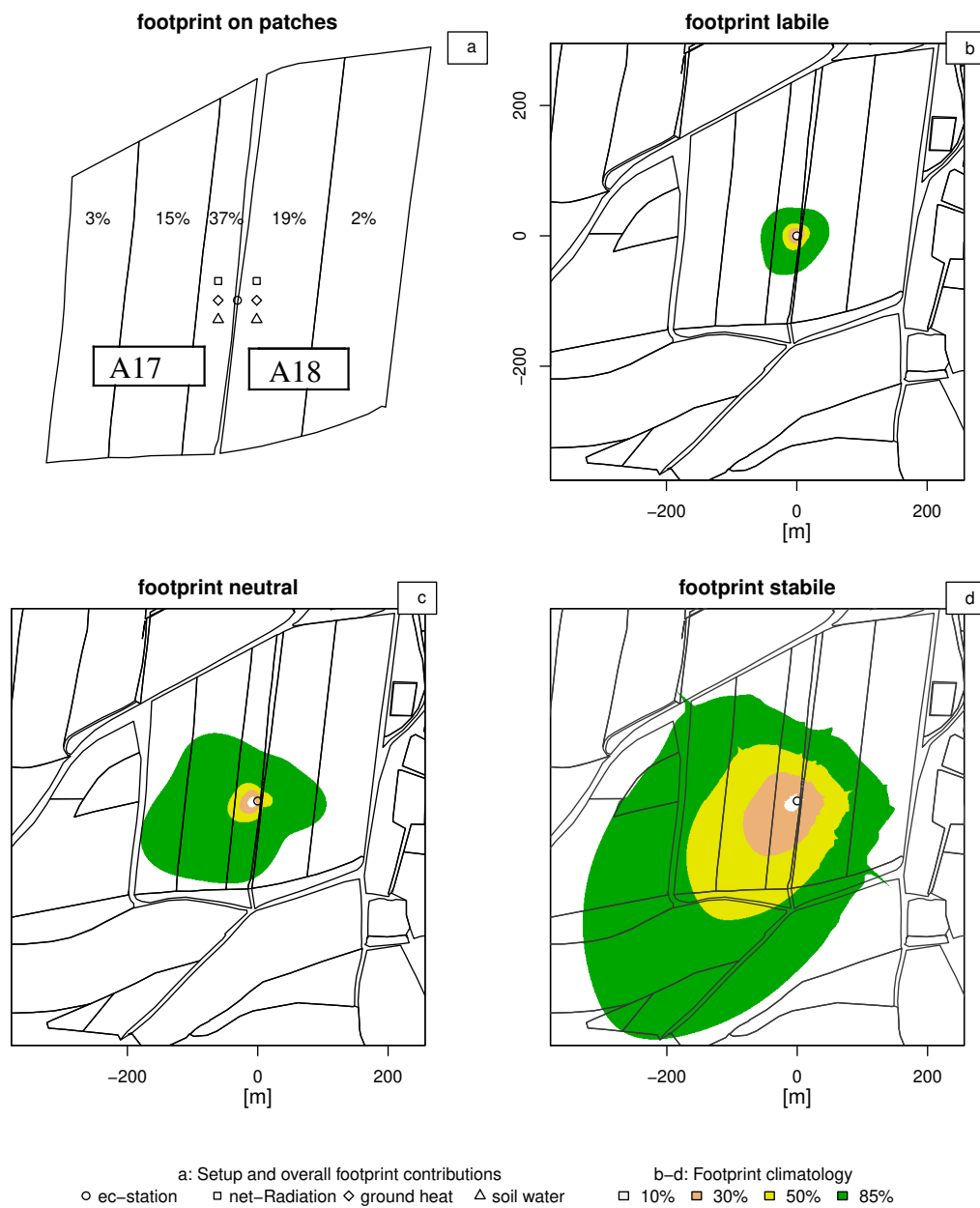


Fig. 3.4 Percentages of the footprint climatology over all stratifications are shown in part a). In total 76 % of the footprint is located within the observed fields over all stratifications (stable, neutral, labile). Footprint climatology during labile, neutral and stable stratification is shown in subfigures b), c) and d), respectively.

3.3 Data splitting into two time series

3.3.1 Multiannual flux data availability between the field A17 and A18, using a simple sorting scheme

Each sub-figure in Fig. 3.5 contains tiles for 40001 possible half-hourly measurements. All following numbers are calculated relative to this number. The number of successful measurements with quality flag 0 or 1 was 78.9% for NEE, 82.4% for Q_H and 72.8 % for Q_E (see Fig. 3.5). The percentage of fluxes that were with a representative footprint within the borders of A17 and A18 (footprint > 80%) were 58.0% for NEE, 56.3% for Q_H and 61.2% for Q_E .

However to obtain reasonable results the data had to be assigned to either A17 or A18, which limits the data availability further. The obtained number of fluxes are shown in Fig. 3.6 and 3.7. According to the sorting scheme in chapter 2.2.6, the percentages available fluxes (flag = 0,1) from A17 were: 25.4% (NEE), 26.4% (Q_H), and 32.4% (Q_E) in Fig. 3.6. Only 7.7% of all NEE fluxes, 8.1% of all Q_H -fluxes, and 11% of all Q_E could be assigned to field A18 (see Fig. 3.7). During night almost no fluxes come from A18 (see Fig. 3.7).

3.3.2 Data quality between the field A17 and A18, using a simple sorting scheme

In Fig. 3.5 the data quality of all processed data is shown in a heat map. On the x-axis time of the day is shown. On the y-axis, days of the years 2013, 2014 and 2015 are shown. The quality flag of the data is shown in color code. Blue represents the best quality (flag = 0), which could be used for model studies and fundamental research (Heinlein, 2018; Klein, 2018). Turquoise represents mediocre quality (flag = 1), this quality flag can be used for example for annual sums of greenhouse gases. Yellow represents bad quality, which is discarded in for any further research. Data that could not be processed is grey.

In the colour pattern, the diurnal cycle is obvious. During day, when the atmosphere is well mixed and the atmospheric conditions are turbulent, data quality is mostly good (flag = 0) on both fields. During night when atmospheric conditions tend to be stable, data quality is worse. Furthermore the quality flags of NEE are more similar to that of Q_E , which makes sense as the same sensor is for the underlying concentration measurements.

The reason for missing nighttime fluxes from A18 is seen in the sloping terrain, and the resulting katabatic winds from the west/south-west (see also chapter 3.2).

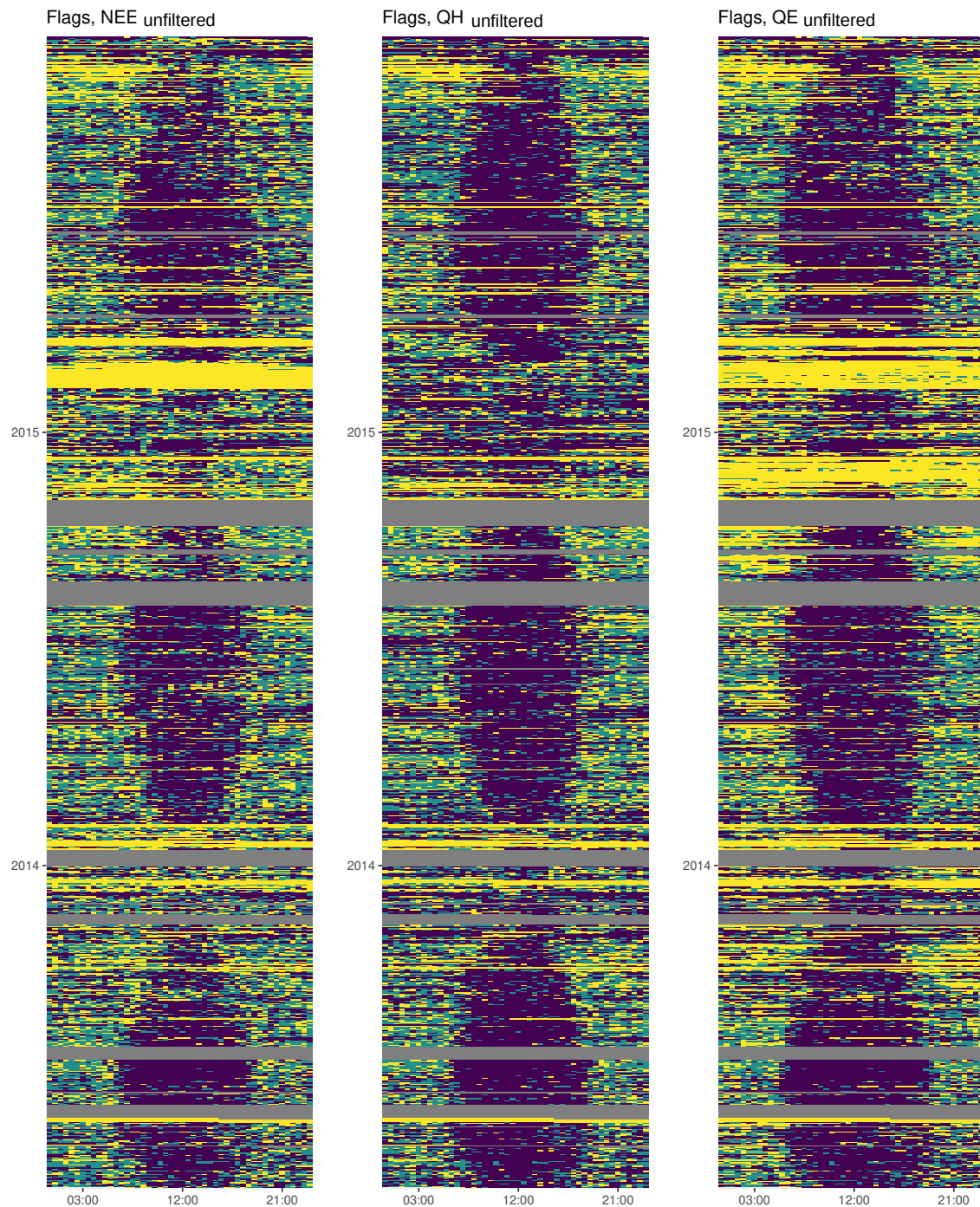


Fig. 3.5 Data quality of NEE, Q_H and Q_E is shown with daytime on the x-axis and days of year on the y-axis. The measurement values are not yet filtered according to their source area. The colours indicate the measurement quality. Dark blue is the best data quality (flag = 0), turquoise colour indicates minor quality but acceptable quality for annual sums (flag = 1), yellow colour indicates bad quality (flag = 2). The number of successful measurements was between 72% and 82.4 %.

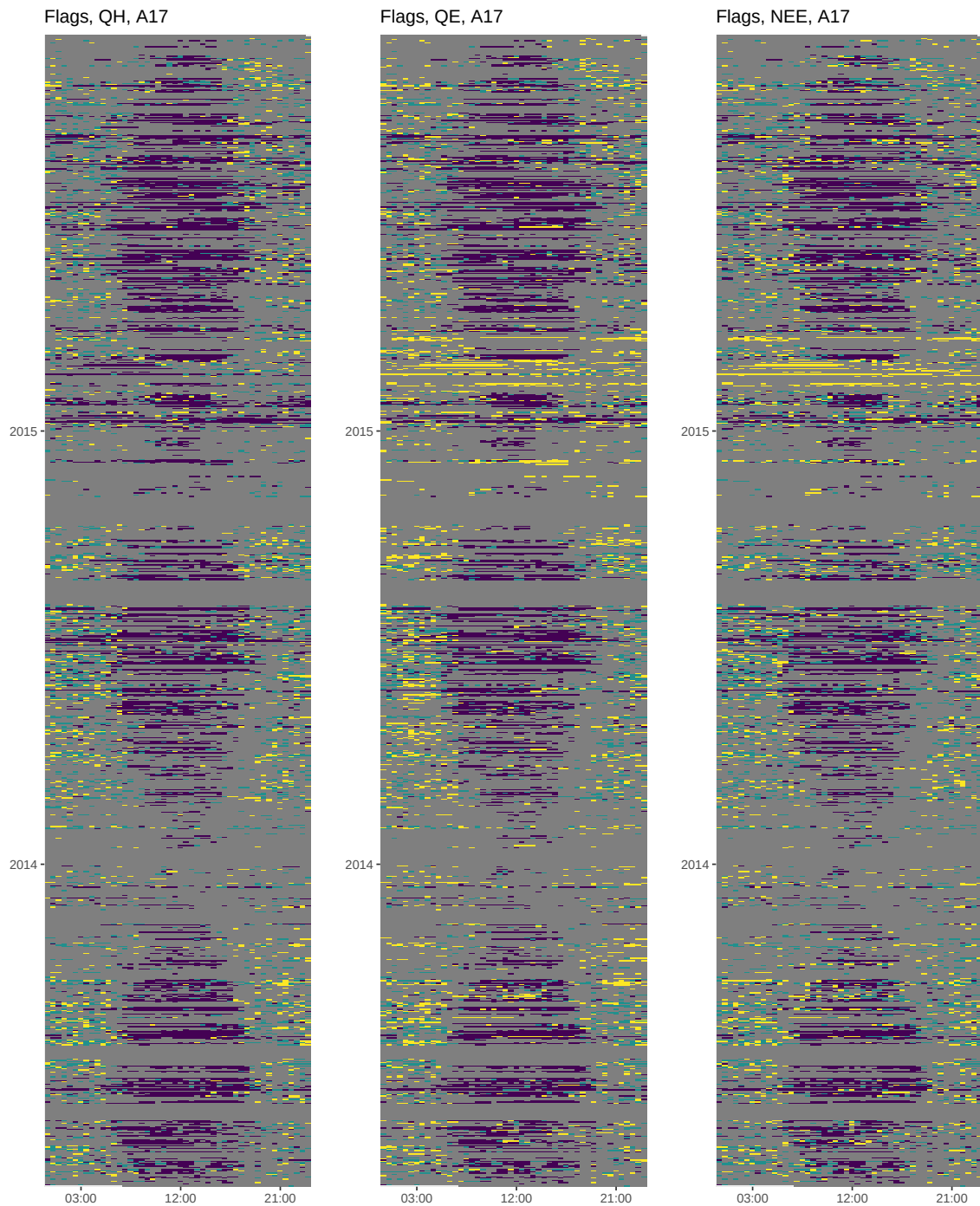


Fig. 3.6 Shown are the fluxes from A17 in color patterns as in Fig. 3.5. Both daytime and night-time fluxes exist from the site. The daytime fluxes are generally better in quality. The percentages of fluxes which are regarded as appropriate quality (flag = 0,1) from A17 were: 25.4% (NEE), 26.4% (QH), and 32.4% for QE.

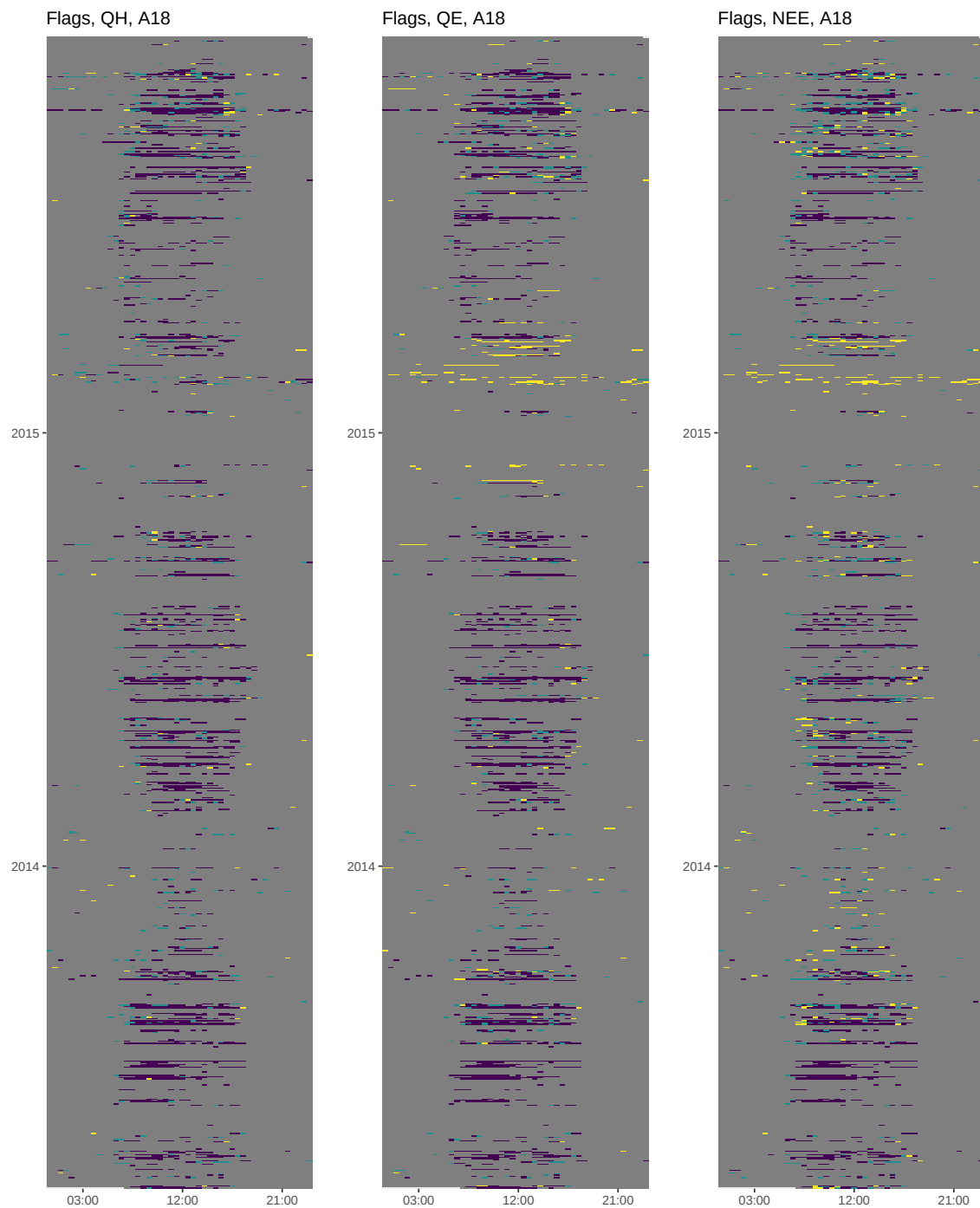


Fig. 3.7 Shown are the fluxes from A18. Mostly daytime fluxes are measured by the eddy covariance station. Dark blue is the best data quality (flag = 0), turquoise colour indicates minor quality but acceptable quality for annual sums (flag = 1), yellow colour indicates bad quality (flag = 2). The data availability for flag 1 and 2 lies between 7.7 and 11% %.

3.4 Multiannual EC-flux measurements (Q_H , Q_E , CO_2)

3.4.1 Net ecosystem exchange measurements of CO_2 from A17 and A18

In Fig. 3.8 and 3.9, monthly averaged fluxes of net ecosystem exchange (NEE) of CO_2 from the fields A17 and A18 are depicted. Hours of the day are drawn on the x-axis. The y-axis depicts monthly NEE measurements in the form of a box-whisker plot. Plots were created with the base package of the programming language "R" (Tippmann, 2015).

The median NEE value of each hour is assumed to be a suitable quantitative measure, which is represented by a horizontal line in the box of the box-whisker plot (see Fig. 3.8). The abbreviations in every plot stand for the planted species: PT = potato, WW = winter wheat, MZ = maize, MT = mustard, BS = bare soil, CC = mixture of catch crops.

Potato (PT): NEE is defined as respiration minus gross primary production (Sands, 1995), therefore plant growth is a major influence on this parameter in crop ecosystems. Plantation, desiccation and harvest of potatoes took place in the same time windows, in 2013 and 2014. Seed potatoes were planted on 2013-04-29 and 2014-04-18 respectively. Desiccation of potato plants was conducted on 2013-08-29 and 2014-08-14/19. Harvest of potato tubers took place in 2013-09-24 and 2014-09-20.

Accordingly, both vegetation periods showed significant CO_2 uptake between June and August (see Fig. 3.8 and 3.9). However in 2014 the uptake of CO_2 throughout the vegetation period was larger and later in time. In 2013, plant and soil (see Fig. 3.8) show the highest uptake-rates of CO_2 during June ($-12 \mu\text{mol } CO_2 \text{ m}^{-2} \text{ s}^{-1}$) and July ($-15 \mu\text{mol } CO_2 \text{ m}^{-2} \text{ s}^{-1}$). Smaller uptake rates are observed in August ($-7 \mu\text{mol } CO_2 \text{ m}^{-2} \text{ s}^{-1}$). In 2014, the monthly median uptake rates of CO_2 were slightly smaller in June $8 \mu\text{mol m}^{-2} \text{ s}^{-1}$, but with $22 \mu\text{mol m}^{-2} \text{ s}^{-1}$ (+22% compared to the previous year) and $24 \mu\text{mol m}^{-2} \text{ s}^{-1}$ much higher during July and August, respectively (see Fig. 3.9 and appendix B). After desiccation, at the end of August, where the plant is treated with a mixture of photosynthesis blockers (Diquat, Reglone, Carfrentazon), daytime fluxes are close to zero for both vegetation periods.

An possible explanation for the delayed and stronger uptake of CO_2 in 2014 is the water availability due to rain during the vegetative phase of potato (see Fig. 3.1). June precipitations were high in 2013 and low in 2014 (2013: 140 mm, 2014: 38 mm), in July the situation was reversed (2013: 18 mm, 2014: 154 mm). During June, the plant leaves of potato were only beginning to emerge. During July the plants flower and have their maximum LAI. Another explanation could be the different varieties of potato, which were Nicola, Cilena, and Krone in 2013 and Burana and Krone in 2014.

Winter wheat (WW): Three vegetation periods of winter wheat (WW) are observed, which show highest median uptake rates of CO₂ between April and July.

In April 2013, the uptake of CO₂ is much lower than in the subsequent years (2013: $-3 \mu\text{mol m}^{-2}\text{s}^{-1}$, 2014: $-20 \mu\text{mol m}^{-2}\text{s}^{-1}$, 2015: $-18 \mu\text{mol m}^{-2}\text{s}^{-1}$). Also the months of May in 2013, 2014 and 2015, showed the least uptake of CO₂ for the year 2013 (2013: $-20 \mu\text{mol m}^{-2}\text{s}^{-1}$, 2014: $-26 \mu\text{mol m}^{-2}\text{s}^{-1}$, 2015: $-48 \mu\text{mol m}^{-2}\text{s}^{-1}$). Also in the following months (June, July), winter wheat in 2013 shows the lowest uptake rates of CO₂ (see Tab. B). Precipitation in

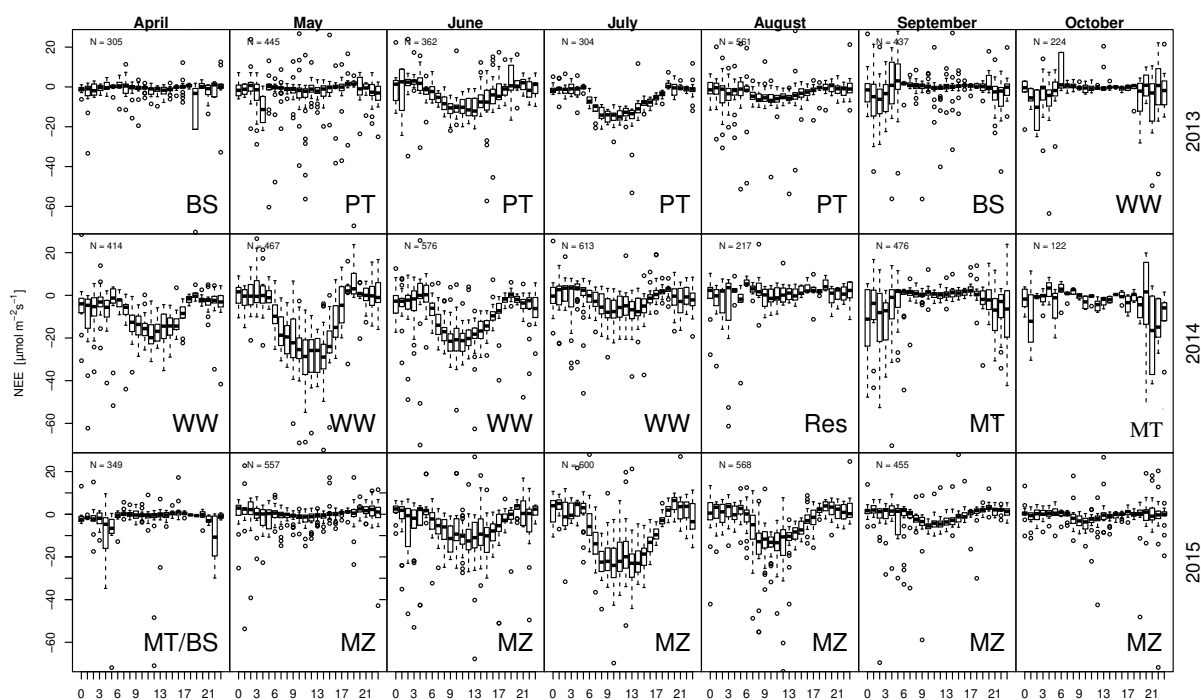


Fig. 3.8 The plot shows monthly averaged diurnal cycles of NEE from A17 during the years 2013 to 2015: Highest uptake rates occur during the vegetative phase of the grown crops (BS = bare soil, PT = potato, MT = mustard, WW = winter wheat, Res = residues, MZ = maize, CC = mixture of catch crops).

the beginning of 2013 is mostly higher than in 2014, thus water is most likely not limiting assimilation (see Fig. 3.1). The most probable reason for the low uptake of CO₂ in 2013 is a delayed plant development due to the rather cold temperatures from January to April 2013 (see Fig. 3.1 a). Thus LAI is smaller and the plant cannot take as much CO₂ from the atmosphere as in 2014. The lower the temperature sums are, the later winter wheat development stages can be reached. Unfortunately no measurements of LAI exist for the years 2013 and 2014.

The yield in 2013 (80.5 dt/ha) is also smaller than the yield in 2014 (85.9 dt/ha), and especially 2015 (96 dt/ha), which makes sense as optimal plant growth goes along with high yield and high uptake of CO_2 .

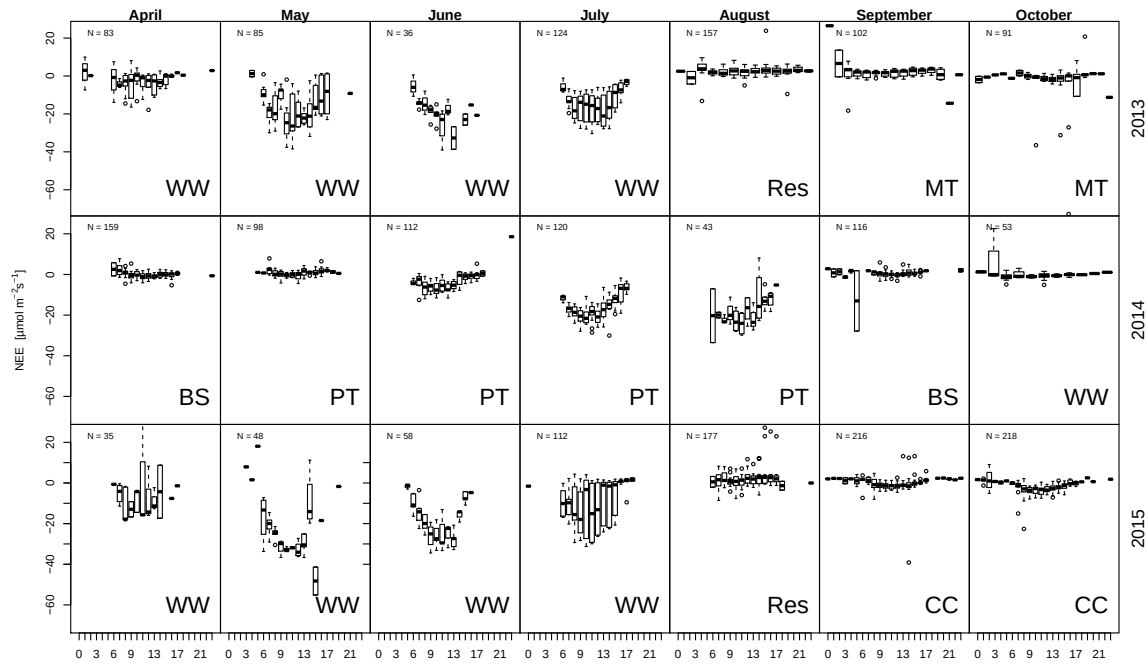


Fig. 3.9 Monthly averaged daily cycles of NEE from A18 during the years 2013 to 2015. While in the beginning of the vegetation period (April), the potato and the maize field is still bare soil with no assimilation, winter wheat is already in the tillering stage with significant CO_2 -uptake.

Maize (MZ): One vegetation period of maize was observed in 2015. Maize was planted at the end of April and emerges in May. Therefore, negative NEE does not occur before May. The vegetation period shows clear negative fluxes during June, July, August and September. Noon values of the monthly averaged diurnal cycles show values around $1 \mu mol CO_2 m^{-2} s^{-1}$ in May, when the small maize plants emerge. In June the maize field already takes up $13 \mu mol CO_2 m^{-2} s^{-1}$ before it reaches its highest value in July with $24 \mu mol CO_2 m^{-2} s^{-1}$. In July the maize plants blossomed and began to fill their fruit biomass. An uptake of CO_2 by the maize field can still be seen in August (maximal hourly median: $15 \mu mol CO_2 m^{-2} s^{-1}$), September (maximal hourly median: $5 \mu mol CO_2 m^{-2} s^{-1}$) and October (maximal hourly median: $4 \mu mol CO_2 m^{-2} s^{-1}$).

Although we cannot compare this maize vegetation period to other vegetation periods of

maize in Scheyern, it is noteworthy that the measurements were conducted in the warmest year that was ever measured in Germany and also in the study area around Scheyern (see 1.1).

Negative fluxes after harvest in 2013 and 2014: It is remarkable that from August to October 2013 and from September to October 2014 strong negative CO₂-fluxes are visible during night-time (see Fig. 3.8). The negative fluxes only occurred, when bare soil and plant residues were present on the soil surface. In 2015, maize was still growing on A17 and no negative fluxes could be detected. As it is known that data quality is worse during night-time, the data was checked by excluding all data of minor data quality (flag = 1). However negative fluxes still appear, when only best data quality (flag = 0) is used.

Variation during the months: Although the plots in Fig. 3.8 and Fig. 3.9 are monthly averaged and variations within months cannot be resolved, the box-whisker plots nicely show the variation of the measurement results in one month. Flux variations during the vegetative phase of winter wheat (May and June) are for example smaller than flux variations in the generative phase (July), which is most probably due to the plant ripening and management impacts (harvest) at the end of July.

Limitations: All in all the obtained measurements compared to their abiotic and biotic drivers seem to make sense and the applied method to assign fluxes either to A17 or to A18 was successful. Beyond this perception, the comparison of abiotic drivers with measured fluxes is interesting but has its limitations. More complex interactions between NEE and its controls cannot be explained as many explanatory parameters influence NEE and the behaviour of controls on NEE is not linear. A further restriction of the setup is that the number of observations for the derived mean diurnal cycles differs between both fields and that the weather conditions during west wind differ from the weather conditions during east wind (Klein, 2018).

It is remarkable that reasonable measurements could be obtained from A18 even though only 10% of the NEE fluxes were available.

3.4.2 Q_H -measurements from A17 and A18 during the years 2013 to 2015

In Fig. 3.10 and 3.11, monthly averaged fluxes of sensible heat from the fields A17 and A18 are shown. The mean value of each hour is depicted as a red dot. Additionally, the number of measurements and the coefficient of variation (CV) of the measurements for each month is given. Similar to CO_2 described in the previous chapter, abiotic and biotic controls (e.g. plant ripening, plant management) can be seen in the sensible heat flux (Q_H) (see Fig. 3.10 and 3.11).

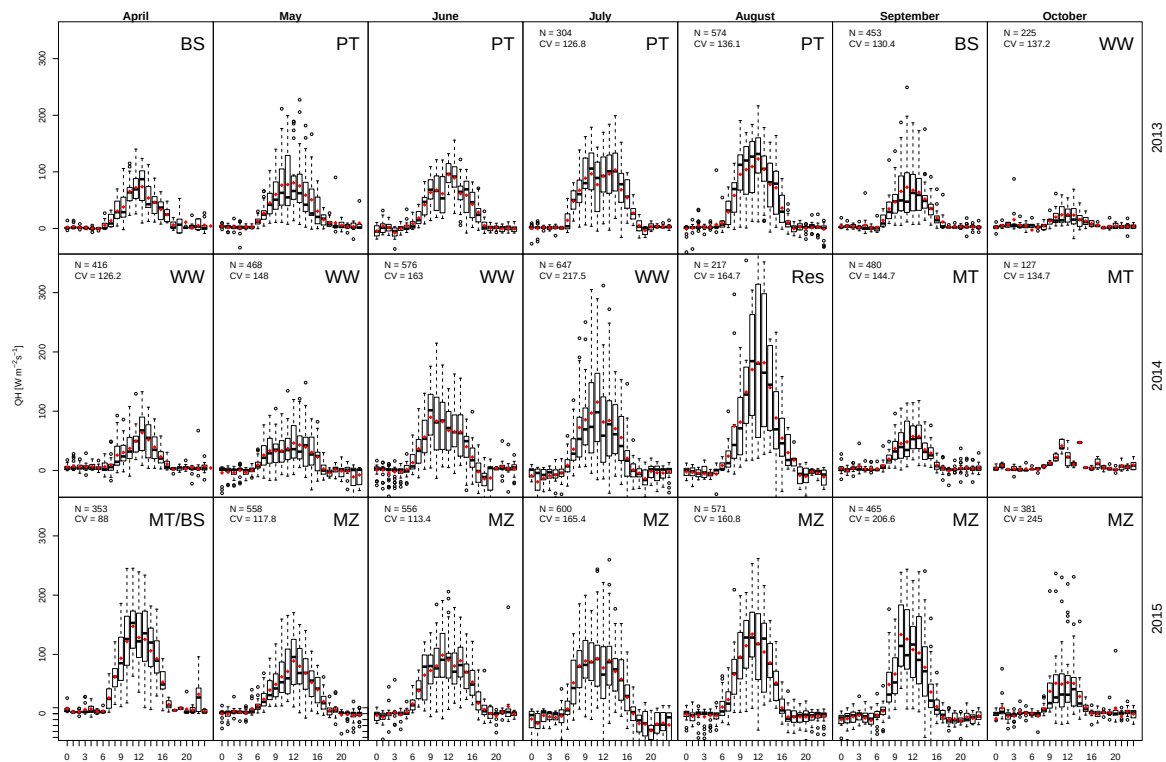


Fig. 3.10 Monthly averaged diurnal cycles of sensible heat from A17 during the years 2013 to 2015 (BS = bare soil, PT = potato, MT = mustard, WW = winter wheat, Res = residues, MZ = maize, CC = mixture of catch crops).

Winter wheat: High mean median Q_H fluxes are generally measured in July (2013: $114 \text{ W m}^{-2} \text{ s}^{-1}$, 2014: $98 \text{ W m}^{-2} \text{ s}^{-1}$, 2015: $269 \text{ W m}^{-2} \text{ s}^{-1}$) and in August (2013: $221 \text{ W m}^{-2} \text{ s}^{-1}$, 2014: $184 \text{ W m}^{-2} \text{ s}^{-1}$, 2015: $254 \text{ W m}^{-2} \text{ s}^{-1}$), when winter wheat is harvested. During this time the soil is most dry and fluxes are high. The energy partitioning shifts due to wilted

wheat plants (end of July) or harvested wheat plants (most of August). Highest Q_H fluxes from winter wheat are also the highest fluxes measured during all vegetation periods.

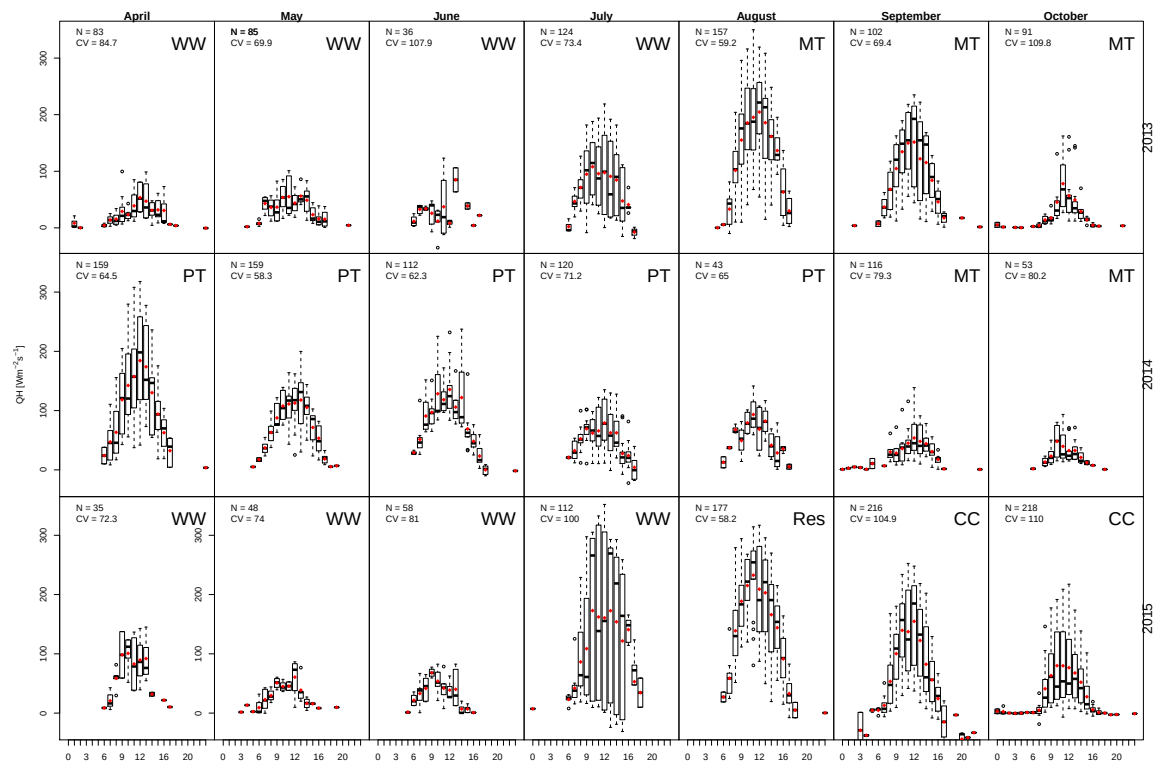


Fig. 3.11 Monthly averaged diurnal cycles of sensible heat from A18 during the years 2013 to 2015. For abbreviations of crop species see Fig. 3.10

Potato: Highest Q_H fluxes from potato occur in April 2014 (highest median per hour is 198.2 Wm^{-2} , see Fig. 3.11), when the soil is still bare. Possible explanations are that transpiration is very low, which favours fluxes of Q_H . On the other hand average global radiation is increased in April 2014 by approximately $20 \text{ Wm}^{-2}\text{s}^{-1}$ compared to April 2013 (see Fig. 3.1). In 2014 the highest hourly median value for any month is in August ($131.6 \text{ Wm}^{-2}\text{s}^{-1}$, see table B.3)

The impact of bare soil on Q_H fluxes at the potato field is also visible if one compares both potato vegetation periods with the vegetated equivalent on the other field. Here, one can see that Q_H fluxes during April 2013 on A17 shows higher values than winter wheat during the same time period on the neighbouring field (compare Fig. 3.10 and Fig. 3.11 in April 2013). The same holds true for the potato field with bare soil on A18 in 2014. It shows higher Q_H fluxes than the respective winter wheat field on A17 (compare Fig. 3.10 and Fig. 3.11 in

April 2013).

Effect of LAI on Q_H -fluxes: The Leaf area index ($m^2 m^{-2}$) is a major biotic control on sensible heat. An example for this control on the measured sensible heat fluxes is winter wheat in July. In July 2015 winter wheat is ripening and the plant leaf is wilting. This goes along with lower values of Q_H in the beginning of July ($LAI = 0.46$, see Appendix F table F.4) as well as high values of Q_H in the end of July ($LAI = 0$). The minimum and maximum values in the first half of July are $-58.9 Wm^{-2}$ $104.6 Wm^{-2}$. The minimum and maximum values in the second half of July is $7.1 Wm^{-2}$ and $352.1 Wm^{-2}$. Although the sub-monthly information is averaged out in in Fig. 3.10, the variation in the Q_H -fluxes is represented by the antennas which are also called whiskers in the box whisker plot.

Oasis effect: On A17, winter wheat and maize show the characteristics of an oasis effect in the years 2014 and 2015, respectively (see Fig. 3.10). In these two months, Q_H -fluxes are negative in late afternoon and early evening. Minimum median values in the late afternoon hours are about $20\text{-}30 Wm^{-2}s^{-1}$ lower than all other time periods. This phenomenon cannot be seen on A18, due to a lack of measurement data in late afternoon. There is also no obvious oasis effect, when potato is planted, which is most probably due to the too small LAI. The oasis effect is a known micrometeorological phenomenon, which is named after the cooling effect in the proximity of vegetated or water surfaces in arid regions. Dry air from a dry surrounding is moisturised under temperature reduction (Potchter et al., 2008). The oasis effect is not limited to deserts and can be also seen in e.g. in urban parks (Oke, 1987) or vegetated islands like maize fiels in dry surrounding (Eigenmann et al., 2011). In the above mentioned months the climate was very dry and the field like a vegetated island between wilted or harvested crops.

Limitations of monthly averaged daily cycles: As described in the chapter before, averaging diurnal cycles over the month (see Fig. 3.10 or 3.11) has the disadvantage of averaging out temporal information. Abrupt changes are muddled out by averaging over the month. However, the variations in the box-whisker plots (whiskers) can be used as an indicator, whether EC-flux data are strongly varying during one month. In this study this was especially the case, when the biosphere or management events (plant growth, ploughing) affected Q_H -fluxes This can help to choose the most interesting time periods for model studies on heat fluxes between land surface and atmosphere.

3.4.3 Q_E -measurements from A17 and A18 during the years 2013 to 2015

Fig. 3.12 and 3.13 are monthly averaged diurnal cycles of latent heat (Q_E). The plot descriptions are analogous to Fig. 3.10 and Fig. 3.11. Compared to the Q_H -fluxes in the previous subchapter, the maximum medians of Q_E -fluxes are generally higher.

Winter wheat (WW): In Fig. 3.12 and 3.13, Q_E -fluxes show the highest values at an earlier stage within the vegetation period, namely, in June (2013: $368 \text{ Wm}^{-2}\text{s}^{-1}$, 2014: $276 \text{ Wm}^{-2}\text{s}^{-1}$, 2015: $370 \text{ Wm}^{-2}\text{s}^{-1}$). Latent heat fluxes during both the warm summers 2013 and 2015 show higher flux rates than during the rather cool summer 2014.

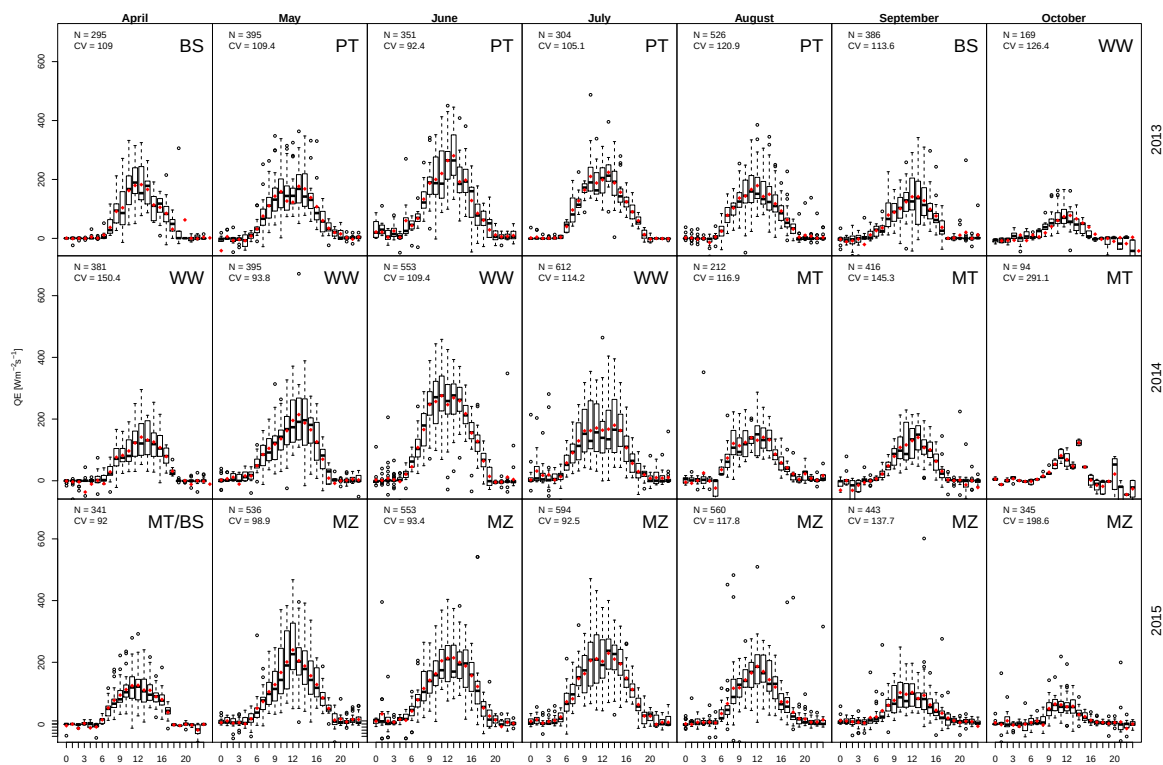


Fig. 3.12 Monthly averaged diurnal cycles of latent heat (Q_E) fluxes during the years 2013 to 2015 from A17. Crop species are abbreviated with WW for winter wheat, PT for potato, BS for bare soil, MT for mustard and MZ for maize and CC for a mixture of catch crops.

Potato (PT): The highest fluxes rates were measured from potato in June 2013 and July 2014 (2013: $276 \text{ Wm}^{-2}\text{s}^{-1}$, 2014: $323 \text{ Wm}^{-2}\text{s}^{-1}$). The Q_E -fluxes from potato are higher in

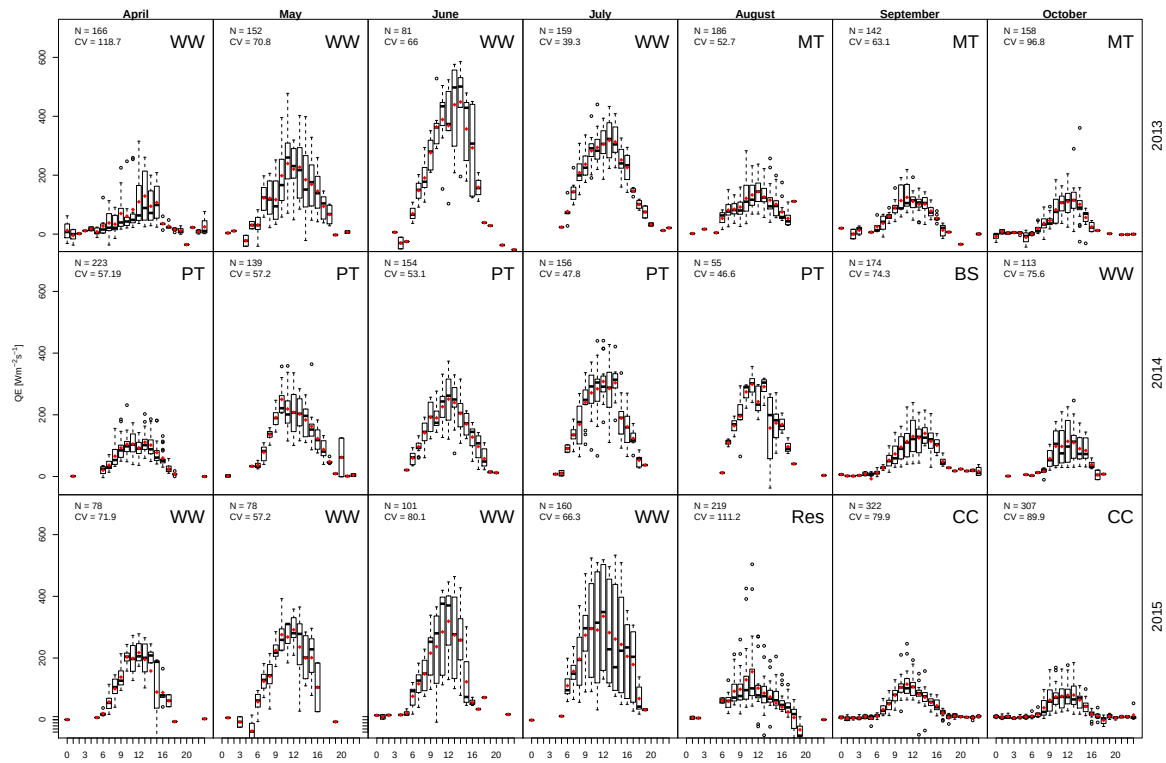


Fig. 3.13 Average diurnal cycles of all latent heat (Q_E) fluxes from A18 from the years 2013 to 2015. Crop species are abbreviated with WW for winter wheat, PT for potato, BS for bare soil and MT for mustard.

2014 and last longer. With the pattern of the uptake rates of CO_2 in mind (see chapter 3.4.1) the most probable explanation for Q_E -fluxes on a higher level throughout summer 2014 is thought to be a consequence of the different impact of the droughts in July 2013 and June 2014. The drought in July 2013 has possibly a more negative impact leading to damages on the potato-plant than the drought in June 2014.

Maize (MZ): In May and to a minor extent in June, the maize plants were small (see Appendix F.3). The highest Q_E -fluxes from maize were measured between June and August. The maximum of the diurnal median values of all monthly averaged diurnal cycles was $237 \text{ Wm}^{-2}\text{s}^{-1}$ in July, when maize is blossoming and the green LAI is highest (see F). In September and October the maize plants are already wilting. Consequently Q_E -fluxes are smaller.

During the main vegetation period of maize in 2015 the temperatures were extremely high and precipitation was extremely low. In July and August, temperatures were 18.0°C and

17.6°C, which is +3.4°C and +3.3°C above the average, respectively. Precipitation was 31 mm in July and 34 mm in August. This value is 73 mm lower than average precipitation in July and 55 mm lower than the average precipitation in August.

Limitations: A limitation of the EC measurements is that the measurement is an integrated signal of both evaporation and transpiration. Hints for this fact can be seen for example in the shape of diurnal cycles. Often these cycles are asymmetric, because the response to the drivers that are often symmetric (e.g. global radiation) is constrained by other factors (e.g. soil water availability during the day).

3.4.4 Bowen ratios for A17 and A18 obtained by a simple splitting scheme

The bowen ratio (Bo) is a measure for the dissipation of energy at the land surface. It has been already mentioned in chapter 1.1.3 that land use influences climate change. Here the relationship between land use and multi-annual Bo is analysed. In contrast to the average diurnal cycles, Fig. 3.14 has the advantage, to show both latent and sensible heat in a continuous time series where rapid changes in Q_H and Q_E are not averaged out.

In this study varying bowen ratios, mostly between -3 and 7 were measured, in the time window between 10 a.m. and 3 p.m.. Very few Bo values are higher or lower than this shown range that appeared in this time frame.

High values appear in almost all vegetation periods (see Fig. 3.14). During the vegetation period 2013 on A17 a peak is visible on 2013-08-29 (see Fig. 3.14 a) which is the day of potato desiccation. The plants are destroyed by photosynthesis blockers and hence transpiration ceases. More energy is now available to be converted into sensible heat (Q_H) and the Bo -value increases. The next period of high Bo -values can be seen at the end of July (see Fig. 3.14, b). This is the time when winter wheat wilts. Also here latent heat decreases, because no green leaves are available for transpiration. Consequently the Bo -ratio rises due to the increase of sensible heat Q_H . The next enhanced bowen ratio values are due to snow and frost. The values of sensible heat are so low that a disadvantage of the bowen ratio becomes visible. When the denominator of the fraction Q_E is close to zero, Bo -ratio gets higher and higher. In Fig. 3.14 d, again mustard is wilting and does not transpire any more, therefore Bo increases. The same is true for maize in Fig. 3.14 e. During the measurement period of maize also sap flow measurements were made by Heinlein (2018). They show that the speed of sap flow decreases from 30 cm h⁻¹ at the end of July to approximately 5 cm h⁻¹ in September.

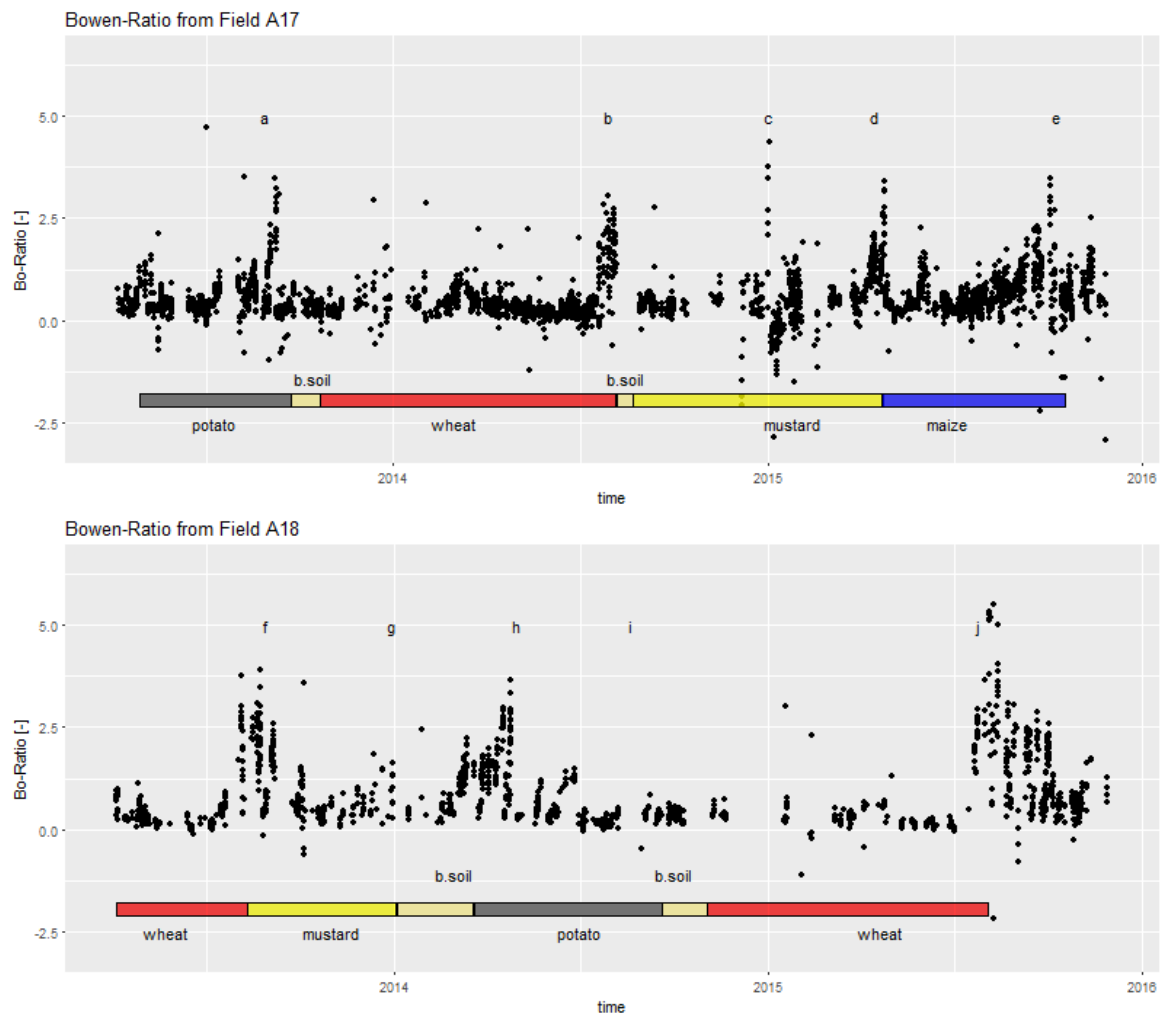


Fig. 3.14 Depicted are the bowen ratios of both field A17 and A18 between 10 a.m. and 3 p.m. o'clock. The diurnal pattern of Q_H and Q_E is most pronounced during that time. Additionally, the planted crops are indicated by horizontal colour bars in Fig. 3.14. The planted crop or land use is written next to the coloured bar. The letters a-j mark management or development stages. a) potato is desiccated b) wheat is ripe and wilted c) snow isolates the surface d) mustard is wilted e) maize is wilted f) wheat is ripe and wilted g) mustard is wilted h) low precipitation for three months i) gap due to fire at the site j) beginning of maize wilting

On field A18, wheat shows an increased in Fig. 3.14 f) as well as mustard in Fig. 3.14 g). In contrast to this general behaviour, potato in 2014 (see Fig. 3.14 h) had the highest bowen ratios at the end of April and in the beginning of May (see Fig. 3.14 h). This can be explained by bare soil and enhanced global radiation during April and May 2013 (see chapter 3.4.3). The desiccation peak is missing due to a lack of data during that short time period. In Fig. 3.14 j) again the increase of Q_H for winter wheat can be seen in the Bowen ratio.

Fig. 3.14 further shows that dissipation of solar energy throughout the vegetation period is strongly bound to plant development. Depending on the footprint, one single EC station detects different and coherent dynamics of plant development on both fields A17 and A18. This again underlines that the sorting scheme chosen in this work gives reasonable results.

3.4.5 Energy balance closure during 4 different observed time periods

The measurements of available energy and surface energy fluxes (see Fig. 3.15) in Scheyern are carried out during the time window between 10:00 and 14:00 o'clock. The sum of Q_E and Q_H are depicted on the x-axis. The available energy is depicted as the difference between net radiation (R_n) and ground heat flux (Q_G) in Fig. 3.15.

The values for the eight plots were measured during four time periods (2014-05-01 to 2014-06-15 for Fig. 3.15 a,b) , 2014-06-15 to 2014-08-08 for Fig. 3.15 c,d), 2015-03-05 to 2015-05-01 for Fig. 3.15 e,f) and 2015-06-15 to 2015-08-08 for Fig. 3.15 g,h). The average energy balance closure (EBC) of all observed periods (four periods and 2 fields) is 0.76 ± 0.09 (see Fig. 3.15). This is a common value for croplands (Stoy et al., 2013). If we only regard the measurements from A17 the energy balance closure is 0.76 ± 0.1 and if we regard only the observed periods from A18 the energy balance closure is 0.77 ± 0.1 . So the average closure of both A17 and A18 is very similar.

If we compare the coefficients of determination R^2 of all correlations, then we see that the top panel from all energy balances from A17 shows the smallest R^2 value of 0.05. A closer look into the data shows that this is due to a systematic behaviour in the data. The maximum values of available energy are systematically higher than the measured energy fluxes and the available energy in the morning and the afternoon is systematically lower than the measured energy fluxes. All other coefficients of determination lie within a range of 0.61 (potato vegetative phase) and 0.76 (mustard generative phase).

Different degrees of closure according to species development (vegetative or generative phase) can be observed in the data. Six of the eight observations are pairs of the same crop in its vegetative or generative phase. Twice wheat in the vegetative phase and once potato in the vegetative phase can be compared with the equivalent in the generative phase. The mean of

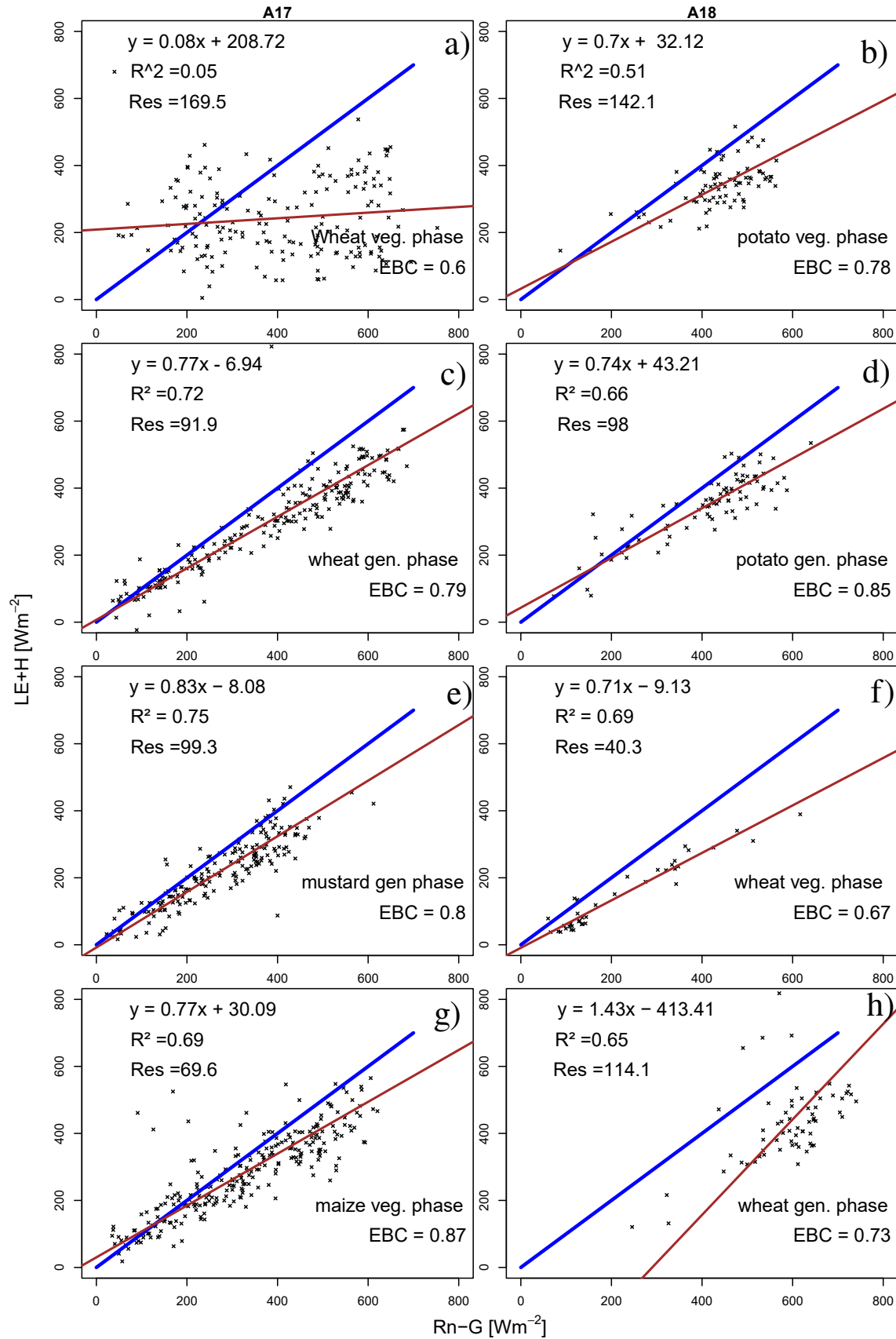


Fig. 3.15 Shown are eight energy balances over 4 different time periods on plot A17 (a,c,e,g) and A18 (b,d,f,h). The time periods are 2014-05-01 to 2014-06-15, 2014-06-15 to 2014-08-08, 2015-03-05 to 2015-05-01, 2015-06-15 to 2015-08-08. The blue line is the $x=y$ line. The brown line is the orthogonal regression.

the plants in the vegetative phase is 0.68 ± 0.09 , the mean of the corresponding three EBCs during the generative phase is 0.79 ± 0.06 . These findings are in accordance with a study of Pardo et al. (2015) who states that energy balance closure is dependent on the development stages of the plant. The above mentioned behaviour, that higher development stages have higher energy balance closures is also in accordance with a study of Imukova et al. (2016)), where winter wheat also has higher EBCs during the generative phase.

A further noteworthy aspect of this work is that although the sampling frequency of the eddy station was set to 5 Hz in November 2014, the energy balance closure did not get worse but rather improved. As a consequence less of the residuum has to be closed for energy simulations modelling study of Heinlein et al. (2017).

3.5 Eddy covariance flux measurements of N₂O on a maize field

A full year of N₂O-fluxes and their known and suspected drivers was recorded at the research station Scheyern. To the authors knowledge, it is the longest observed N₂O-flux time series, which includes maize measured using the eddy covaraince method. Furthermore, the fluxes are simulated using the ecosystem model Expert-N 5.0 and are also estimated by applying a neural net.

3.5.1 Quality analysis of the QCL-Laser and the eddy covariance setup

Allan variance: A known problem of QCLs is a lack of stability in concentration measurements. Therefore the Allan Variance, a measure of instrument stability, was calculated. With an accuracy of 0.12 ppb for the integration time of 1s and 0.004 ppb for 5120s the accuracy is considered to be within the expected range for an instrument from 2010, which was updated in 2013 (see chapter 1.2.2). As expected, the Allan variance in the investigated time of series of N₂O decreases with the observation time, τ , until signal drift at bigger time scales (larger τ) becomes more dominant and Allan variance increases again. A graph of the Allan Variance over different integration times can be seen in Fig. 3.16.

Spectrum of the eddy covariance system: The power spectrum of the measurement can be used to check which parts of the frequency range are captured by the measurement setup. For this purpose in Fig. 3.17 a power spectrum of the N₂O signal is depicted. The power spectrum is a converted time series, where the x-axis is transformed from time to frequency

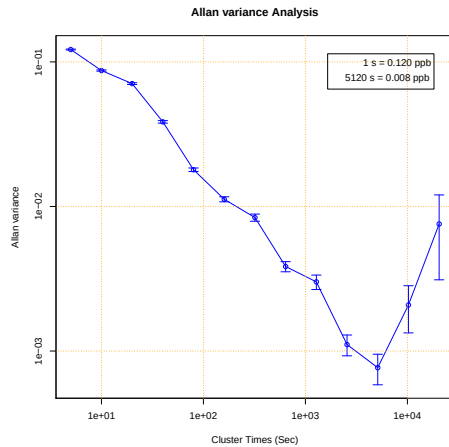


Fig. 3.16 A log-log graph with the Allan variance [ppb] on the y-axis and observation time, τ , on the x-axis [s]. The precision of the instrument is 0.12 ppb for an observation time (τ) of 1s and reaches its minimum 0.004 ppb for an observation time of 5120s

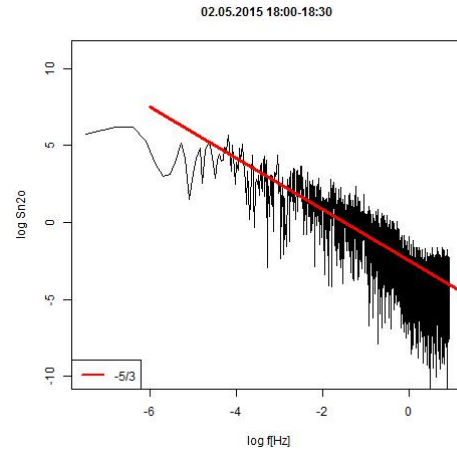


Fig. 3.17 Depicted is a plot of the the measured signal spectrum of N₂O [-] against the frequency [Hz] of the measured turbulent signal. The red line shows the slope (-5/3) which is expected for correct measurements in the inertial subrange.

by Fourier Transformation. The red line indicates a -5/3 slope, which is a property of the inertial-sub-range. The fact that the spectrum follows the expected slope until the sub seconds range is the proof that we capture the desired signal is indeed detected.

Data gaps and data availability for N₂O: The eddy covariance station for N₂O consists of multiple components (see Fig. 2.7). Most of them are crucial for the functioning of the measurement process (see chapter 2.6). Most important examples in our case are: i) energy supply, ii) flow in sample tube, iii) no contamination of the measurement cell of the instrument. iv) quality flag of at least 0 or 1 v) footprint on target area and vi) random error at least smaller than measurement value. Due to these reasons the number of detected half-hourly fluxes in the vegetation period November 2014 to October 2015 is 1758, which is comparably low in contrast to the possible number of measurements during 1 year (number of possible measurements = 17520). The measurements with a representative footprint in field A18 is only 2 % for A18. Due to the much better data basis for the field A17, the work in this chapter concentrates on the field A17.

Stationarity flags during fertilized and unfertilized periods: Stationarity is a prerequisite for eddy covariance measurements. In table 3.1, stationarity flags of two time periods accord-

Table 3.1 Shown are the frequencies of stationarity flags in percent during an unfertilized period and a fertilized period. The unfertilized period covered the measurements from February to April, the fertilized period covered the whole month of May.

stationarity flags	1	2	3	4	5	6	7	8	9
fluxes in spring (unfertilized field)	4.2	5.5	9.6	19.4	23.2	25.2	1.6	0.4	10.8
fluxes during May (fertilized field)	6.5	6.2	8.3	13.0	11.7	11.4	2.9	0.9	40.0

ing to the scheme of Foken are depicted (Foken and Wichura, 1996; Mauder et al., 2013). The first time period covers the months of March and April. During that time the field was not fertilized. The second time period covers the month of May.

The stationarity flags shown in table 3.1 decrease from flag 1-9. In the used scheme, all time periods with a flag higher than 5 are discarded. Differences in both time periods are visible. In case of the unfertilized field the discarded fluxes sum up to 38.0 percent. In the case of fertilisation, the discarded fluxes sum up to 55.2 %. Notably the worst stationarity flag 9 is four times higher in the fertilized case. The tendency towards non stationarity is thought to be a consequence of highly variable N_2O sources in time.

3.5.2 Measurements of N_2O -fluxes and their drivers from October 2014 to November 2015

Statistics: The minimum N_2O -flux value was $-6.4 \text{ nmol m}^{-2} \text{ s}^{-1}$. The maximum flux measurement was $33.2 \text{ nmol m}^{-2} \text{ s}^{-1}$. The majority of the measurement data was close to zero between minimum uptake (higher than $-3 \text{ nmol m}^{-2} \text{ s}^{-1}$) and minimum emission of N_2O (smaller than $3 \text{ nmol m}^{-2} \text{ s}^{-1}$), which can be seen in the histogram of N_2O -fluxes in the appendix (see Appendix D.1). The coefficient of variation (CV) is 311 % for the month with the highest fluxes. This range is comparable with literature values (Huang et al., 2014). In order to derive an annual sum ($0.21 \text{ kg-N ha}^{-1} \text{ a}^{-1}$), a neural net is used in chapter 3.7.4.

N_2O -fluxes in winter before snowfall: Although the water content in the soil was around 80% WFPS (see Fig. 3.24 b), which is a favouring condition for N_2O formation by denitrification, several factors were limiting. Strong frost seldomly occurred and temperatures were mostly between 0°C and 10°C . It can be assumed, that nitrogen availability is very low, as the last fertilisation was six months ago (see Appendix F.3) and additionally mustard is growing as catch crop since summer 2014 (see Fig. 3.18). As a result of this microbial activity is regarded to be low and consequently no high fluxes of N_2O were detected (see Fig.3.24).



Fig. 3.18 Green mustard (2014-12-24) **Fig. 3.19** Snow on mustard (2015-01-01) **Fig. 3.20** Wilted mustard (2015-04-01)

N₂O-fluxes in winter after snowfall: With the falling of snow on 2014-12-25 (see 3.19), a further limiting factor was added. In January, N₂O-fluxes differed from the baseline measurements only once. It seems unlikely that these variances from the baseline are due to frost-thaw events, as the air temperatures and soil temperatures in 10 cm are over zero degree °C (see Fig. 3.24 c and 3.24 d). Better conditions for frost thaw events appear in early February. Evidence for freezing can be seen in Fig. 3.24 b) and d). Decreasing WFPS (see Fig. 3.24 b) coincides with air temperatures under 0°C (see 3.24 d). Unfortunately, during that time, N₂O-fluxes could not be measured by the QCL system (defect pump). However the formation of N₂O was detected during by soil gas measurements in the proximity of the measurement station (see Appendix: table E.3). No significant frost-thaw peaks were detected from January to March. After the melting of the snow, plant residues remained at the wet soil surface. Temperatures were low enough to limit microbial activity and not low enough to trigger N₂O formation by freezing and thawing (see Fig. 3.20). All in all low nitrogen contents, temperatures near the zero degree treshold and subsequently snow cover hampered N₂O formation in the soil. In March 2015 mustard residues began to mineralize visibly on the field.

N₂O-fluxes during fertilisation period: Only one freeze-thawing event could be observed in the morning hours of 2015-04-01. The camera (see Fig. 3.20) shows wilted mustard pressed to the soil and a wet soil, which are considered to be good conditions for denitrification.

After this day, temperature values increased. N₂O peaks by freezing and thawing became more and more unlikely. On 2015-04-22, the residues of mustard were finally harrowed into the soil (see Fig. 3.20). On the same day the soil was prepared for sowing (cultivated), fertilized (93 kg – Nha⁻¹) and maize was sown. Maize emerged in the beginning of May. With high substrate contents in the soil (fertilization and mineralized mustard) and good conditions for N₂O-formation, first N₂O-fluxes could be detected on 2015-05-02. Also the highest flux value for N₂O from field A17 (33.2 nmol m⁻² s⁻¹) was measured at that day.



Fig. 3.21 Residues tilled into **Fig. 3.22** Dry soil for one **Fig. 3.23** Rewetted soil with soil and subsequent rainfall month after 2. fertilisation on small maize plants (2015-06-15-05-02) 2015-05-19 (2015-06-07) 08)

The delay between fertilization and N_2O -peak can be explained by the rainfall pattern. In the days after fertilization only few liters of rainfall were observed (see Fig. 3.24). This on the one hand didn't dissolve the solid fertilizer grains to enhance reactive nitrogen in the soil nor did it lead to a wet soil, which is favourable for denitrification. However, on the last day of April and the first days of May rainfall was heavy (see Fig. C.6 in the appendix for a higher temporal resolution). The solid fertilizer grains dissolved in rainwater and the reactive nitrogen became available for plants and microorganisms. Finally fluxes of N_2O could be detected. After fertilization, nitrogen was taken up by the biosphere. Further sinks from the perspective of the upper soil layers are nitrogen losses into other compartments (groundwater, atmosphere, etc.). As a consequence it is consistent that nitrogen contents in the upper soil layers decrease (see Fig. 3.28). It is also consistent that nitrous oxide fluxes decrease until the next fertilization at 2015-05-19. Like in the first fertilisation event we did not detect high fluxes of N_2O . The most probable explanation is that water contents are often too low for denitrification.

The next N_2O -flux events were detected on 2015-06-17. Although nitrogen content in the soil was already decreasing, WFPS was varying around 80% and temperature was between 10 and 20 degrees.

N_2O -fluxes in July to October 2015 N_2O -flux ranged between $4.5 \text{ nmol m}^{-2} \text{ s}^{-1}$ and $-5.7 \text{ nmol m}^{-2} \text{ s}^{-1}$. The low flux values are most probably due to the low rainfall and thus soil moisture values in summer 2015. In July and August, the cumulative precipitation was 31 mm and 36 mm respectively. Average temperature was 21.4 and 21.0 $^{\circ}\text{C}$, respectively. Compared to the monthly means from 1992 to 2015 at the research site, the temperature was 3.4 and 3.3 $^{\circ}\text{C}$ higher and the precipitation was 73 mm less in case of July and 55 mm less in case of August (see Appendix A.1). The water filled pore space of the loamy soil was

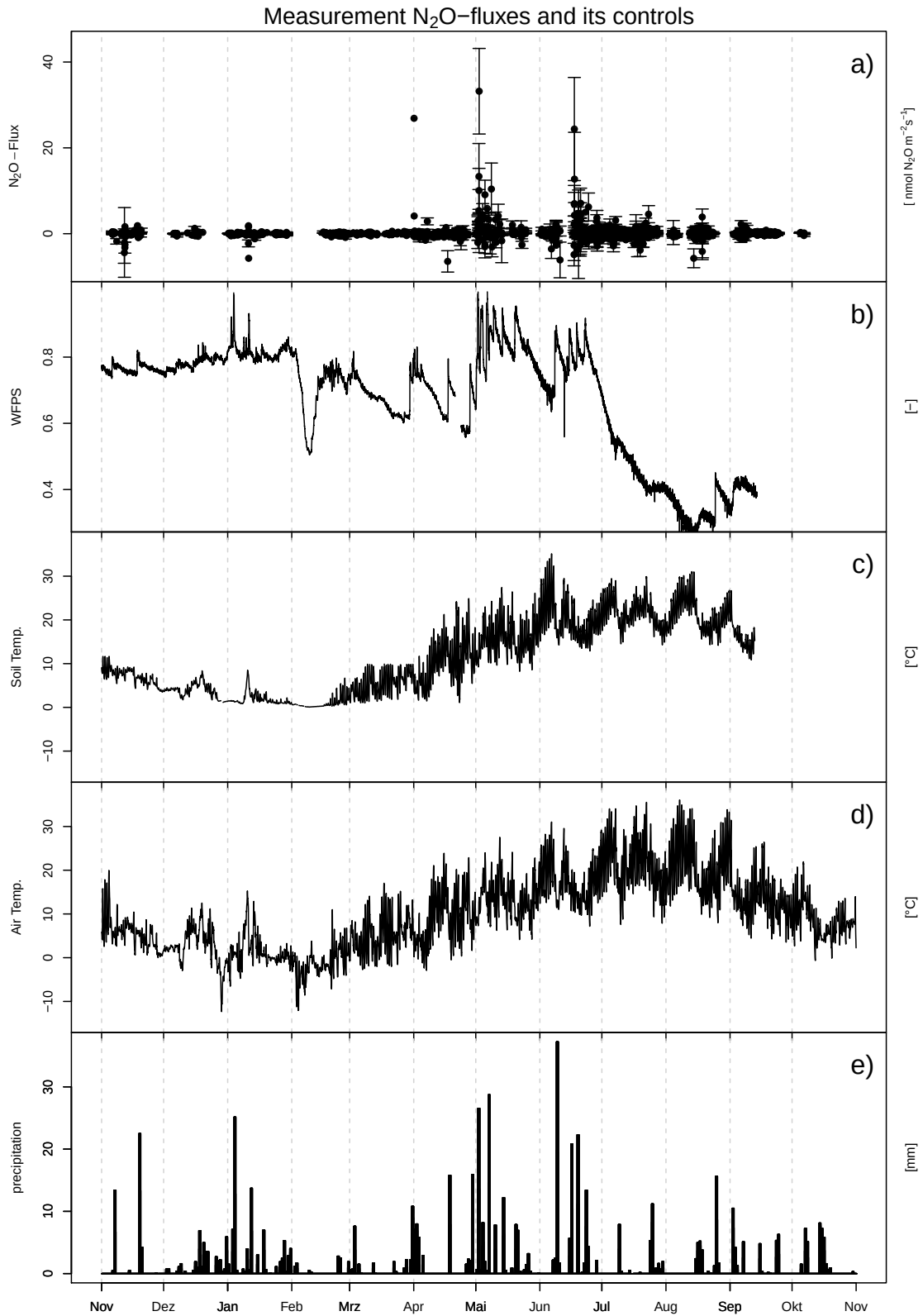


Fig. 3.24 Depicted are the measurements during the vegetation period 2014/2015 on the maize field. During wintertime mustard was cropped. Subfigure a) shows N₂O-flux [$\text{nmol m}^{-2}\text{s}^{-1}$], b) WFPS in 10cm [-], c) soil temperature in 10 cm [$^{\circ}\text{C}$] d) air temperature [$^{\circ}\text{C}$] and e) rainfall [mm/d]

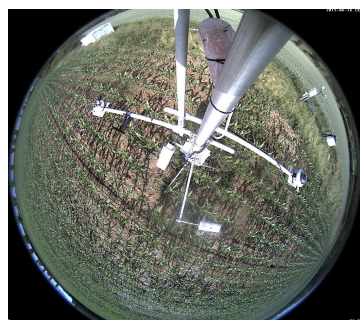


Fig. 3.25 Photo: Drying soil on 2015-06-16

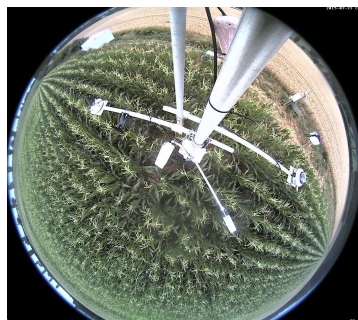


Fig. 3.26 Photo: Anthesis of maize on 15-07-23

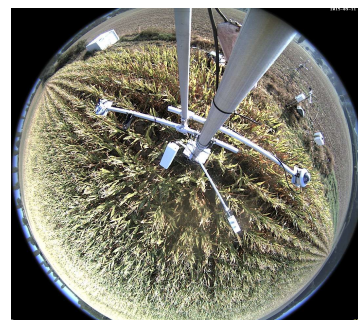


Fig. 3.27 Photo: Wilting maize on 15-09-11

minimal in August with around 10 % (see Fig. 3.24).

Due to the above mentioned drought, the conditions for denitrification are unfavourable and thus N_2O fluxes were not detected. Obviously fluxes from nitrification, which can be produced in the case of low WFPS values are not measured.

3.5.3 Correlations of measured controls on N_2O -fluxes

The drivers for N_2O emissions are nonlinear and multicausal (see Fig. 3.34). Therefore, good correlations cannot be expected when one plots N_2O -fluxes against another single entity. Nevertheless, the plots show us at which conditions N_2O -fluxes are favoured.

Driver 1, Soil temperature and air temperature: Soil temperature as well as air temperature was correlated against N_2O emissions (see Fig. 3.28 a,b). We can see in both panels that there are two regions where N_2O is formed. The first range is around 0 °C and the second range is 10-30°C. The enhanced values in the first range can be explained by frost-thaw peaks. It is remarkable that high N_2O -fluxes coincide much more accurately with the value of 0 °C of T_{air} than with soil temperature in 10 cm Fig. 3.28 a)b). A probable explanation might be that in 10cm depth, the soil was not freezing, which can be seen by the soil temperature measurements in Fig. 3.24. The main result of both plots therefore is that frost-thaw events measured in 2015 only come from the surface and not from the deeper soil.

Driver 2, WFPS: In Fig. 3.28 c, water filled pore space in 10 cm (WFPS) is plotted against N_2O -emissions. It was found that all emissions higher than $5 \text{ nmol m}^{-2} \text{ s}^{-1}$ are located between a WFPS of 0.7 and 0.9, the typical range for denitrification. The rare measurement of N_2O emissions close to water saturation (WFPS = 0.9-1) of the soil are

smaller, which is also reasonable. On the one side a wet soil can severely limit diffusion from the soil into the atmosphere (Bakker and Hidding, 1970) and on the other side denitrification from N₂O to N₂ is almost complete (Davidson et al., 2000). No N₂O-fluxes higher than 5 nmol m⁻² s⁻¹ were measured within the range of 0.2 to 0.6 WFPS, where emissions from nitrification would be expected.

In former studies at the research site Scheyern, Ruser et al. (1998) found maximal N₂O-flux rates at WFPS about 60-70 %, which is lower than the maximum found in this study. However, in laboratory experiments he also found the maxima at higher WFPS with soils from Scheyern. His explanation was the different sampling depth, which was smaller in laboratory experiments than in field experiments. In this context, both the former correlations and the correlations of this work seem consistent, which underlines the functioning of the measurement method. While Davidson et al. (2000) assumes soils to have optimum WFPS values for maximal N₂O emission between 60 and 80%, Butterbach-Bahl et al. (2013) finds in a review study most emissions under conditions of 80% WFPS.

Driver 3, Available reactive nitrogen: Reactive nitrogen species (e.g. nitrate, nitrite, urea, amino acids) serve as basic substrate for transformation processes within the nitrogen cycle, where N₂O is emitted. The peaks that follow the two fertilisations in Fig. 3.24 clearly underline this common knowledge. As only measurements are presented in this sub-chapter and nitrogen measurements were not conducted during the measurement period, correlations between simulation and measurement are renounced to be shown.

Driver 4, Atmospheric stability: Atmospheric turbulence controls gas fluxes from the soil. In Fig. 3.28 (lower right panel), N₂O-fluxes are shown on the y-axis and the stability parameter ξ (zL^{-1}) is shown on the x axis. As written in the lower part of the picture, fluxes smaller than -0.0625 are labile, between -0.0625 and 0.0625 they are regarded as neutral, fluxes bigger than 0.0625 are regarded as stable. Only one value higher than 3 nmol m⁻² s⁻¹ is observed during stable stratification. During neutral stratification and labile stratification, all other fluxes which are higher than 3 nmol m⁻² s⁻¹ are observed.

Summary of abiotic drivers influencing N₂O-fluxes: As a general result of the abiotic drivers one can say, that the known drivers of N₂O-formation, as rapid changes of WFPS or frost thaw stimulations are confirmed. Furthermore the atmospheric stability parameter ξ correlates with the fluxes that are measured by the eddy covariance technique.

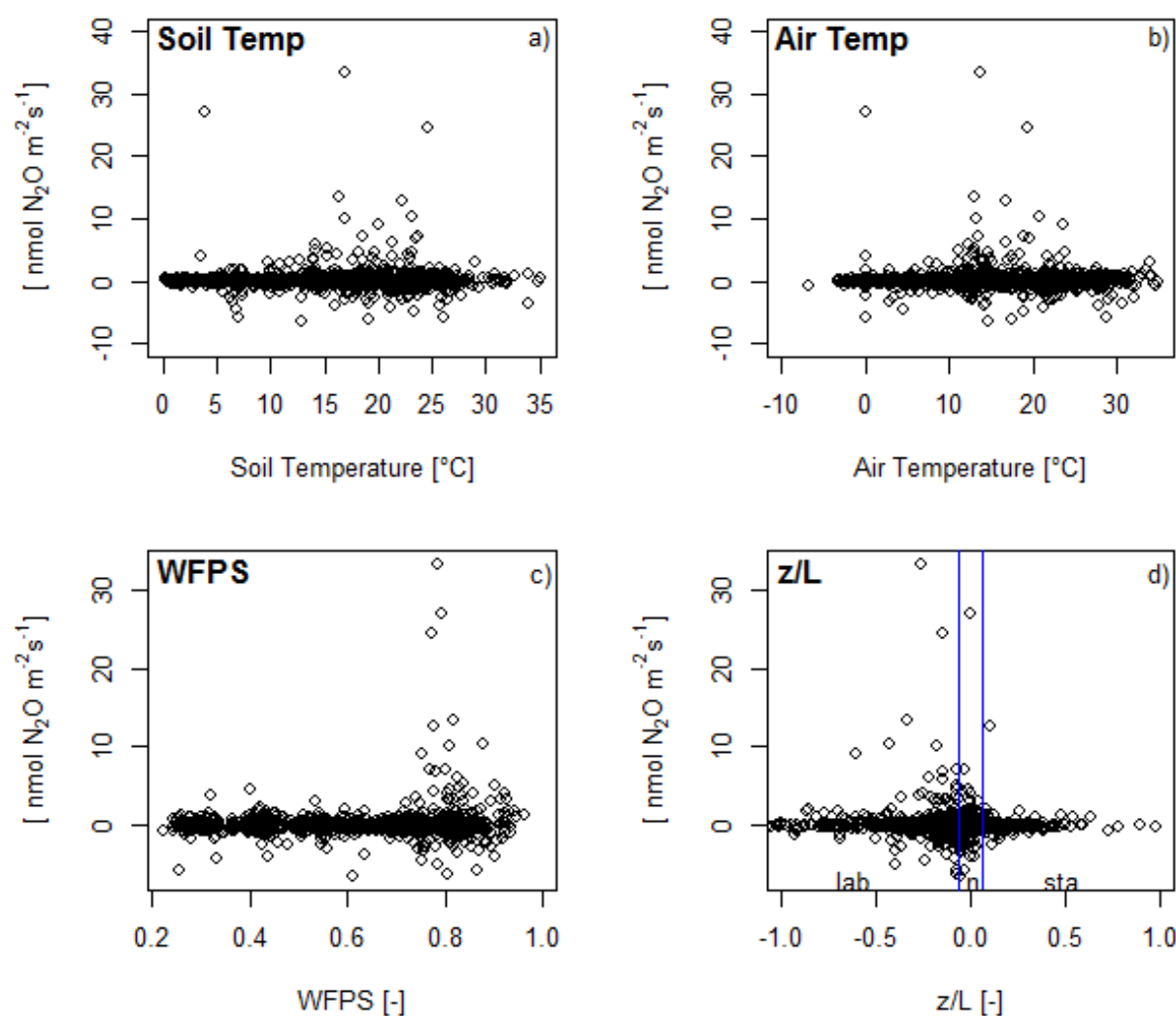


Fig. 3.28 Steering factors influencing N_2O -fluxes: Depicted are soil temperature (upper left panel), air temperature (upper right panel), water filled pore space (lower left panel), and the stability parameter, z/L (lower right panel) as x-y plots against measured N_2O -fluxes with the eddy covariance method. In the latter mentioned plot, lab. = labile stratification, n. = neutral stratification and sta. = stable stratification.

3.6 Measurement method comparison: eddy covariance vs. static chamber

3.6.1 Diurnal Cycle in both N₂O-flux measurement methods

High frequent measurements of greenhouse gas fluxes up to 48 halfhourly fluxes (EC) allow the observation of existing diurnal cycles better than measurements with lower frequency (automated chamber method). Nevertheless, in order to compare both methods it is assumed in this chapter, that only enough hourly measurements are needed to detect an existing diurnal pattern. This of course implies, that a longer time series of N₂O-fluxes measured by the automated chamber method needs to be chosen, because of its lower sampling frequency. Fig. 3.29 shows diurnal cycles of N₂O-fluxes measured with the eddy covariance technique during the vegetation period 2014/2015. Fig. 3.30 shows automated chamber measurements from the years 2008 to 2015. In the case of the eddy covariance measurements, the number of measurements ranges between 80 and 295. In case of the automated chamber measurements the number of measurements ranges between 294 and 310.

As already shown in Fig. 3.28, N₂O-fluxes correlate to atmospheric stratification, soil

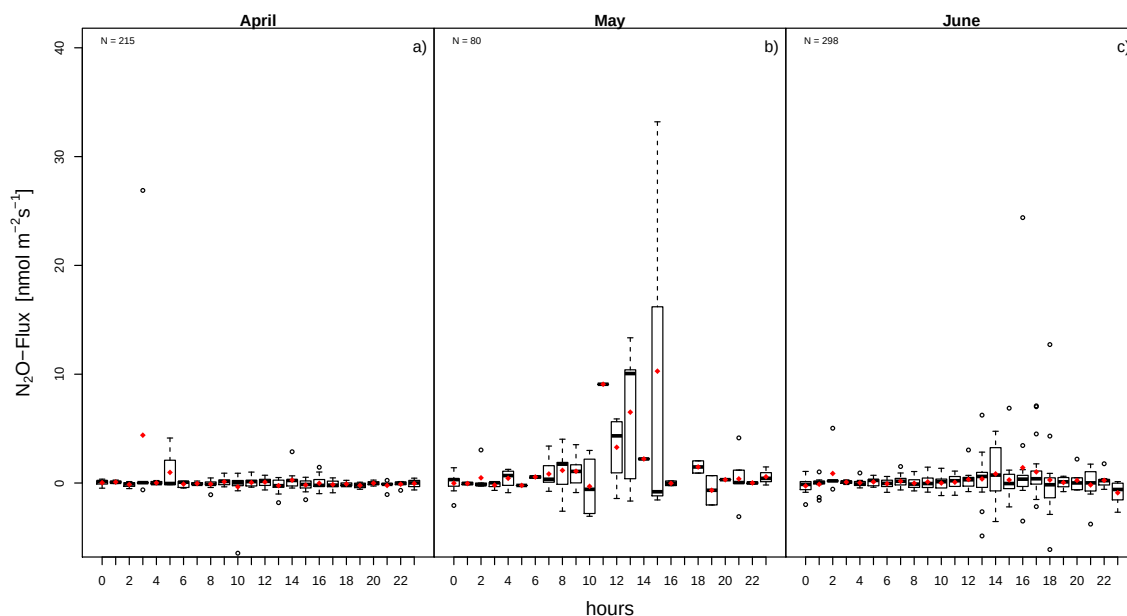


Fig. 3.29 Monthly averaged diurnal patterns of N₂O-fluxes: Depicted are measured N₂O-fluxes in the months April, May and June in 2015. During May and June a daily cycle can be seen. During April most of the few enhanced N₂O-fluxes happen at night

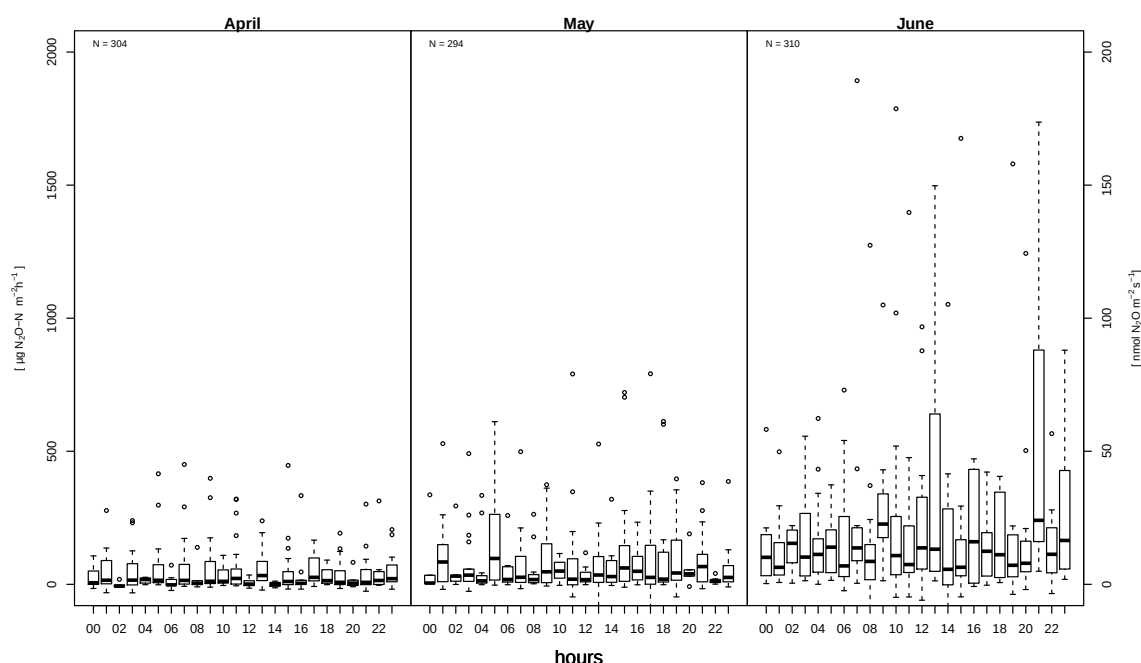


Fig. 3.30 Monthly averaged diurnal patterns of N_2O -fluxes: Depicted are measured N_2O -fluxes in the months April, May and June from 2008 to 2015 measured with the automated chamber technique. A diurnal daily pattern is not visible for N_2O -fluxes. Also fluxes are often higher during nighttime than during daytime.

temperature, air temperature and WFPS. Apart from WFPS, these state variables have a diurnal pattern. Thus it is not surprising that the measured EC values in Fig. 3.29 also show a diurnal cycle.

In April few fluxes measured with the EC method are higher than $3 \text{ nmol m}^{-2} \text{ s}^{-1}$ (see Fig. 3.29). However the variation of the hourly values that were measured with the eddy covariance are enhanced during daytime. Such a behaviour cannot be seen for the fluxes measured with the static chamber method for 7 years (Fig. 3.30). The highest measurement values are distributed over the whole day. An explanation for the higher daytime fluxes in the eddy covariance measurements is atmospheric turbulence that enhances the exchange of N_2O between the soil and the atmosphere (see also Fig. 3.28).

Higher average N_2O -flux values can be observed in May. This is true for both eddy covariance and chamber measurements. Also here a diurnal cycle can be seen in the eddy covariance measurements and a diurnal cycle in the chamber measurements is not visible.

In June, the highest measurement values with the eddy covariance method are also during the day. Most of the enhanced values happen during the afternoon.

The reason for higher daytime values could be higher soil temperatures, diurnal cycles of root

exsudates that stimulate microbial activity (Shurpali et al., 2016), changing WFPS values in the soil or the evolving mixing layer in the boundary layer, which makes the transport of greenhouse gases from soils to the atmosphere more effective (Riederer et al., 2013).

3.6.2 Comparison of half-annual sums between both measurement methods

In Fig. 3.31, both measurement methods are shown. In the upper panel static chamber measurements are shown and in the lower panel eddy covariance measurements are shown. The measurements begin in November 2014 and end in April 2015.

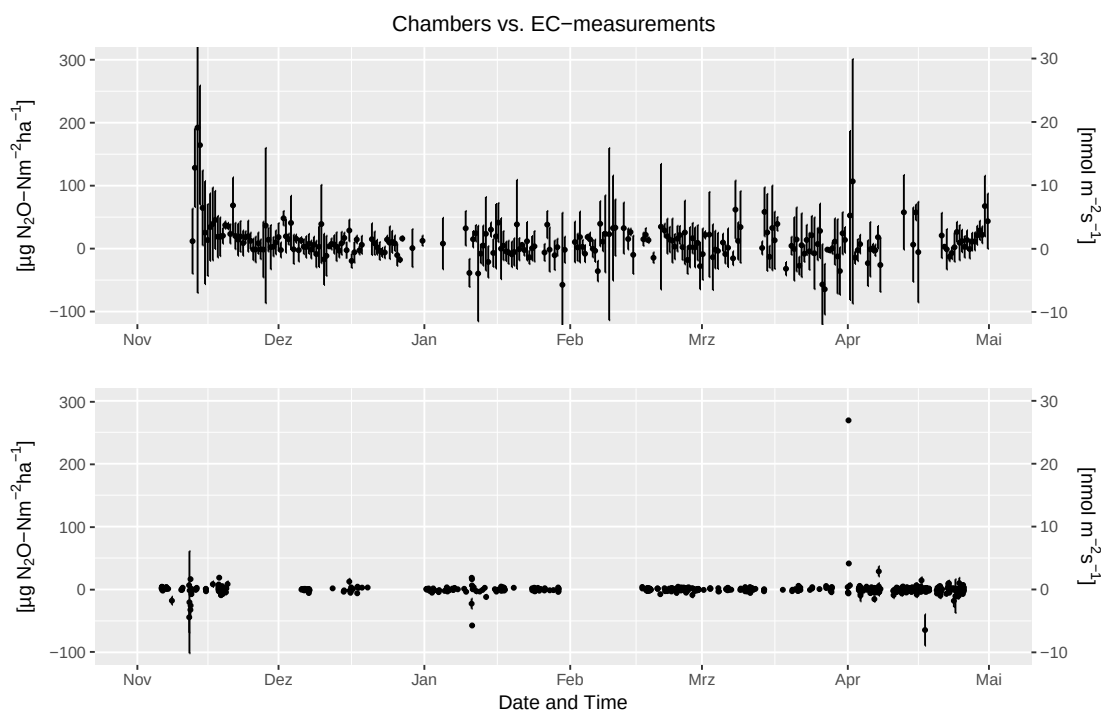


Fig. 3.31 Comparison of EC and chamber measurements during winter 2014 and 2015. Hot moments where fluxes are higher than baseline emissions partially agree (mid of November and begin of April) and are partially similar in flux magnitude.

Measurement frequency: With the EC-method, 580 measurements were taken within half a year on A17, which are rather few measurements for the eddy covariance technique. The reason for the low number of measurements are primary the bad meteorological conditions (no turbulent atmosphere) during wintertime. This effect is also visible in the the heat map in chapter 3.5, where less measurements were successful during wintertime, than during summertime. With the automated chamber technique 300 average flux measurements (derived

from 3-4 synchronous chamber measurements) were taken within the same timeframe (see also table 2.5).

Hot moments: Both time series show similar hot moments (middle of November, beginning of April). The behaviour of both time series support the assumption that the relevant controls that drive N₂O-fluxes in winter (freeze-thawing, snow) are similar at the two studied fields. As there is no soil management (e.g. tillage, fertilisation, etc.) on both sites between October and April the weather is seen as a main driving force of N₂O – fluxes (frost-thaw emissions).

Half-yearly sums: The mean value of N₂O-fluxes measured with the chamber method is $0.45 \text{ kg-N} \pm 8.1 \text{ kg-N ha}^{-1}$. The mean value of the EC-measurements is $0.048 \text{ kg} \pm 0.04 \text{ kg N}_2\text{O} - \text{N ha}^{-1}$. Both measurements are within the same range if one takes into account the measurement error of the chamber measurements.

A magnitude und 0.5 kg-N ha^{-1} is very small compared to earlier measurements. In winter 2008/2009, $9.9 \text{ kg N}_2\text{O} - \text{N ha}^{-1}$ were measured with the same chamber system (see chapter 3.8). The two independent measurements in Scheyern underline the reliability of the relatively small halfyearly sums in Scheyern compared to the much higher winter sums in earlier winters.

3.7 Energy and greenhouse gas flux simulations from field A17

3.7.1 Simulations of the plant model

LAI: In 2013 and 2014, development stage measurements of LAI are not available from the site, however camera photos exist from the first vegetation period of potato in 2013. From these photos it becomes evident that it takes only two days to destroy the whole LAI after desiccation. Such an abrupt decrease cannot be seen in the simulation with Expert-N 5.0 (see arrow, Fig. 3.32 a, desiccation).

In 2014, LAI measurements of A18 from 2015 are used to answer the question whether the LAI are at least in the range of values measured at the site. The simulations of this study exceed the maximum winter wheat measurement from 2015 values for LAI of the next year by about the factor 4 (see also table F.3 in Appendix F). Although there is annual variation a variation about the factor four is seen as rather unrealistic.

In the vegetation period 2014/2015, 10 measurements of LAI during the maize vegetation period were made (see also table F.3 Appendix F). In 2015, simulations showed a similar dynamic as the measurements. An overestimation of the simulation against the measurements of a maximum LAI of 2.5 can be shown for 2015. In the end of the vegetation period, the LAI values for both measurement and simulation are very similar. It is possible that the measured LAI values were lower during 2015 because of the severe drought.

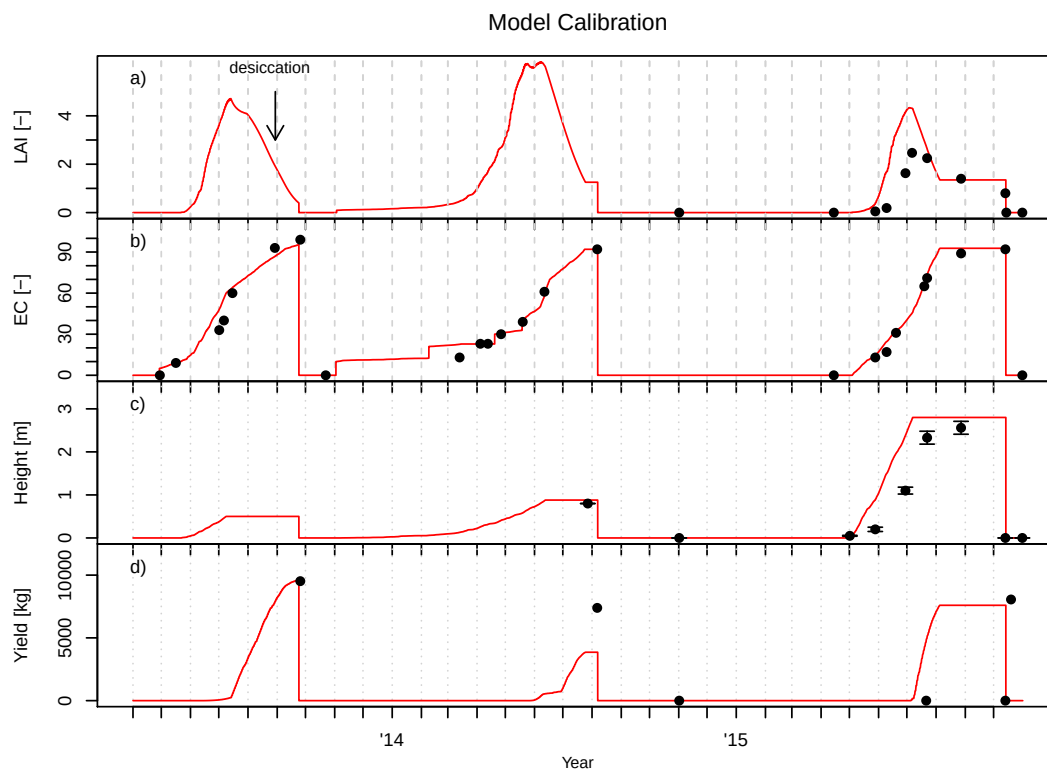


Fig. 3.32 Measured (black) and simulated (red) values of potato, winter wheat and maize using the SPASS model within Expert-N 5.0. LAI [-] is depicted in part a), $EC_{plant}[-]$ b), height[m] c) and yield [kg] d).

Development stages: The development stages (EC_{plant}) of all modelled plants fit well to the observed development stages. In the years 2013 and 2014 the development stages were determined together with the farmer of the research farm depending on plant treatment and on-site camera pictures.

Potato in 2013 could be simulated well from emergence until desiccation. Also the development stages of winter wheat could be modelled well from autumn 2013 to harvest in summer 2014. Maize emerges in the beginning of May 2015. On the 2015-06-19, the maize plant

has already several leaves ($EC_{\text{plant}} = 13$). At 2015-06-19, the plant is in the one-node-stage ($EC_{\text{plant}} = 31$) and in the second half of July (2015-07-16, $EC_{\text{plant}} = 65$) the plant is flowering (see also Fig. 3.26, anthesis). After that the plant transcends into the generative phase and fills its corn. Until corn is ripe at the end of August ($EC_{\text{plant}} = 89$) and can be harvested afterwards ($EC_{\text{plant}} = 92$).

Height: The simulated values of potato (2013) and wheat (2014) are within a reasonable range (see Fig. 3.32). However a permanent observation of the plant height was only conducted in 2015. Although the development stages of the plant are simulated rather accurately, the height of maize is significantly overestimated. Especially at the beginning of the vegetation period, the growth rate of maize did not agree with the measured values. At the end of the year the simulation model and measurement data match better.

Fruit Biomass and Yield: The simulation of the potato yield fits well with the potato yield measurements, which was 96 dt ha^{-1} . In contrast to that, the simulation of winter wheat yield in 2014 underestimated the measured yield of 85 dt ha^{-1} . The simulation of maize yield at A17 was slightly lower than the measured value of 96 dt ha^{-1} , in 2015.

3.7.2 Simulations of bowen ratios from field A17 with Expert-N 5.0

One of the most obvious results from the comparison of both measured and simulated bowen ratios (see Fig. 3.33) is that the simulated bowen ratio values are much more scattered and show higher values than the measured bowen ratios. A second general result is that the impact of plant growth on the bowen ratio (see also 3.33) cannot be seen as consistently in the simulation as in the measurement.

For example the clearly enhanced Bowen ratio values, which are visible in the measurement data after desiccation of potato (see Fig. 3.33 a, upper panel) cannot be found in the simulation (see Fig. 3.33 a, lower panel). A probable explanation is that the rapidly decreasing LAI after desiccation (on site camera photos not shown) is not implemented in the potato model of the SPASS model (see Fig. 3.32). Also during June/July 2014, when bowen ratios are increased for the second time in the time series (see Fig. 3.33 b, upper panel), the simulations do not show similar behaviour. This is more astonishing, as the decreasing LAI with ripening of the plant is simulated by the SPASS model (see Fig. 3.32).

In general the simulations exceed bowen ratio values over 1 much too often. This supports the finding of Lokupitiya et al. (2016) that fluxes of Q_H are often overestimated. Vice versa the capacity of high bred plants to transpire water is often underestimated (Lokupitiya et al.,

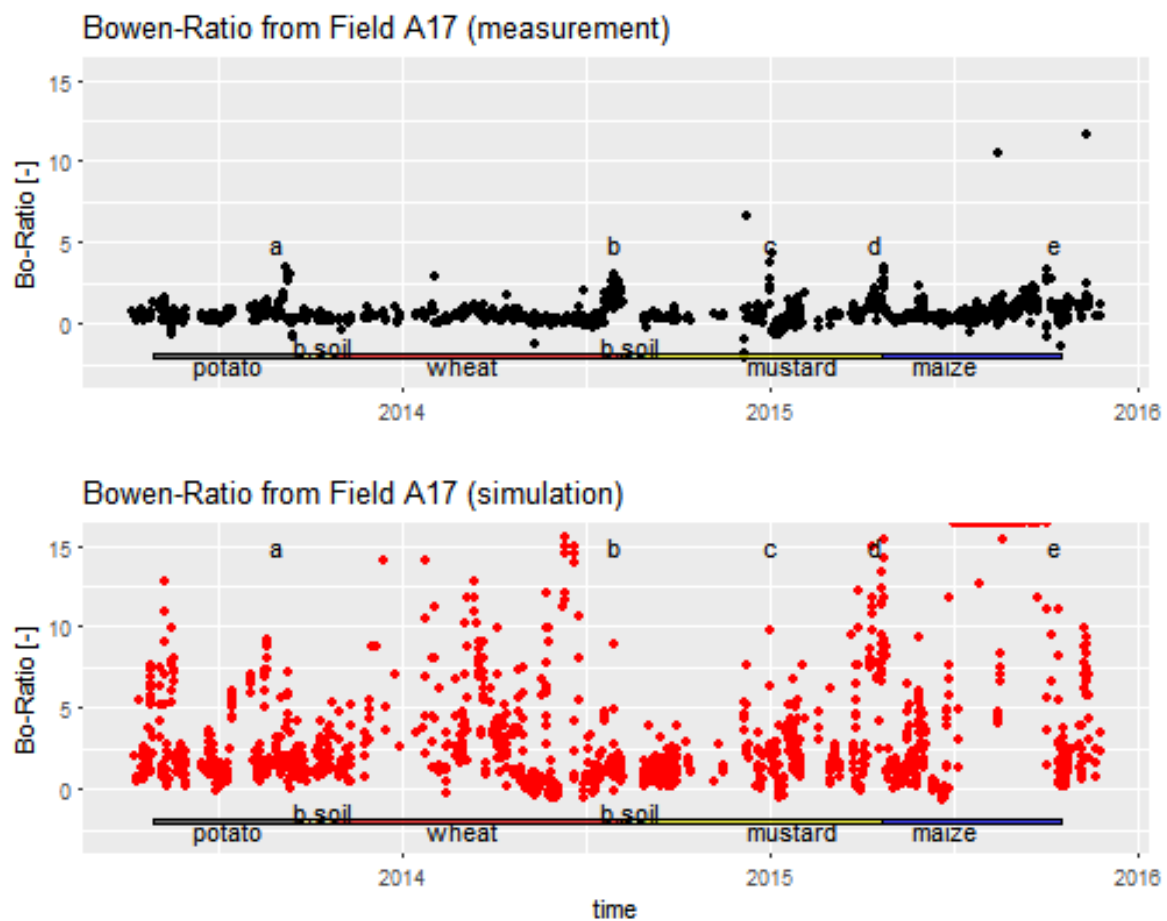


Fig. 3.33 Depicted is the measured bowen ratio at field A17 (black) and the modeled bowen ratio at field A17 (red). In the measured data a) is desiccation of potato b) is ripening of wheat c) is enhanced bowen ratio during snow cover, d) is ripe mustard and e) is ripening maize.

2016). Thus it is explainable that high values up to $Bo = 15$ throughout the vegetation period are possible. Furthermore it has to be stated that only one model configuration was used in the simulations. A study of Heinlein (Heinlein et al., 2017) showed that different evapotranspiration algorithms used in SPASS-Expert-N show different behaviour in resulting evaporation.

3.7.3 Simulations of nitrous oxide fluxes with Expert-N 5.0

N₂O-flux simulations: Fig. 3.34 a) shows measurement and simulation values from November 2014 to March 2015. Both are on a very low level and close to background fluxes. The

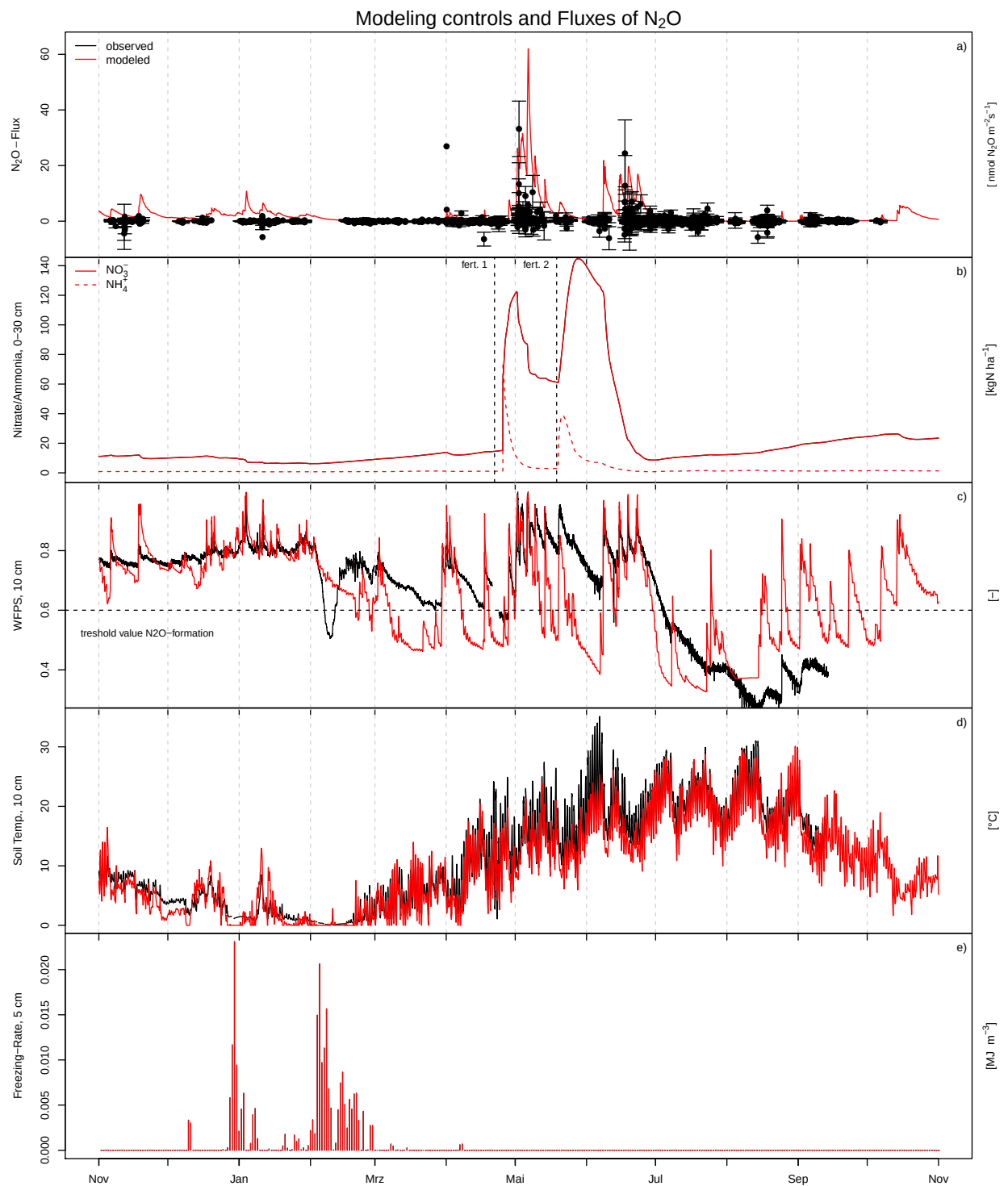


Fig. 3.34 Modelling controls and fluxes of N₂O: Measurement values are shown in black colour. Model results of the ecosystem model Expert-N are shown in red colour. All values are half-hourly values. Fig. 3.34 a) shows the modelled emissions and measured N₂O emissions with uncertainties (not available in case of no bar), b) the modelled NO₃ values (straight) and NH₄ values (dashed) are shown. The dashed lines are fertilization events with 131 and 105 kg N ha⁻¹, respectively. Fig. 3.34 c) shows measured and modelled WFPS in 10 cm depth, d) measured and modelled soil temperature in 10 cm depth, e) latent heat flux in the soil during soil freezing is shown as freezing rate [MJ m⁻³ h⁻¹]

highest N_2O -flux simulations did not exceed values of $10 \text{ nmol N}_2\text{O m}^{-2}\text{s}^{-1}$. The simulation dynamics are mostly due to changes in water content.

The highest peak to that date, occurred on 2015-04-01 at night after a rainy day (10 mm) and air temperatures around 0°C . The model simulated slightly enhanced N_2O -fluxes and underestimated the measurement value by far.

The timing of the first peak on 2015-05-02 was correctly simulated with a delay of a few days after fertilization on 2015-04-22, when WFPS rapidly increased from values around 0.5 to values around 0.8. The dashed line in the third panel of Fig. 3.34 marks the threshold value in the simulation for the formation of N_2O from denitrification. This first peak was the highest measured and the highest simulated peak within the period. The maximal simulated values are around $60 \text{ nmol N}_2\text{O m}^{-2}\text{s}^{-1}$. The simulation during the second N_2O -fertilization peak showed a similar behaviour. When the fertilization was conducted by the farmer, the soil was dry and the value of the simulation was again below 0.6. After the highest daily rain sum of the whole year on 2015-06-08 (38 mm h^{-1}) the water filled pore space increased again rapidly over 0.6 and a second fertilization peak was simulated. The simulation gave higher values for the first fertilisation peak than for the second fertilisation peak, which agrees with the measurements.

After the fertilization events no N_2O -fluxes are measured and simulated. A main reason might be the drought during July, August and September 2015, since the weather conditions, the summer was extremely hot and dry chapter 3.1. As a result conditions for denitrifications were very unlikely. Evidence for significant emissions from metabolic pathways when soils are dry (e.g. nitrification) are not observed. Although the overall dynamics of model and simulation partially agreed well, a NSE of -30.7 shows that the model has to be further adapted towards eddy covariance measurements.

Simulation of nitrate and ammonia The second panel of Fig. 3.34 shows the simulation of NO_3 and NH_4^+ . The input for both fertilizations was 131 kg-N ha^{-1} and 105 kg-N ha^{-1} , respectively. The dynamics of both nitrogen peaks differs due to the fertilizer type. In the first case solid N-fertilizer (Blaukorn) had to be solved by rainfall before it was washed into the soil profile. In the second case the fertilizer (UAN) was applied in liquid form. NSE for nitrate and ammonia are not available as no measurements exist during 2015.

WFPS simulations The model was optimized to reproduce the crucial dynamics for N_2O -formation, which are e.g. the water dynamics during the time period with high fertilization (e.g. fist days of May NSE = 0.47) and the drought situation in summer 2015. The overall NSE over the whole year is 0.31, which is slightly smaller than the NSE value in a study of

Klein (2018), which was conducted from 2013 to 2014.

In Fig. 3.34 it can be seen that from November to February the water model simulates WFPS sufficiently well, however a decrease of WFPS in early February due to frost could not be captured by the model. In spring and summer the simulations of WFPS show much higher dynamics compared to the measurements.

As the Hydrus 1-D in Expert-N 5.0 has problems to reproduce extreme drought situations which might have been caused by preferential flow (Heinlein, 2018), the model parametrization was adjusted with a relatively high K_{sat} in the lowest numerical layer of the considered soil profile so that the soil drying could be simulated in summer.

Soil temperature simulations The yearly dynamics of the simulated soil temperature fit well to the measured soil temperature in 10 cm. During the main part of the simulated time series, the simulation agrees well with the measured values in 10 cm. Only in June 2015, the simulated soil temperature is permanently lower than the measured soil temperature.

An interaction which is not considered by the model study might be the effect of leaf-shading on the soil surface. Leaf shading is a reasonable cause that influences the top-soil temperature. In June the maize plants are relatively small. In contrast to that, the maize plant is fully grown in July (see Figs. 3.24 and 3.25).

An improvement by a simple boundary condition that assumes 0°C air temperature in case of snow, when snow cover occurs was not observed (see Appendix 3.15).

Frost simulations Frost was simulated in December, January, February, March, and to a very small extent in April. Simulated frost, shown in Fig. 3.34, did not have a significant impact on N₂O emissions in the simulations. The reason is seen in the rather small amount of freezing which is also less pronounced than in previous winters, such as 2008/2009 (see chapter 3.8.3).

3.7.4 Simulations of nitrous oxide fluxes with an artificial neural net

Training the artificial neural net

In this study, 20 fits of a neural network were conducted. Training and evaluation was done as described in chapter 2.6. The calculated NSE for the comparison of predicted value of the ANN and the test data set ranged from -7.9 to 0.12. The single NSE were -7.9, -2.5, -2.34, -4.07, -2.45, 0.12, -1.35, -0.08, -0.04, 0.11, -10.3, -6.8, 0.0, -0.4, -0.11, 0.05, -0.16, 0.10, -4.6 and 0.08. The Nash-Sutcliffe efficiency answers the question whether the model is a better estimator than the mean. If the NSE is bigger than 0 it is better to use the model.

The span of the NSEs is amongst others a consequence of the training of the neural network. The input data for the 20 model runs was chosen randomly. As neural network depends strongly on the input data of the training data set the performance of the network is different. If the input for the test data set does not represent the whole observation span, the neural network cannot predict the test data set.

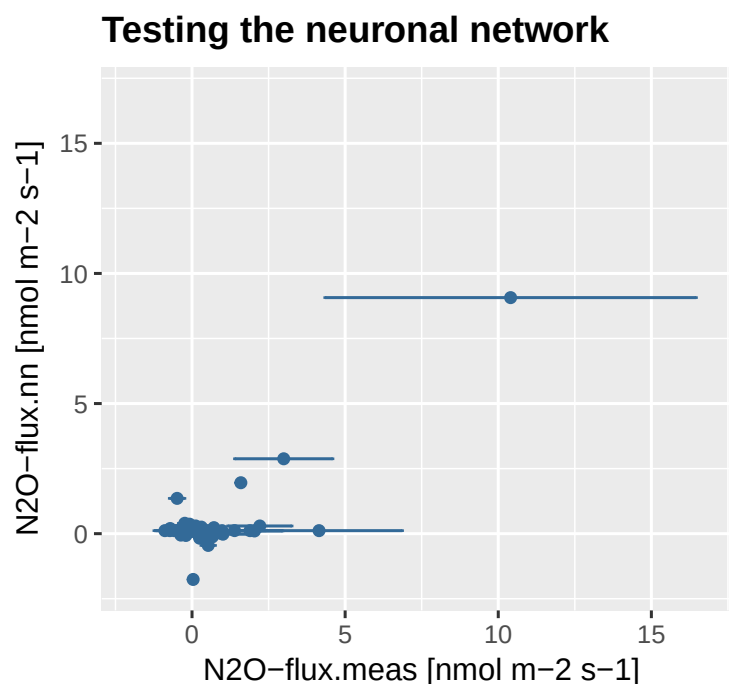


Fig. 3.35 Testing the neural network: The picture shows the performance of the ANN against the test data set. Vertical bars are calculated errors of the EC-method calculated by the TK3 software.

The fact that fluxes could be predicted with a NSE of 0.12 but not higher is thought to be a consequence of probably missing explanatory variables and an imperfect match of explaining variable and explained variable. Finally, the best trained network was chosen to predict the data gaps. Fig. 3.35 shows that the ANN can estimate low flux values well within the boundaries of the measurement errors.

Gap filling and annual sum

The mean of the 1758 measured N₂O-fluxes is $0.135 \pm 0.04 \text{ nmol m}^{-2}\text{s}^{-1}$. The mean of the predicted values for the data gaps is $0.25 \text{ nmol m}^{-2}\text{s}^{-1}$ (no error given). In total, the gap

filled time series adds up to $0.21 \text{ kg N}_2\text{O} - \text{N ha}^{-1} \text{ a}^{-1}$, which is an extremely low value for a fertilized site. An explanation for such a small annual flux may be the topography of the

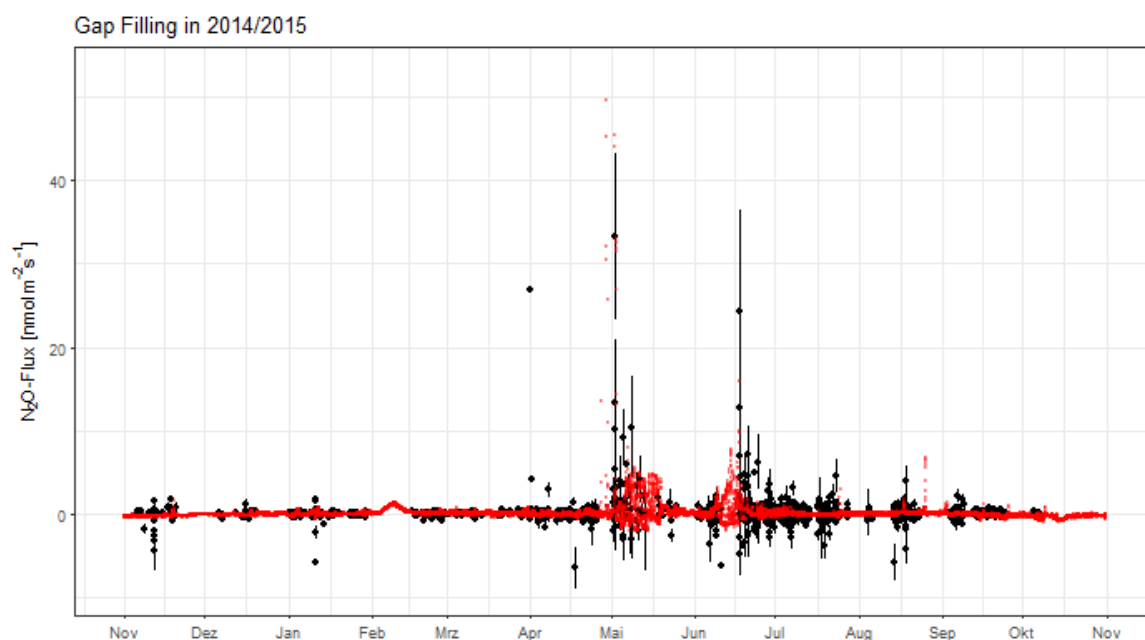


Fig. 3.36 Depicted are the N_2O -fluxes (black dots) that were detected from 2014-11-01 until 2015-10-31, with their uncertainties (black lines). In order to fill the gaps during the year a neural network was employed (red line).

site, which is located on a hill ridge. Hills are known to be sites where less N_2O is formed. Hot spots of N_2O -formation are often found in low elevations (Yanai et al., 2003).

The annual performance of the ANN fits well to the measured pattern. It can be clearly seen in Fig. 3.36 that the ANN predicted both fertilization peaks within a reasonable range and also at the right time. Furthermore enhanced fluxes during the beginning of February 2015 are estimated by the ANN. These estimations make sense increased N_2O soil gas concentrations were measured during that time (see Appendix E.3). Also time periods when N_2O -fluxes were low are generally estimated well.

However, the ANN which is shown in 3.36 could not reproduce the frost-thaw events. A reason for this is possibly the lack of hot moments due to frost-thaw in the training data set.

The half-hourly fluxes values of this study ($-6.4 \text{ nmol m}^{-2} \text{ s}^{-1}$ to $33.2 \text{ nmol m}^{-2} \text{ s}^{-1}$) are within the same range as the values reported in a recent study by Cowan et al. (2016). He found fluxes ranging from 0 to $8.8 \text{ nmol m}^{-2} \text{ s}^{-1}$ after fertilization of a pasture ecosystem. It is interesting, that this study was also conducted with an eddy covariance station between two landuses. Both landuses were pastures with different tillages.

Table 3.2 Review over micrometeorological measurements (EC = eddy covariance, Gr = Gradient Method) and selected chamber measurements (Ch) methods and ecosystems. The studies of (Meurer et al., 2016) and (Jantalia et al., 2008) are again review studies.

Method	obs. time	Author	Fertilizer kg-N ha a	Fluxes kg-Nha ⁻¹	crop type
EC	1 year	this study	236	0.2	maize
EC	6 months	(Huang et al., 2014)	217	6.9	maize
EC	3 months	(Grant and Pattey, 2003)	155	2.2	maize
EC	3 months	(Grant and Pattey, 2003)	99	1.2	maize
EC	2 months	(Cowan et al., 2016)	200	1.5	pasture
EC	1 year	(Merbold et al., 2014)	197.8	29.1	pasture
Gr.	6 months	(Wagner-Riddle et al., 2007)	150	1.2	maize
Gr.	6 months	(Wagner-Riddle et al., 2007)	110	1.0	maize
Gr.	6 months	(Wagner-Riddle et al., 2007)	150	1.6	maize
Gr.	6 months	(Wagner-Riddle et al., 2007)	110	1.8	maize
Ch.	6 months	this study (winter '10/11)	0	5.9	maize
Ch.	6 months	this study (summer '10)	135	3.4	maize
Ch.	6 months	this study (winter '14/'15)	0	0.5	bare
Ch.		(Jantalia et al., 2008)	256	0.7	corn/wheat
Ch.	1 year	(Meurer et al., 2016)	80	0.5	maize

Although the range of values after fertilisation in this study is similar to the study of Cowan, the annual flux is much lower (one magnitude). The obtained annual nitrogen sum ($0.21 \text{ kg-N ha}^{-1} \text{ a}^{-1}$) is furthermore lower than the sums for 11 other studies reported in similar agroecosystems (see table 3.2).

Compared to the default tier 1 emission factor, which assumes that approximately 1% of the applied nitrogen is lost by gaseous emissions of nitrous oxide, the percentage of lost nitrogen in this study it is only 0.1 %. The great variability of this factor can be shown by studies, where the default emission factor is either much higher (e.g. 15% of the applied nitrogen in the study of Merbold et al. (2014) or lower as 1 (Ruser et al., 2017).

There are several explanations for the relatively low N_2O -fluxes compared to other studies. The first argument is that the footprint of the tower is located over the hill ridge (see Fig. 3.4). It is possible that the soil is more aerated at the hill ridge than in the lower parts of the field. This hypothesis is supported by soil gas measurements during summer 2015, that show lower concentrations of N_2O over the hill ridge than in lower elevations (see Appendix E). Furthermore the annual fluxes of N_2O are generally decreasing in Scheyern since years (see also chapter 3.8.4).

A further aspect lies in the special measurement setup. In contrast to other fluxes N_2O peaks

are highly episodic and characterised by low background fluxes. This in turn means that if one misses one or two time periods of high fluxes an essential part of the annual flux can be missing. In our time series there are two gaps that contain possibly high N_2O -measurements.

Daily cycle in the neural net

Apparently, in both fertilization periods the neural network learnt that high WFPS and high reactive nitrogen loads lead to high N_2O -fluxes. However, due to the nature of the ANN, the underlying relationship for the prediction of the ANN is not transparent and without further statistical methods, sensitive controls on the N_2O -flux cannot be derived. Such a statistical method is for example the application of Garson's algorithm, which is described by Olden and Jackson (2002) with the words "illuminating the black box".

An astonishing behaviour of the ANN is that the neural network predicts a pronounced daily

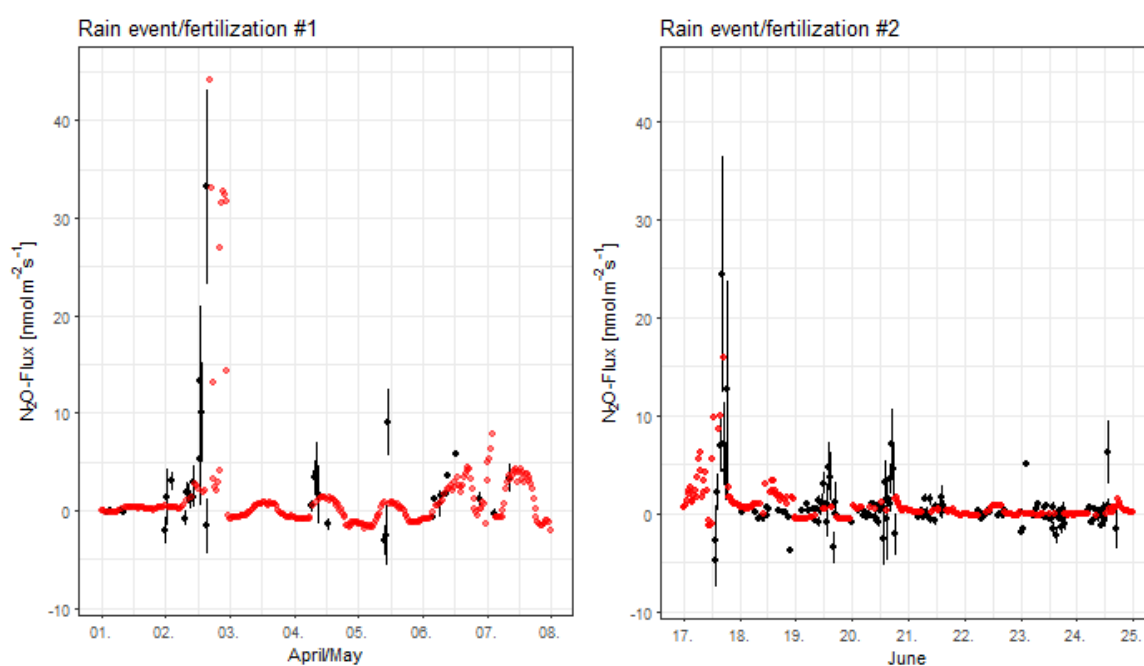


Fig. 3.37 Depicted are the two time windows when N_2O -fluxes (black dots) and estimated errors (black lines) were detected after the fertilization of the maize field. In order to fill the gaps during the year a neural network was employed (red line).

cycle (see Fig. 3.37). This is in contrast to Expert-N 5.0 simulations, where no daily cycle is simulated. This predicted diurnal cycle is most pronounced during the two fertilization periods in early May and June, see Fig. 3.37.

3.8 Evaluation of hourly N₂O-flux simulations with long-term automated chamber measurements

3.8.1 Meteorological model driver data

The drivers of the model system were temperature, precipitation, relative humidity, wind speed, and global radiation (see Fig. 3.38). Temperatures filled with red colour are below 0 °C, temperatures above 0 °C are black (Fig. 3.38 a)). Further meteorological driver data were precipitation (b), relative humidity (c), wind speed (d) and global radiation (e). Snow height as an additional driver for the model run with boundary condition 2 at the soil surface (see chapter 2.4.5) is depicted in Fig. 3.40

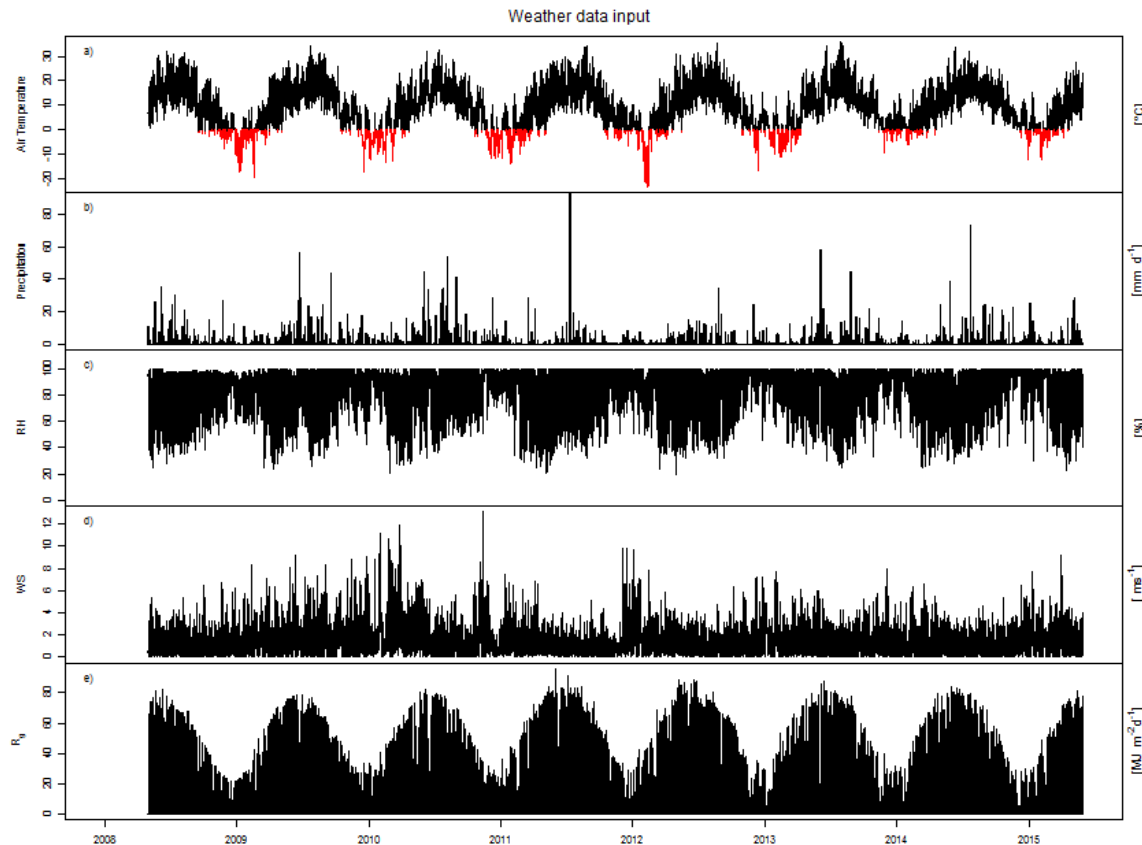


Fig. 3.38 Depicted is the hourly weather data input for the simulation over 7 years. Since 2012 TERENO data consisted of complete weather data. Since TERENO data availability for weather data were 100 %. From 2008 to 2012 hourly data availability for temperature, precipitation, relative humidity and global radiation are 82.5 % for all covered hours. For wind speed 65.1 % of all hours was covered.

Since 2012 when the TERENO instruments were finally installed at the research station, the availability and quality of the weather data is very good in Scheyern. As several weather stations exist within a few hundred meters we do not have any gaps in the weather data from 2012 to 2015 (acquisition time = 10 min, model input = averages of 1 h).

Before 2012 the driver data is a compilation of data, which is mainly from a weather station at a hilltop near A17. Between 2008 and 2012, 65.1 % of the hourly wind data were recorded and over 80 % of the hourly data are available for global radiation, wind direction and humidity. The remaining gaps were filled with data from the weather station Voglried and the DWD stations Hüll and Altomünster, which are already mentioned in chapter 1.1.2.

3.8.2 Model calibration and drivers of the N₂O model

In order to simulate N₂O-fluxes successfully, the underlying parameters that determine N₂O fluxes in the model have to be simulated as accurately as possible. In Fig. 3.39 simulations of water filled pore space, nitrate content and yield, as an indicator for adequate plant simulation are depicted by red lines. Data used for the evaluation of the simulation are depicted by black open circles. The evaluation data for WFPS and NO₃⁻-N refers to the ploughing horizon (0-25 cm).

WFPS: Fig. 3.39 shows measurements and simulations of WFPS. An evaluation of the volumetric water contents in all seasons and years can be found in chapter 3.8.5.

Nitrate content: Nitrogen dynamics are driven by fertilisations (see table F.2).

In 2008, one NO₃⁻-N peak-value of 132 kg-N ha⁻¹ after two fertilisations was measured (50 kg-N ha⁻¹ + 150 kg-N ha⁻¹). The simulations (154 kg-N ha⁻¹) agree in magnitude but appear slightly after the highest measurement. After harvest, slightly rising nitrogen contents appear both in the simulations and the measurements.

In 2009, no peaks of NO₃⁻-N higher than 25 kg-N ha⁻¹ were measured. Urea-ammonium-nitrate was applied thrice in smaller applications (50, 45 and 90 kg-N ha⁻¹). It is possible that the plants were able to take up the comparable small amounts of nitrogen before the measurements were conducted. Surprisingly, also the simulations are very low with small peaks after the three fertilisations events. Later in autumn and winter, the simulations underestimate the measurements.

In winter 2010, nitrate measurements show maximum NO₃⁻-N values up to 40 kg-N ha⁻¹, whereby simulated NO₃⁻-N values are lower (0 kg-N ha⁻¹ - 10 kg-N ha⁻¹). After the first two fertilisations with a urea-ammonium-nitrate solution (UAN) in February and March

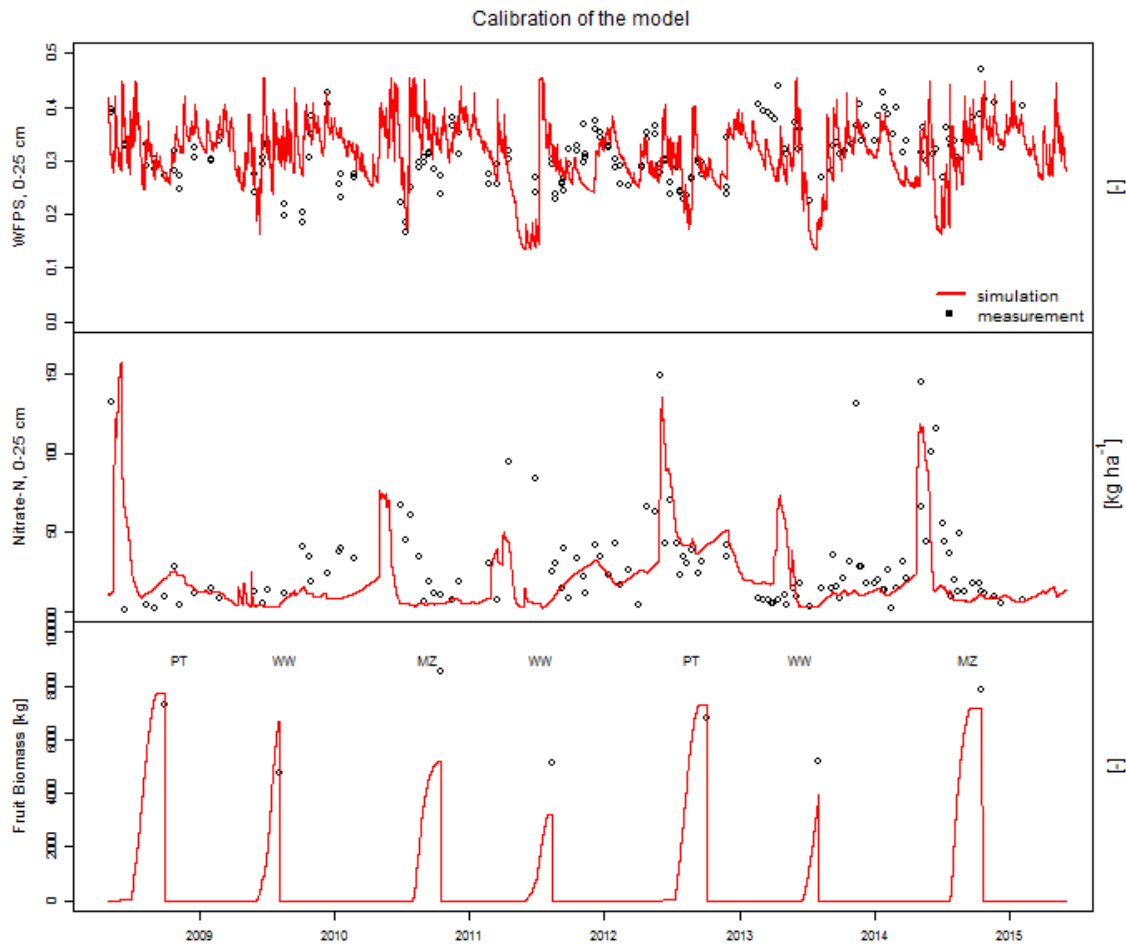


Fig. 3.39 Calibration of the model: Shown are the simulations (red) and measurements (black) of water filled pore space [-], nitrate [$\text{kg-N ha}^{-1} \text{a}^{-1}$] and yield [kg]. Crops are abbreviated with PT for potato, WW for winter wheat, and MZ for maize.

2010 (50 and 40 kg-N ha^{-1}) measurement and simulation did not increase significantly. However after the application of 100 kg-N ha^{-1} in June measurements were 67.7 kg-N ha^{-1} and simulations were 73.5 kg-N ha^{-1} . All in all, measurements and simulations in 2010 agree in magnitude, but disagree in dynamics. Simulations also decrease too early after the fertilisation events.

In 2011, the highest measurement amount of $\text{NO}_3^- \text{-N}$ 94.3 kg-N ha^{-1} occurs after the fertilisation of winter wheat. The highest simulated amount is 47.1 kg-N ha^{-1} . Although the simulated summer values clearly underestimate the measurements, the dynamics of autumn values is simulated quite well.

In 2012, the complete year could be simulated well. Measured peak value of $\text{NO}_3^- \text{-N}$ (132.3

kg-N ha⁻¹) and modelled peak value of NO₃⁻-N (149.1 kg-N ha⁻¹) agree within a reasonable range.

In 2013, measured nitrate dynamics during the vegetation period are similar to the year 2009, where no increased values were measured (max = 35.8 kg-N ha⁻¹). However in autumn 2013 a very high nitrogen amount was measured (131.6 kg NO₃⁻-N ha⁻¹).

In 2014 measured and simulated nitrogen are coherent, however the fertilization peak is lower compared to the measurements. The maximum measured value is 144.8 kg-N ha⁻¹ and the maximum simulated value is 116 kg-N ha⁻¹.

As a main result, one can conclude that the model simulates the dynamics of mineral nitrogen dynamics with varying success over the 7 years. In 2008, 2009, 2012, and 2014, the nitrogen dynamics were simulated well. During 2010, 2011 and 2013, the nitrogen dynamics were simulated worse compared to the previous mentioned measurements.

Yields: In 2008, the measured potato yield (dry mass) was 7310 kg ha⁻¹ while the simulated value was 7738 kg ha⁻¹ (+6%). Also in 2012 simulated potato yields are with 7321 kg ha⁻¹ close to the measured values of 6800 kg ha⁻¹ (+8%).

The simulations of winter wheat yields deviate more from the measured values. In 2009, which was the first year when winter wheat was cultivated, the measured values were 4760 kg ha⁻¹ and the simulated values were 6707 kg ha⁻¹ (+41%). In 2011, the measured plant yield was 5100 kg ha⁻¹ and the simulated values are 3069 kg ha⁻¹ (-39%). In 2013, the measured yield was 5190 kg ha⁻¹ and the simulated value was 4092 kg ha⁻¹ (-21%).

In case of maize during 2010, the yield simulation with 5176 kg ha⁻¹ was much lower than the measurement of 8540 kg ha⁻¹ (-40%). In 2014 however the model, 7136 kg ha⁻¹, and measurement, 7870 kg ha⁻¹, agreed better (-9%).

3.8.3 Impact of snow on simulated soil freezing

Snow measurements: The maximum snow height in the observed period was 30 cm and measured in winter 2010/2011 (see Fig. 3.40 a). Additionally this year was also the year with most snow days (79 days) and the most hours under zero degree (1713 hours). During winter 2013/2014 maximal snow height was lowest with 9cm. With 14 days also snow days were lowest (Wetterdienst, 2018a).

Snow cover was present on 386 days over the whole observed period. On average this is 55.2 days per year or 15% of the time of the year. As soil frost is a major control on N₂O formation, the effect of snow cover on soil frost was investigated with two boundary conditions in Expert-N 5.0.

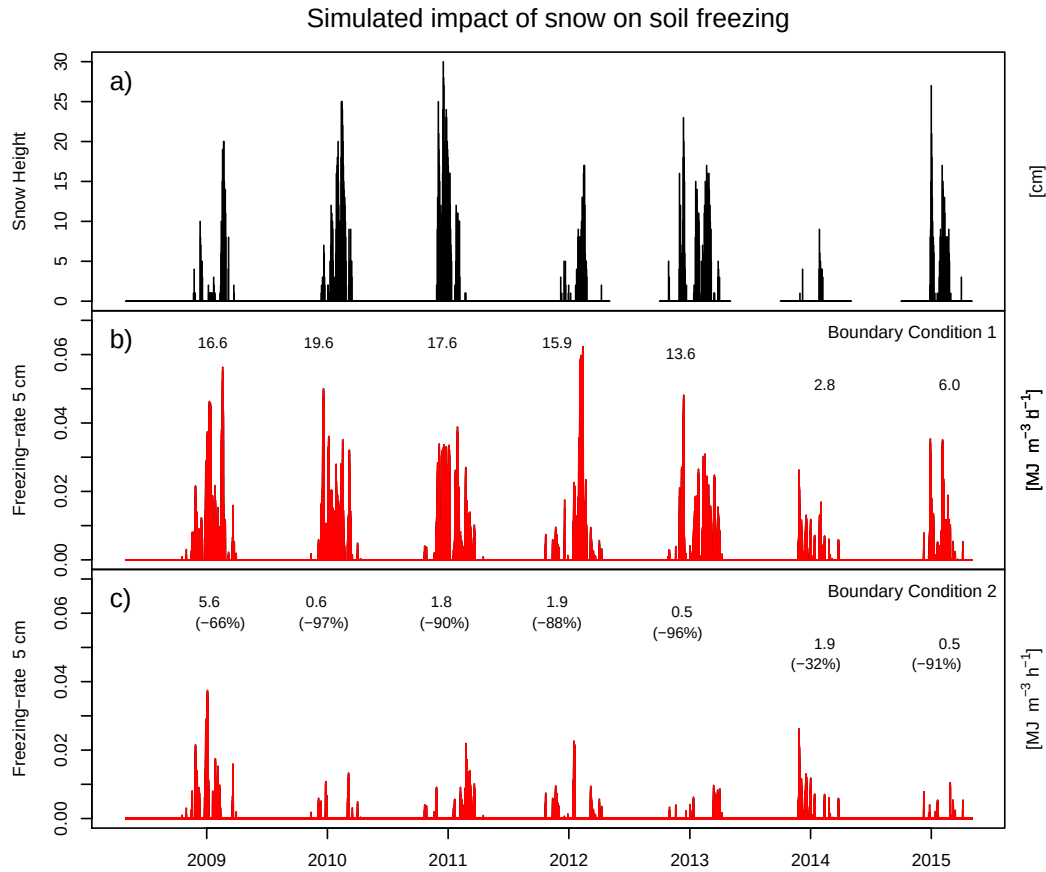


Fig. 3.40 Impact of snow on frost simulations: In subfigure a) snow height [cm] is depicted. Data are taken from the climate data server of the german weather service (Wetterdienst, 2018a). The impact on hourly frost simulations is depicted in the two panels below. Fig. 3.40 b) shows the behaviour of frost-rate for the model configuration with BC1 as upper boundary condition for the soil. Fig. 3.40 c) shows the impact of BC2 on soil freezing. Freezing rates [MJ m⁻³d⁻¹] are given as the latent heat needed for soil freezing referred to time. The cumulative freezing rate per winter is written over the winter peaks of freezing [MJ m⁻³a⁻¹]. Under the cumulative freezing-rates, the percentual decrease of the cumulative freezing rate by using BC2 is written.

Frost simulations with BC1: In the model configuration with boundary condition 1 air temperatures under 0°C lead to soil freezing even if snow is lying on the soil surface. In this case cumulative soil freezing was strongest in the winter 2009/2010 with $19.6 \text{ MJ m}^{-3} \text{ a}^{-1}$ and weakest in the winter 2013/2014 with $2.8 \text{ MJ m}^{-3} \text{ a}^{-1}$ (see Fig 3.40 b). An important shortcoming of the model implementation so far is that the freezing rate does not become negative and therefore no thaw occurs in the model. This limits the performance of the frost-thaw model to a frost model. For an improved model performance the model should be able to simulate negative frost (=thaw).

Frost simulations with BC2: In the model configuration with boundary condition 2, the temperature of the upper soil layer is exposed to 0°C "air temperature" in case of snow cover. In this case, soil freezing is strongest in the year 2008/2009 with $5.6 \text{ MJ m}^{-3} \text{ a}^{-1}$, and weakest in 2014/15 with $0.5 \text{ MJ m}^{-3} \text{ a}^{-1}$. The highest differences between boundary condition 1 and boundary condition 2 can be found in the second year. In this year the relative decrease of the cumulative freezing-rate is -97%. Snow cover prevented freezing in the model very efficient in this year. The lowest decrease of freezing rate can be seen in the winter 2013/2014, which is the year with the lowest snow heights and snow days. In general, this model experiment shows us over 7 years how snow cover can influence soil temperature in a simple model approach. To further verify the accuracy of the modelled data, soil temperature measurements should be used to evaluate the impact on soil freezing.

3.8.4 Evaluating simulations with automated chambers I: Half-yearly N₂O-flux sums from 2008 to 2015

Fig. 3.41 shows the measured N₂O-fluxes in Scheyern over a period of 7 years. The flux measurements were divided into summer and winter emissions. As these numbers refer to a half-year, the annual flux is equal to the sum of both winter and summer emissions. The emitted amounts of N₂O measured between 2008 and 2015 range over almost two orders of magnitude ($0.1 - 9.9 \text{ kg-N ha}^{-1}$). The dynamic range of emitted amounts of N₂O during summer is similar but slightly smaller ($1.2 - 8.3 \text{ kg-N ha}^{-1}$).

The measured N₂O-fluxes are not arbitrary distributed over time. A clear trend towards smaller amounts of N₂O emitted per half-year can be seen in the measurements. This downward trend notably occurs in wintertime (November-April). While in the beginning of the time series (2008/2009, 2009/2010, 2010/2011) the winter and summer emissions are more or less in the same range, winter emissions almost disappear in the last four years (2011/2012,

2012/2013, 2013/2014, 2014/2015). In 2008/2009, the amount of N₂O emitted in "summer" (1/2 year) was 7.3 kg-N ha⁻¹. The amount of N₂O emitted in "winter" was even higher with 9.9 kg-N ha⁻¹.

In 2009/10, emitted amounts of N₂O were 8.3 kg-N ha⁻¹ in summer and 4.7 kg-N ha⁻¹ in winter. After the first two years a significant decrease of N₂O-fluxes begins.

In 2010/2011, summer amounts are 4.3 kg-N ha⁻¹) and winter amounts are 5.0 kg-N ha⁻¹. In winter 2011/2012, 2012/2013 and 2013/2014 the winters emit very small amounts of kg-N ha⁻¹ (0.1 kg N₂O-N, 0.2 kg N₂O – N, 0.2 kg-N ha⁻¹. Summer emissions in the according three years are rather small 4.0, 1.2 and 1.4 kg-N ha⁻¹).

The measurement of the N₂O-trend is contrary to an investigation of (Grandy et al., 2006), who investigated measured fluxes from 1989 to 2002 and found no trend in N₂O-fluxes. However their resolution was weekly to monthly samples, which is probably inadequate for episodic measurements (Barton et al., 2015).

Fig. 3.41 (middle panel) shows the simulation for the boundary condition 1, where no influence of snow cover on soil frost was assumed in the model. The absolute values of the half-yearly sums are shown in the appendix in table H.1.

It is clearly visible that neither the decrease of the half-yearly sums of winter fluxes nor the decrease of summer fluxes is reproduced by the model. The highest observed winter fluxes (2008/2009) do not agree with the highest simulated winter fluxes. Also the smallest measured winter fluxes (2011/2012) do not agree with the smallest modelled winter fluxes for boundary condition 1 (2013/2014). The annual sums show a good agreement in 2010/2011. The NSE value of the half-annual sums is 0.14.

Simulated winter emissions for the boundary condition 2 were also highest in the first year (2008/2009), which is in agreement with the measurements. The lowest emissions in the simulations were found in 2011/2012, which is again in accordance with the measurements. However, the magnitude of the measurements is still far from the measured values. In particular, the high amounts of N₂O-N emitted in the first 3 years could not be captured by the model simulations.

The NSE value of the halfannual sum is lower than zero with this parametrisation. However with small changes in the parametrisation (e.g. changing the denitrification factor by 2.7), the NSE can be improved to 0.29.

In general, the implementation of an upper boundary condition which includes the impact of snow layer on the soil surface temperature is seen as a useful model extension as higher NSEs in the half-annual simulations can be reached.

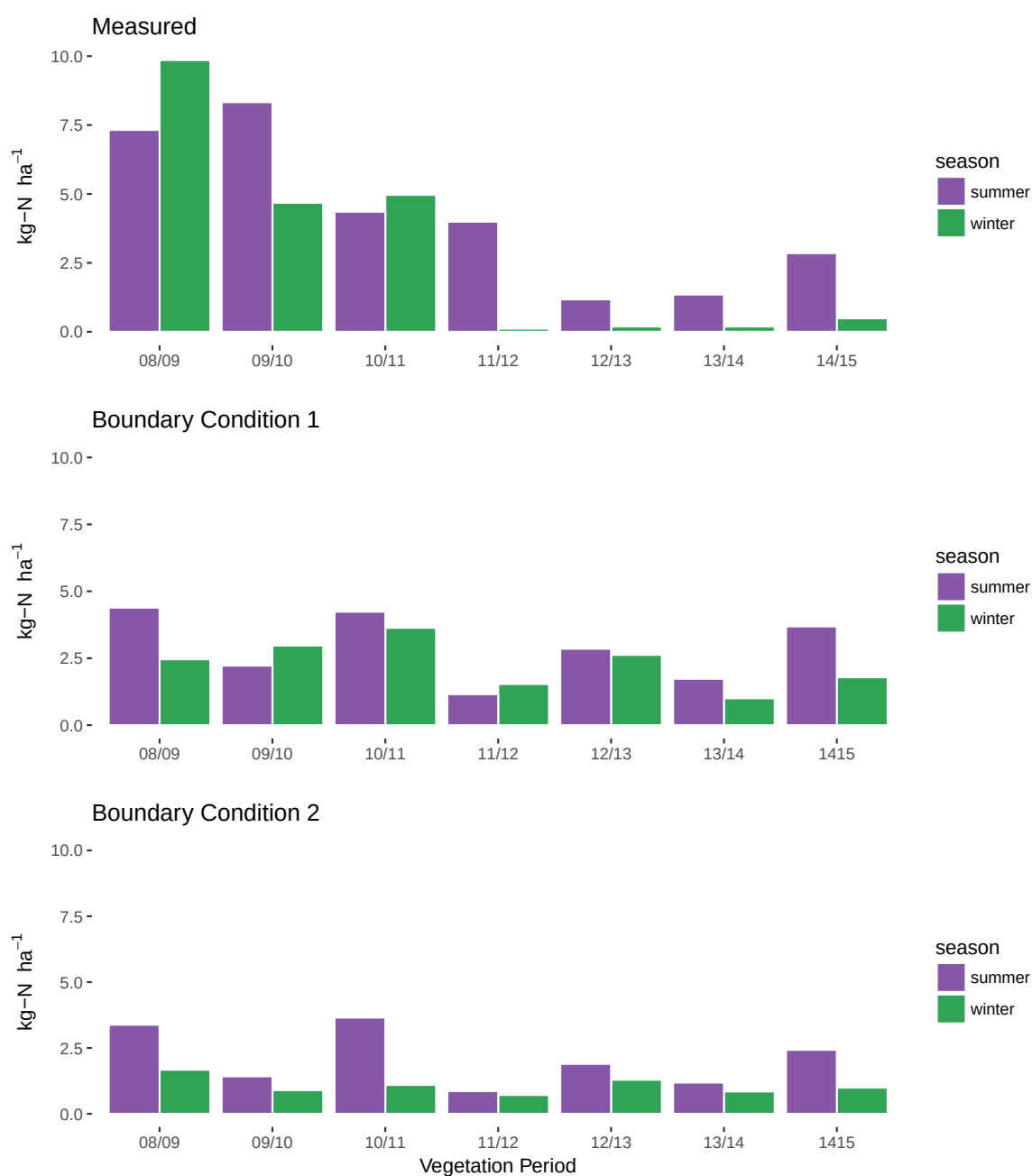


Fig. 3.41 Winter and summer emissions from 2008/2009 to 2014/2015. The amounts, which are emitted during summer are depicted in violet colour. The amounts, which are emitted during winter are shown in green colour. The upper panel depicts the measurements and the lower two panel depict the simulation results. The amounts of the half-yearly sums kgN₂O – Nha⁻¹

3.8.5 Evaluation of hourly simulations

Table 3.3 shows NSE values for N₂O simulations with boundary condition 1 show negative values in every winter from 2008/2009 to 2014/2015. The worst NSE value is -33.0, the best NSE-value is -0.17. In contrast to this, summertime NSEs are higher. The worst NSE value is -2.7 and the best NSE-value is 0.45.

The normalized root mean square errors lie between 75.3 and 193 for the winters from 2008/2009 to 2014/2015. The summer values are higher in all years except the years 2009/2010 and 2010/2011. In the latter mentioned years, the NRMSE values are slightly smaller.

The NSE values with boundary condition 2 are shown in Table 3.4. One can see that the NSE values during winter are better compared to BC1 in almost every winter and summer over the 7 years. Despite this it has to be noticed that the NSE values are still negative. Furthermore a NSE of approximately 0 is not as bad when most of measured values lie around the mean of the measurements.

As a general result one can conclude that the NSE values of the hourly values are worse than the NSE values of the half-annual sums. This is in accordance with a study of (Molina-Herrera et al., 2016). The model still needs improvements as almost all NSE values have values lower than 0. However, a decreasing NSE for decreasing time steps (months, weeks, days) in models is known. Daily NSE values show often only slightly better NSE values (Molina-Herrera et al., 2016). Therefore, it is not surprising that simulations with hourly time steps have NSE values around and under 0.

The same holds true for NO₃ values. In comparison to the model study of Molina-Herrera et al. (2016), who found within 6 sites thrice NSE values smaller than 0 and thrice NSE values between 0.13 and 0.28.

NSE values of simulated NO₃ values are mostly negative. The NSE values of most winters are very close to zero. The range of the winter NSE values for NO₃-N range from -2.83 to 0.60. The range of the summer NSE values reach from -18.0 to 0.12. From all 14 seasons 12 negative NSE values and 2 positive NSE values exist. The most positive value of all winter values is found during winter 2012/2013 with an NSE value of 0.60 and most positive value during summer 2010/2011 with an NSE of 0.12.

Furthermore, it was found that the water model has a massive impact on the simulations of the NO₃ values. This suggests that the NO₃-simulations could be further improved by choosing different water models with different parametrisations. However, it would be even more important to improve the water models in the unsaturated zone as many drawbacks still exist (see chapter 3.7.3).

Between boundary condition 1 and 2 no significant difference is found for the evaluation parameters for predicted NO_3 values. However with an implementation of water reduction by frost in the HYDRUS model a difference between boundary condition 1 and 2 in the NO_3 -statistics is to be expected.

Table 3.3 Boundary Condition 1: Shown are the evaluation parameters (NSE [-], NRMSE [%]) for N_2O and NO_3 for hourly simulations in both winter and summer. The parameters are calculated for the boundary condition 1, when snow cover was not taken into account.

	N_2O NSE winter	N_2O NSE summer	N_2O NRMSE winter	N_2O NRMSE summer	NO_3 NSE winter	NO_3 NSE summer	NO_3 NRMSE winter	NO_3 NRMSE summer
2008/09	-0.45	0.43	75.3	120.4	-0.42	-5.45	219.9	108.8
2009/10	-0.17	-0.34	115.4	108.1	-0.46	-18.02	377.6	111.9
2010/11	-0.39	-0.62	127.1	117.5	-1.48	0.12	84.1	147.3
2011/12	-12.40	-0.05	102.5	365.5	-1.08	-0.16	102.0	133.7
2012/13	-33.03	-2.75	193.2	582.3	0.60	-1.90	159.3	60.4
2013/14	-15.87	-0.04	102.0	410.0	-2.83	-0.30	109.3	188.0
2014/15	-3.82	-0.82	134.6	219.1	-0.02	-1.16	120.0	98.2

Table 3.4 Boundary Condition 2: Shown are the evaluation parameters (NSE [-], NRMSE [%]) for N_2O and NO_3 for hourly simulations in both winter and summer. The parameters are calculated for the boundary condition 2, when snow cover was taken into account.

	N_2O NSE winter	N_2O NSE summer	N_2O NRMSE winter	N_2O NRMSE summer	NO_3 NSE winter	NO_3 NSE summer	NO_3 NRMSE winter	NO_3 NRMSE summer
2008/09	-0.44	0.36	79.8	119.9	-0.43	-5.79	109.0	225.6
2009/10	-0.35	-0.41	118.6	115.8	-0.44	-15.46	110.9	351.4
2010/11	-0.16	-0.51	122.8	107.6	-1.48	0.20	147.3	80.2
2011/12	-2.11	-0.10	104.8	176	-1.08	-0.13	133.4	101.0
2012/13	-5.60	-1.27	150.3	256.5	0.59	-2.49	61.1	174.8
2013/14	-9.67	-0.01	100.3	326.1	-4.06	-0.28	216.1	108.8
2014/15	-0.31	-0.05	102.5	114.3	-0.02	-1.09	98.1	118.1

3.8.6 The winter of 2011/2012 as an example for the effect of snow on N₂O-fluxes

Fig. 3.42 a) shows that water simulations in 10 cm are almost not affected by using either boundary condition 1 (BC1) or boundary condition 2. It also does not make a difference whether soil water freezes or not (see Fig. 3.42 d). A missing water sink in the model implementation is obvious (see also 3.7.3). Fig. 3.42 b) shows the expected air temperature drop under zero degree in case of the first boundary condition 1 and permanent 0°C during snow cover in case of BC2.

N₂O-fluxes significantly improved (see Fig. 3.42 c) by implementation of boundary condition 2 (see chapter 2.4.5). The major effect behind this improvement in the simulation is seen in the prevention of unrealistic freeze-thaw peaks during snow cover and thus reduced soil frost (see Fig. 3.42 d).

An example for such a peak, which is not simulated due to the fact that snow cover exists, can be seen in the first two months of 2012 in Fig. 3.42. It is astonishing that a second peak in the time series, which is mostly due to a rapidly increased soil moisture content in the model simulation with BC1 also did not appear in BC2. The very few peak values could be modelled well with boundary condition 1. Moreover it is astonishing that in the winter 2011/2012 it seems as if neither BC1 nor BC2 is totally wrong as also in BC1 some peak values are simulated very good.

For further model improvements one should test the circumstances under which BC 1 or BC 2 might be right. Possible variables which are not regarded here are the exact snow height and also the effect of thawing as triggers for N₂O peaks instead of frost.

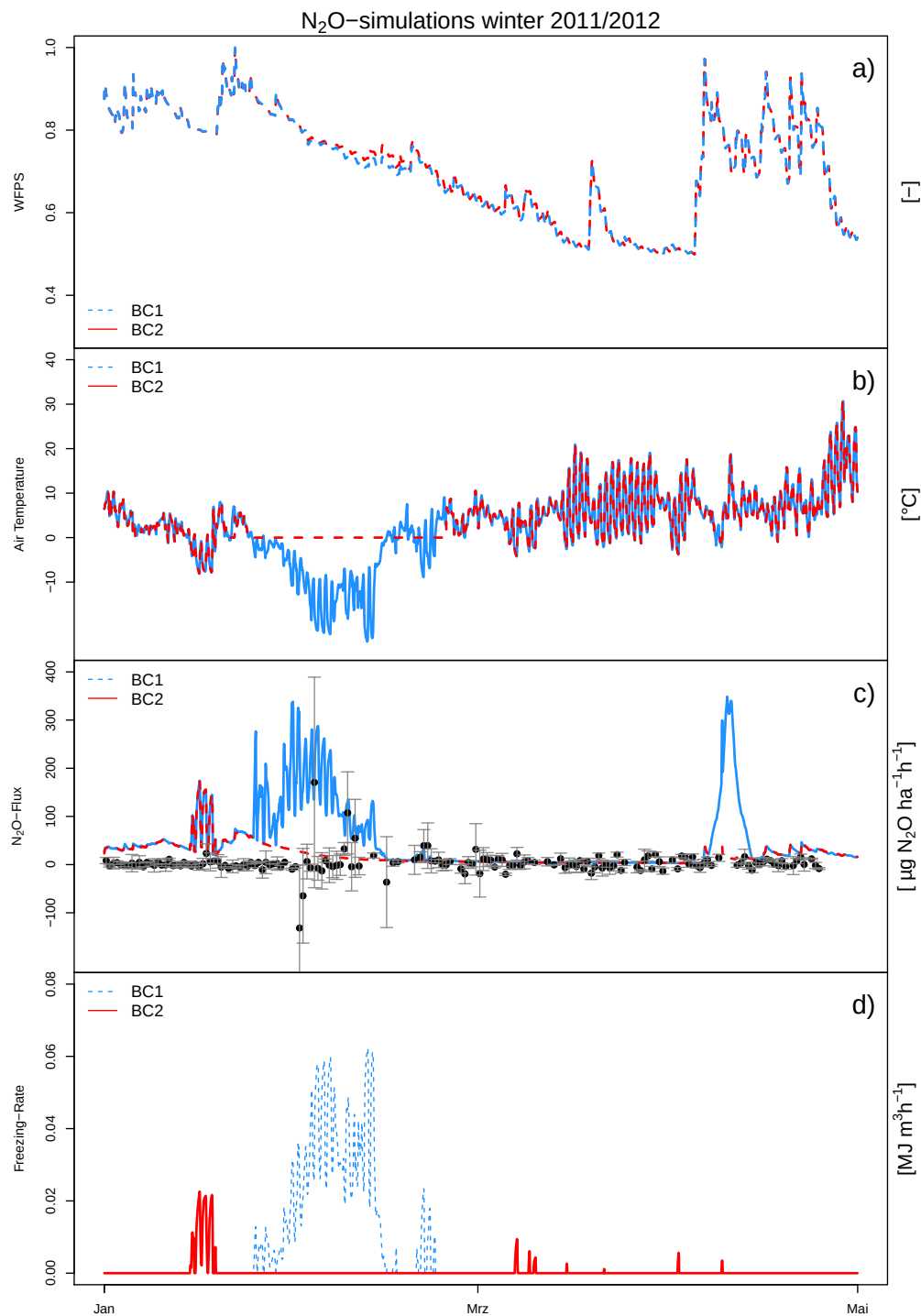


Fig. 3.42 N₂O simulation during winter 2011/2012. Water filled pore space (WFPS) in subfigure a) air temperature in b) N₂O-flux in c) and the simulated soil freezing rate in 10 cm

Chapter 4

Conclusions and Outlook

4.1 Measurement and modelling fluxes of Q_H , Q_E and CO_2 in complex terrain

Simple sorting scheme allows the investigation and modeling of ecosystem processes with limitations

At common eddy covariance sites data gaps for surface energy and NEE fluxes are reported to lie between 20% and 60% percent of the annual sums (Moffat et al., 2007). The complex setup in Scheyern leads to data gaps that lie around 70% for A17 and 90% for A18 (see chapter 3.3). Nevertheless, the data allows us to quantify the flux of energy and greenhouse gases from the two fields.

The simple sorting scheme (80%-footprint) proved to be a useful tool to split one time series into two time series. The sorted fluxes measured at the complex site gave similar results compared to sites that did not conduct their measurements in complex landscape (see chapter 3.4.1). However, the used approach has two main disadvantages: 1) a certain extent of data has to be dismissed because the footprint is a mixture of A17 and A18, and 2) a percentage (< 20%) of each single footprint can be located in another field with a different land use compared to A17 or A18.

NEE measurements in a complex cropland

Due to the setup, 6 main vegetation periods could be measured instead of 3 vegetation periods. CO_2 -fluxes of potato are less negative than winter wheat fluxes, which is in accordance with the measurements published in Moureaux et al. (2012). This is true for both fields, although

the data availability of (A17 = 25.4%; A18 = 8%) is very low (see also chapter 3.3.1). The uptake of maize in this study is comparable to that of winter wheat which is in contrast to literature values from North America, where maize is reported to have much higher annual uptake rates than winter wheat (Lokupitiya et al., 2016).

Energy flux measurements in extreme summers

Until 2015, the three measured years in this work contained the two hottest years on record in Scheyern (see chapter 1.1.2) and Germany as well. Both in the Q_E as well as in the Q_H high measurement values could be observed during all summers.

Special landuse can help to mitigate the impact of global and regional warming. As shown in table F.3 and F.4 only rotor harrowing was conducted. Harvest residues are left on the field. Davin et al. (2014) states that this management (crop residues and reduced tillage) can mitigate both the regional as well as the global warming effect. The global warming is mitigated by binding carbon in the soil (Davin et al., 2014). However, it has to be said that increased soil carbon can also trigger N_2O formation in soils. More full greenhouse gas balances in agroecosystems are needed to better understand the connection of management and climate warming effects.

A further positive effect of reduced tillage, which is probably more important is the increase of albedo and subsequently the decrease of soil temperature. The impact of this management is in fact lower than 1 °C if one regards longer time periods, but the cooling effect during very hot days is more than 2°C (Davin et al., 2014).

Considering initial aims of the FAM research farm, one can conclude, that a sustainable landuse according to energy fluxes was followed now for more than 25 years.

Model input and evaluation data

For model studies, the two mentioned problems in complex landscapes (see above) can be overcome by footprint weighted modelling. Simulated energy fluxes are obtained by simulating the flux as a sum of different fluxes, which are weighted by the modelled footprint contribution. This approach was already applied for two complex ecosystems. Kirschbaum et al. (2015) simulated fluxes of an assembly of differently managed pasture parcels and Biermann et al. (2014) simulated a complex landscape containing water surface and pastures. Recently, Klein (2018) showed for the fields A17 and A18 in Scheyern that footprint weighted modelling increases the comparability of model and measurement. Fluxes of Q_E and Q_H have been modeled for each sub-field (see Fig. 2.3) with the input data measured in this study. Subsequently the fluxes were weighted with the footprints calculated in this study and

compared to the original measurements. The weighted modelling improved the agreement between measurement and simulation results and could be shown for the first time in the case of croplands.

In a further study of (Heinlein, 2018), simulated latent heat fluxes which were simulated with a newly developed model could be evaluated.

Outlook: The weighted modelling for surface energy fluxes based on this data (Klein, 2018) provides already the parametrisation which could be used to study CO_2 -fluxes between two differently managed fields. The amount of data is seen as suitable. Until now, there is no study investigating NEE with footprint weighted modelling in croplands and only one study in grasslands (Kirschbaum et al., 2015).

It is seen as challenging to train a model in case of N_2O for both fields as the amount of available data from A18 is very limited. However footprint weighted simulations are seen as reasonable if enough data for model training and evaluation existed.

Measured bowen ratio shows consistent variability of land surface fluxes but is challenging to model accurately

The dynamics of the measured bowen ratio at mid-day could be consistently sorted according to their underlying source area. The main differences detected between the two fields in Scheyern are due to different plant development (ripening of plants) or management impacts (desiccation). As the mid-day bowen ratio shows the impact of land surface on energy fluxes so well, it is seen as a good measure to evaluate the bowen ratio of surface energy models.

Simulations of Q_E and Q_H have been excessively conducted since decades without dynamic vegetation (Arora, 2002). At the moment studies with dynamic vegetation show that they can either reproduce surface energy dynamics at the multi-annual time scale by showing averaged diurnal cycles (Krinner et al., 2005) or at the sub annual time scale by showing diurnal cycles of latent or sensible heat (Casanova and Judge, 2008; Klein, 2018).

In this study, the simulation of the bowen ratio proved to be a good measure to compare the dominance of either Q_E or Q_H in the simulations against measurements. However the simulation results in this study gave in many cases very high bowen ratios compared to the measurements, which has been reported before by (Lokupitiya et al., 2016), who states that Q_H is often overestimated in ecosystem models and Q_E is often underestimated.

For an improvement of the simulated energy fluxes and thus the simulated bowen ratio one should test the ability of footprint weighted simulations to better reproduce the bowen ratio. Furthermore improved LAI values and improved soil water simulations by preferential flow (Bogner et al., 2007) as well as improved micrometeorological steering parameters as canopy resistance and atmospheric resistance should be used for further model optimization. Furthermore this model run uses a one dimensional representation of plants. It is very likely that model performance will improve when the exact architecture of the plant is considered (Heinlein, 2018).

Energy balance closure is very similar and coupled to growth stages

The outcome of the investigation of the energy balance closure is that the energy balance is equally closed on both fields if one regards a longer temporal scale. With an EBC of 0.79 on both fields, the value obtained in this study is very similar to findings in other croplands. Stoy et al. (2013) calculated an average value of 0.78 ± 0.18 for 25 croplands. Furthermore, the study shows that different crop species and development stages (vegetative phase/generative phase) have different EBCs. We measured generally higher EBC with higher development stages. The highest energy balance closure however was measured during summer 2015 over maize, which is especially favourable for the modelling study of Heinlein (2018).

It is assumed that the closure of the energy balance can further be improved by enhancing the comparability of available energy (R_n-G) and measured fluxes (Q_E , Q_H). As we measured in a hilly landscape, some slopes are more or less exposed to the sun. Radiation measurements for both fields were only conducted at a single location next to the eddy covariance station. In order to increase the comparability of measured and modeled data, the available energy can be corrected according to the slopes. In a recent study Wohlfahrt et al. (2016) showed, that footprint-weighted slope corrected available energy data shows better closure values than the uncorrected equivalent in complex terrain.

As a general result, one can conclude that an energy balance closure of 0.79 is a good value for a site in such a complex terrain. This in turn is favourable for model studies, especially when the energy balance closure is as high as in case of maize in the year 2015.

4.2 Measurement of N₂O fluxes with the eddy covariance method and the modelling in complex terrain

Stationarity in measurements often not fulfilled

A major reason for the limited data availability in case of N₂O-flux measurements by the eddy covariance technique in complex terrain is the lack of stationary conditions. Up to 50 % of the data measured in May 2015 had to be discarded because of this problem. This is especially unfavourable as it was the month after the first of two fertilisations.

An option to overcome this problem could be flux calculation by wavelet transformation, which is not depending on stationary conditions. This method was already proposed by Desjardins (1977). Schaller et al. (2017) found excellent agreement of eddy covariance fluxes and fluxes obtained by wavelet transformation. The mentioned study was conducted with CH₄ which can show similar behaviour, i.e. non stationary conditions, as N₂O in this study.

Eddy covariance measurements of N₂O using a quantum cascade laser

The measured time series of N₂O-fluxes from 2014-11-01 to 2015-10-01 is up to now one of the longest time series known in croplands measured with the eddy covariance method. The first gap is in the beginning of February (see also Appendix, Fig. C.4). Soil measurements of N₂O show that high quantities of N₂O were formed during that time, however we do not know whether the N₂O was transported out of the soil. The second time period is in June. During that time the source area for the measurement was unfortunately over field A18 (see Appendix, Fig. C.7).

Observed N₂O-fluxes allows the investigation of abiotic drivers, notably atmospheric processes

From the literature, the relationship between WFPS and N₂O-fluxes is known. It is also known, that the maximum N₂O production during denitrification is not necessarily bound to a fixed value of water filled pore space, but rather to the water filled pore space at field capacity (Davidson et al., 2000).

In this study highest emission occurs between 60 and 80% water filled pore space. These findings are partially consistent with the literature

An explanation for the different WFPS optima is that the concept of water tension is more appropriate for N₂O emissions than WFPS. It has been proposed, that the maximum values

of N₂O emissions lie around field capacity by several authors. Also the DNDC model uses this relationship, because it sets the maximum N₂O emission to field capacity.

Besides the formation conditions of N₂O the transport conditions from the soil into the atmosphere are equally important. A major resistance against transportation of N₂O out of the soil can for example be a wet soil crust which limits N₂O diffusion very effectively (Bakker and Hidding, 1970).

Besides WFPS, N₂O-fluxes are influenced by temperature. In 2015, N₂O-fluxes are more bound to air temperature than to soil temperature measurements. Freezing was only superficial in 2015 (see also chapter 3.5.3). This could be seen in better correlations between N₂O-fluxes at 0 °C air temperature. N₂O-fluxes did not correlate with soil freezing in 10 cm depth. This superficial freezing is in contrast to the literature, where 46% of the annual emissions are reported for December and January for the field A18 (Flessa et al., 1995).

In addition the influence of stratification on land-surface fluxes is a key component of fluxes between land surface and air (Monin and Obukhov, 1954). In micrometeorological models, the influence of stratification is introduced since the late 1970ies (Eugster and Hesterberg, 1996; Garland and Monteith, 1977; Louis, 1979). Accordingly, Denmead (2008) showed in a previous study how different ventilation or no ventilation might bias static chamber measurements.

Neural network successfully applied to fill measurement gaps

A neural net was applied to fill the measurement gaps between eddy covariance measurements of N₂O. The same type of network was already successfully applied to eddy covariance fluxes measurements of CH₄ before (Dengel et al., 2013). In Fig. 3.37 both a daily cycle can be seen in the ANN as well as in the measured data. The neural network with multiple hidden layers proved to predict N₂O-fluxes with an NSE of 0.12 at the hourly time scale. The benefit from this is that the annual sums are more accurate than the simple averaging approach.

The disadvantage of neural networks is that although very good fits can be achieved, the neural networks resemble black boxes and an understanding about the processes is not easily possible (Feraud and Clerot, 2002). In the future a sensitivity analysis of the drivers of the neural net could be conducted. If a neural net is further used this sensitivity analysis of the differently weighted input parameters could be done e.g. by "Garson's algorithm" (Olden and Jackson, 2002). However this is not possible with all kinds of neural nets.

Furthermore other machine learning techniques such as boosted regression trees or random

forest models could be used.

Modelling eddy covariance measurements of N₂O-fluxes with Expert-N 5.0:

A model study with hourly resolution was successfully conducted with the measured driver data at field A17. The magnitude of the measurements and the simulations of Expert-N is approximately within the same range. Furthermore the beginning of the hot moments of N₂O-formation could be simulated very accurately. Also the duration of fertilisation events was modelled with the accuracy of very few days.

The model could not capture the diurnal variations of the N₂O-flux. This is reasonable as the model was developed on basis of automatic chamber measurements that cannot resolve a diurnal cycle. Future attempts to further develop the nitrous oxide formation model in Expert-N 5.0 should also include variations of the diurnal patterns. As a reproduction of the diurnal cycle was already possible using the neural network (see chapter 3.7.4) it is assumed that the additional measurements in Scheyern contain the relevant data and model development can be conducted based on the newly gathered high resolution N₂O data in Scheyern.

Model improvements should not only include an improvement of N₂O formation but also improve the transport of N₂O from to the atmosphere. First, the more mechanistic transport model of N₂O from the soil should be used also for Expert-N 5.0 instead of the emit all function, as it is known that diffusion is limited in the case of a wet soil crust (Bakker and Hidding, 1970). A more mechanistic model for N₂O transport was already tested for Expert-N 3.0 by Klier et al. (2011). A further control on the transport of N₂O is atmospheric stability. This can be for example introduced by a resistance approach according to Eugster and Hesterberg (1996). However a limitation for all modelling approaches of N₂O-fluxes will be the high measurement errors.

4.3 Modelling N₂O-fluxes of seven years obtained by the automated chamber method

Decreasing longterm trend is not reproduced by the model

A clear reason for the decreasing longterm trend of N₂O fluxes in the 7 year time series (see Fig. 3.41, upper panel) cannot be found. Also the model did not reproduce the dynamics of the decreasing N₂O emissions.

It is possible that the weather conditions which were very warm and dry in the summers created bad conditions for denitrification and therefore reduced N_2O -fluxes in summer. A decrease of N-min in the measurements cannot be seen although the fertilisation was low. For further insights into the dynamics of N_2O emissions also further treatments that were conducted at the automated chamber site should be taken into account. Additionally, three analogous datasets for lower fertilisation and different management (no till) exist that cover the same time period. Management is known to be a major steering parameter for longterm dynamic of NO_3 and N_2O -fluxes.

Furthermore, these measurements can be completed with N_2O -flux measurements that were conducted since the 1990ies. This in turn would be a unique N_2O time series in the literature for any ecosystem.

For model studies, the underlying time series is already a very long time series with good resolution. Further development of the submodels in Expert-N 5.0 are seen as a possibility to gain an understanding of the observed decreasing longterm trend. A better modelling of the water contents during freezing in winter or during time periods with preferential flow in summer is seen as a crucial task. Furthermore, soil structure and microbial activity are not taken into consideration yet. A further simplification of the model is, that all models are 1-D models.

Included snow cover improves simulation of N_2O -fluxes

It can be concluded from the simulations in chapter 3.8.3, that snow cover is a main control on soil freezing in every winter from 2008 to 2015.

In future studies the focus should lie on developing a more accurate N_2O formation model as a very complete data basis was put together in this study. A possibility to further improve winter flux simulations is to investigate the correlation of exact snow height and the occurrence of N_2O -fluxes. In some years of the modelling study (see Fig. 3.42) both applied boundary conditions seem to reproduce N_2O -fluxes well for some cases. A different insulation effect of the soil dependent on more or less thick snow heights was already mentioned in Yu et al. (2016).

A changed temperature at the soil surface (0°C) due to snow cover also improved the halfyearly simulation results in 6 of 7 winters. However, the magnitude of the frost thaw peaks cannot be simulated with the exactly same model which is used during summertime. It was furthermore observed that half yearly sums could be simulated with NSE values of 0.14 (BC1) and 0.29 (BC2) respectively if one allows a minor change in the model configuration

in the second case (see chapter 3.8.4).

In order to further improve simulation results a more sophisticated frost thaw model should be implemented in Expert-N 5.0. Important in this context are improvements by reduced water content in the soil while the soil is freezing.

In this simulation, the "emit all approach" for N_2O -transport from the soil into the atmosphere was chosen. This is a very simple approach. In the further development of the Expert-N model the more sophisticated soil transport-scheme used in Klier et al. (2011) might also improve the simulation results.

4.4 Comparison of automated chamber versus eddy covariance method

In this study enhanced daytime eddy covariance fluxes of N_2O were found during May and June, after fertilisation, when nitrogen supply was high. The eddy covariance flux values before the fertilisation period happened during the early morning hours. In contrast to eddy covariance measurements increased flux values were not detected for averaged diurnal cycles of automated chamber measurements in this study.

The existence of a diurnal cycle, which was already stated by Blackmer and Cerrato (1986) is especially important for the annual sum of greenhouse gases (Ruser et al., 1998). Ruser et al. (1998) already discussed the meaning of enhanced daytime values for annual budgets of N_2O -fluxes. In his study diurnal cycles were measured after desiccation in August with the automated chamber method. Ruser (1999) shows the correlation between temperature and N_2O emissions.

In a study of Shurpali et al. (2016) the diurnal cycles are measured with eddy covariance during winter and summer. They found that wintertime N_2O -fluxes are higher during night. Summertime N_2O -fluxes are higher during day, which agrees with our study as far as data is available. In the study of Shurpali et al. (2016) nitrogen availability and the role of plants is seen as the major reason for the reverse diurnal patterns, which is supported by isotopic analyses. Shurpali et al. (2016) and already Blackmer and Cerrato (1986) describe tight connection of the diurnal patterns of root exsudations of C and the microbial activity. Meanwhile further studies also suggest plants as drivers for N_2O -fluxes.

In the future it is recommended to rethink the possibility to model the microbial activity in soils. If the evidence of the role of plants is increasing in further studies it could be rewarding

to implement the microbial activity as a function of plant activity and their possibility to provide root exudates to the soil.

Comparison of annual sums

N₂O-fluxes measured with the automated static chamber method are higher than N₂O measurements measured with the EC-method (0.45/0.05 kg-N ha⁻¹). In addition, both automated chamber and eddy covariance measurements gave much smaller measurement values during winter compared to values found in the literature.

Current findings in the literature describe differences between chamber measurements and eddy covariance measurements for several gases (Laville et al., 1999; Podgrajsek et al., 2014; Riederer et al., 2013; Wang et al., 2013). Yet, the fact that the measurements by both measurement methods are in the same range is already an important information.

Chapter 5

Abstract

Currently 12% of the terrestrial land on planet earth is covered by primary intensively managed crops and their area is further increasing. According to the aims of TERENO (terrestrial environmental observatories), this work was designed to both study the influence of croplands on climate and to study the influence of climate on croplands, especially their biogeochemical fluxes. Therefore, eddy covariance measurements and model simulations were conducted. Additionally, long-term automated chamber measurements were used to study greenhouse gas emissions during 7 winters with differing soil freezing.

Eddy covariance (EC) measurements of N_2O were conducted for 12 months. EC-measurements of Q_H , Q_E and CO_2 -fluxes were conducted for 33 months. A special focus of the measurements work was the feasibility of the flux measurements in this complex terrain, as the measurement station was established between two adjacent fields. An outcome of this part of the work was, that the setup is suitable to detect seasonal and multi-annual patterns of CO_2 , Q_H and Q_E for two fields during the same observation period. Energy balance closure as well as energy flux partitioning (bowen ratio) was found to be dependent on the growth stages of plants. The data, gathered in this work, was already used to further develop surface energy flux simulations within the software framework Expert-N (Heinlein, 2018; Klein, 2018).

As one of the core tasks of this work, N_2O -fluxes with the eddy covariance method were measured for the first time between two croplands. Spectral analysis of the measured fluxes showed that turbulent exchange between land surface and atmosphere can be captured with this measurement setup. However a drawback of this setup is that stationarity conditions are often not fulfilled in case of N_2O -measurements between two fields. A possible solution of this problem might be data analysis via wavelet analysis instead of eddy covariance analysis. The obtained N_2O -fluxes measured by the eddy covariance method showed a consistent

behaviour according to well known drivers as water filled pore space or soil temperature. Frost thaw effects were found to be due to superficial frost in the year 2014/2015. As the eddy covariance method is an *in situ* measurement method also atmospheric controls on N₂O-fluxes could be observed. Under labile and neutral stratification higher N₂O-fluxes were observed as under stable stratification.

Simulations of N₂O with the ecosystem model Expert-N showed that the model successfully captures the seasonal variability in the measurements. However diurnal variations were not reproduced in the model and the NSE for hourly simulations was low. In contrast to the process based model, a fitted artificial neural net could reproduce the diurnal cycle. The main profit of the fitted neural network was the possibility to fill measurement in order to calculate gaps to calculate an annual sum of N₂O emissions. The annual sum was 0.21 kg-N ha⁻¹m⁻², which is one order of magnitude smaller than the value obtained by the default emission factor of the IPCC for fertilized croplands.

Half-yearly comparisons between static automated chamber measurements and EC measurements of N₂O show that fluxes from croplands in Scheyern are permanently decreasing, which fits to the low measurement values in Scheyern with the EC method. Both winter sums of static chamber and eddy covariance measurements are with 0.48 kg-N ha⁻¹ and 0.04 g-N ha⁻¹ significantly under 1 kg-N ha⁻¹ and approximately within the same measurement range. Thus it can be concluded, that the measurements conducted with the eddy covariance are reliable within the boundaries of the described limitations such as the availability of measurements.

Simulations of N₂O-fluxes measured with automated chambers showed that an inclusion of the effect of snow on the upper boundary condition of the soil is relevant for the accuracy of N₂O-flux simulations. However the model should be further developed in order to simulate the absolute winter and summer sums more correctly.

Together the measurement and modelling results of N₂O-fluxes highlight the importance of long time measurements of greenhouse gases, for a better evaluation of model simulations on the multi-annual scale. At the moment, Expert-N does not reproduce multi-annual trends correctly. Both high resolution data obtained by the eddy covariance method and multi-annual chamber measurements would be ideally suited to develop a new N₂O formation model. Moreover, short time measurements can be put into context with longer time series. The different measurement and modelling experiments also show that Expert-N should be further improved to also reproduce the diurnal cycles of N₂O-formation.

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Appendix A

Mean monthly temperatures and precipitation from 2013 to 2015

Table A.1 shows the mean monthly temperatures and precipitation compared to the multi-annual mean from 1991 to 2015. The 3- years measurement was measured in the course of this work. The longer time series is a compilation from several time series recorded directly in Scheyern and in the proximity of Scheyern.

T2 [°C]	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	mean
2013 [°C]	0.0	-1.6	1.1	8.7	11.6	15.2	20.3	18.2	13.4	9.8	4.0	1.5	8.6
2014 [°C]	1.8	3.3	6.7	10.4	12.4	17.3	18.8	23.9	18.7	13.3	6.9	3.2	10.1
2015 [°C]	1.5	-1.4	5.1	9.0	13.6	17.3	21.4	21.0	13.3	8.3	7.1	4.4	10.1
1992-2015 [°C]	-0.6	0.0	4.0	8.4	13.1	16.3	18.0	17.6	12.9	8.5	3.6	0.4	8.6
ΔT2 [°C]	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	mean
2013 [°C]	+0.7	-1.6	-2.8	+0.3	-1.5	-1.1	+2.4	+0.6	+0.6	+1.3	+0.4	+1.1	+0.1
2014 [°C]	+2.5	+3.2	+2.7	+2.1	-0.7	+1.0	+0.8	-1.2	+1.3	+2.7	+1.9	+2.7	+1.6
2015 [°C]	+2.2	-1.4	+1.2	+0.6	+0.5	+1.1	+3.4	+3.3	+0.4	-0.3	+3.5	+4.0	+1.6
Precipitation [mm]	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	ΣYear
2013 [mm]	22	21	21	42	117	140	18	86	80	58	56	5	665
2014 [mm]	49	8	12	20	130	38	154	92	61	83	41	44	732
2015 [mm]	81	11	35	57	109	114	31	36	38	39	63	3	617
1992-2015 [mm]	42	32	53	50	84	98	104	91	63	58	53	48	778
Δ Precipitation [mm]	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	ΣYear
2013 [mm]	-20	-11	-33	-8	33	42	-86	-5	17	0	2	-42	-113.1
2014 [mm]	6	-23	41	-30	42	-61	50	1	-2	25.2	-12.1	-3.8	-45.6
2015 [mm]	38	-21	-19	-7	25	16	-73	-55	-25	-19	10	-44	-161

Table A.1 Average temperatures and precipitation for every month from 2012 to 2015 are shown. Additionally the deviation from the average values are calculated. This average value is calculated from the 24 years time series that was put together for Scheyem during this work.

Appendix B

Median values of EC measurements

B.1 NEE-minimum median values of hourly averaged diurnal cycles

Table B.1 Minimum median values of NEE, CO₂ uptake is given as $\mu\text{mol m}^{-2}\text{s}^{-1}$

	04	05	06	07	08	09	10
2013 (PT)	-0.003	-0.011	-0.012	-0.015	-0.007	-0.006	-0.010
2014 (WW)	-0.020	-0.029	-0.022	-0.008	-0.002	-0.011	-0.016
2015 (MZ)	-0.011	-0.001	-0.013	-0.024	-0.013	-0.005	-0.004

Table B.2 Minimum median values of NEE. CO₂-uptake is given as $\mu\text{mol m}^{-2}\text{s}^{-1}$

	04	05	06	07	08	09	10
2013 (WW)	-0.005	-0.026	-0.033	-0.021	-0.001	-0.014	-0.011
2014 (PT)	-0.001	-0.0001	-0.008	-0.022	-0.024	-0.013	-0.001
2015 (MZ)	-0.018	-0.048	-0.029	-0.018	-0.001	-0.002	-0.004

B.2 Maximum and minimum hourly median values of Q_H -fluxes

Table B.3 Maximum median values hourly averaged diurnal cycles of Q_H from A17. The measurement values are given in $Wm^{-2}s^{-1}$.

	04	05	06	07	08	09	10
2013 (PT)	87.1	66.2	96.4	105.9	131.6	62.7	22.8
2014 (WW)	67.6	42.4	101.5	98.1	184.4	54.9	47.2
2015 (MZ)	153.2	95.6	94.1	92.3	128.5	116.7	41.4

Table B.4 Minimum median values hourly averaged diurnal cycles of Q_H from A17. The measurement values are given in $Wm^{-2}s^{-1}$.

	04	05	06	07	08	09	10
2013 (WW)	51.7	55.5	84.9	114.6	221.5	192.6	68.0
2014 (PT)	198.2	131.3	124.4	78.0	86.4	45.0	48.7
2015 (WW)	111.9	73.1	67.8	269.3	254.4	184.9	61.2

B.3 Maximum and minimum median values of Q_E -fluxes

Table B.5 Maximum median values hourly averaged diurnal cycles of Q_E from A17. The measurement values are given in $\text{Wm}^{-2}\text{s}^{-1}$.

	04	05	06	07	08	09	10
2013 (PT)	189.5	168.0	264.9	212.8	159.1	136.5	69.8
2014 (WW)	130.9	196.1	276.7	165.5	150.6	149.6	122.5
2015 (MZ)	120.9	226.3	210.1	237.4	185.5	98.5	61.9

Table B.6 Maximum median values hourly averaged diurnal cycles of Q_E from A18. The measurement values are given in $\text{Wm}^{-2}\text{s}^{-1}$.

	04	05	06	07	08	09	10
2013 (WW)	135.2	251.2	368.5	326.1	150.2	116.3	122.6
2014 (PT)	100.9	237.6	262.1	323.8	313.0	128.7	152.3
2015 (WW)	238.5	330.7	370.4	336.8	104.5	106.8	74.4

Appendix C

Measured N₂O-fluxes with the eddy covariance technique and measured drivers

In contrast to Fig. 3.24 N₂O-fluxes and the drivers are depicted over a shorter time scale of one month.

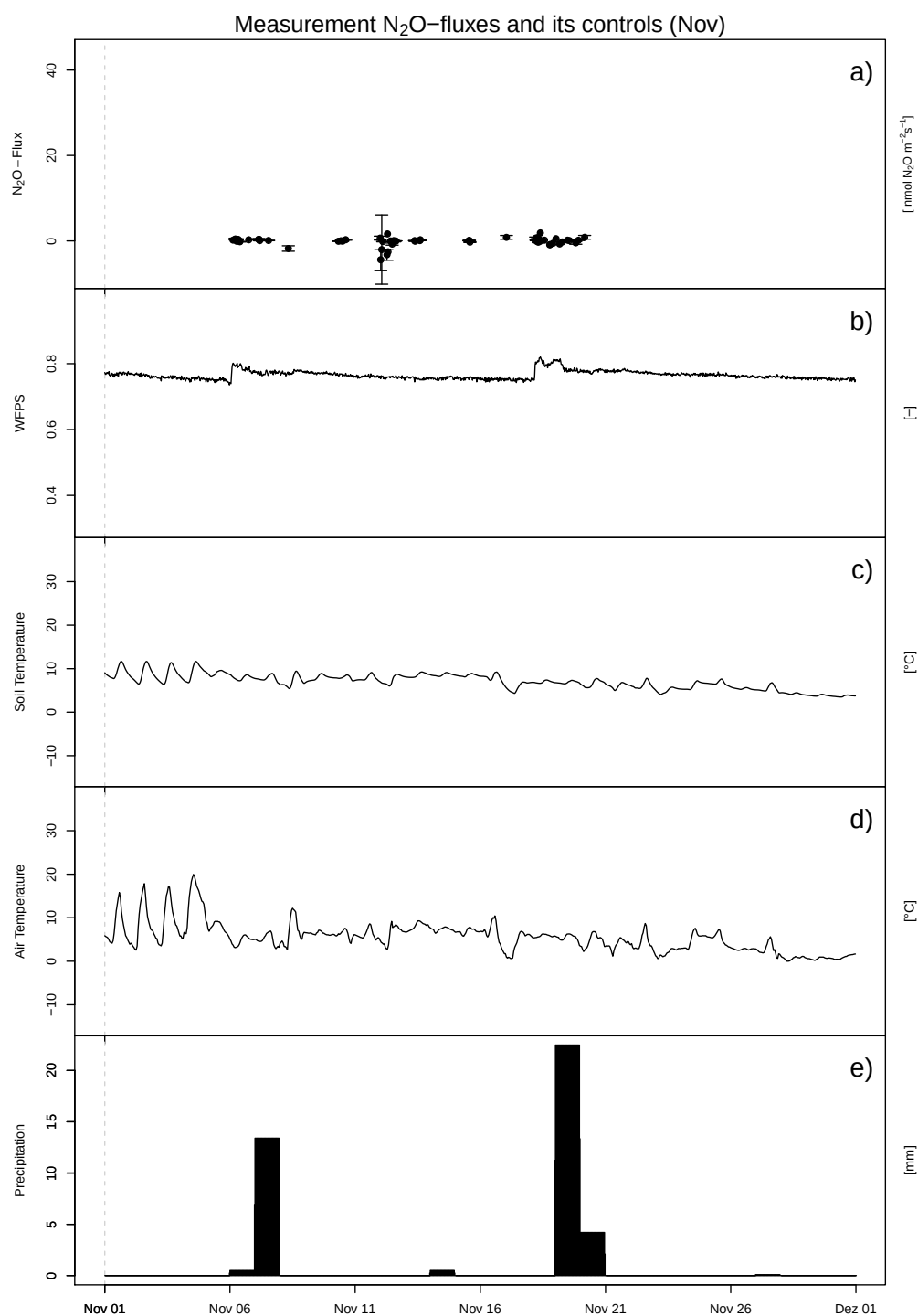


Fig. C.1 In November, almost all emissions are close to the baseline. The deviation of N_2O in the middle of November shows no relationship to the drivers in the lower panels.

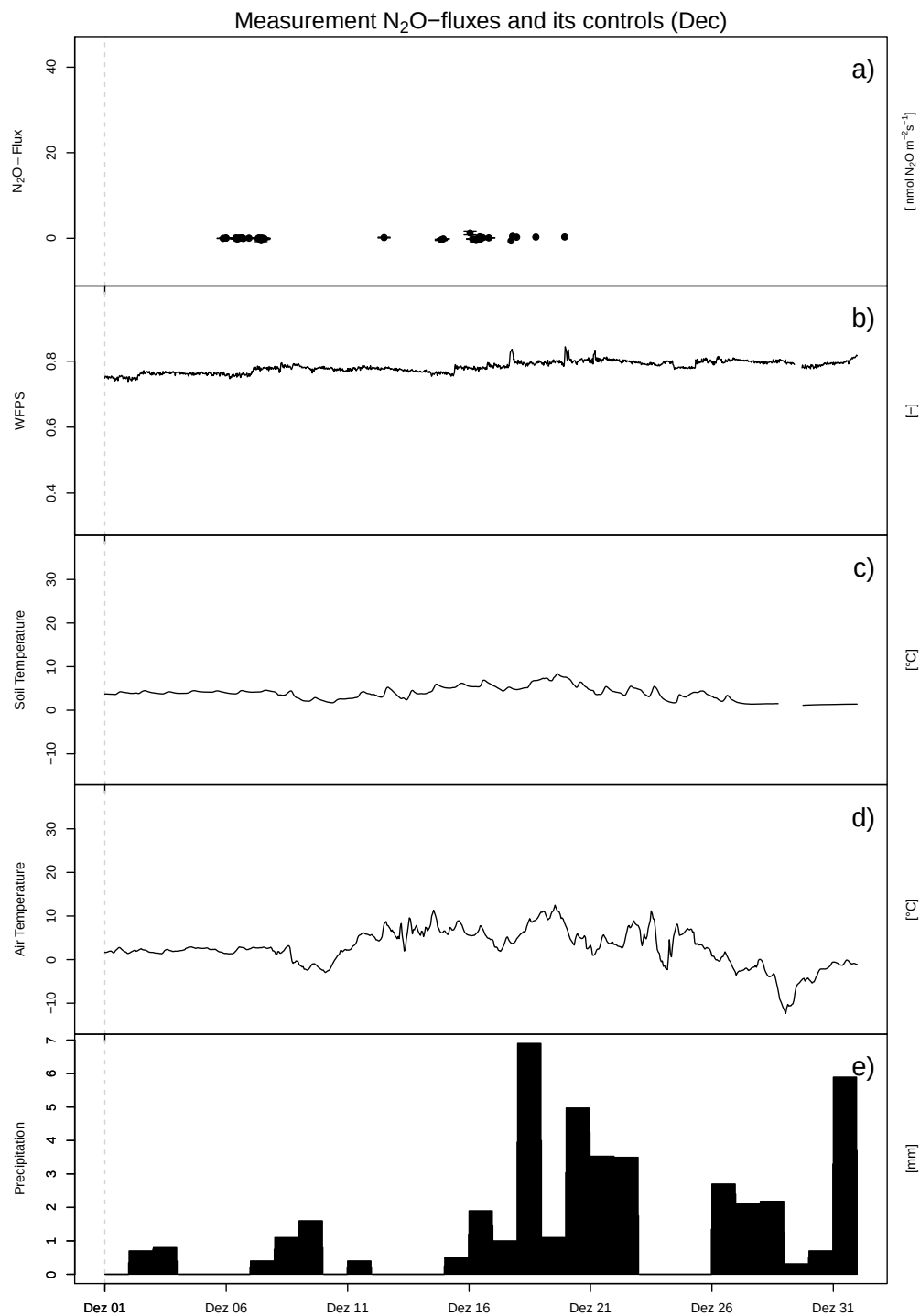


Fig. C.2 During December only low fluxes were observed. In the the second half of December no fluxes were measured due to no energy supply at the EC-site. The precipitation at the end of December fell as snow.

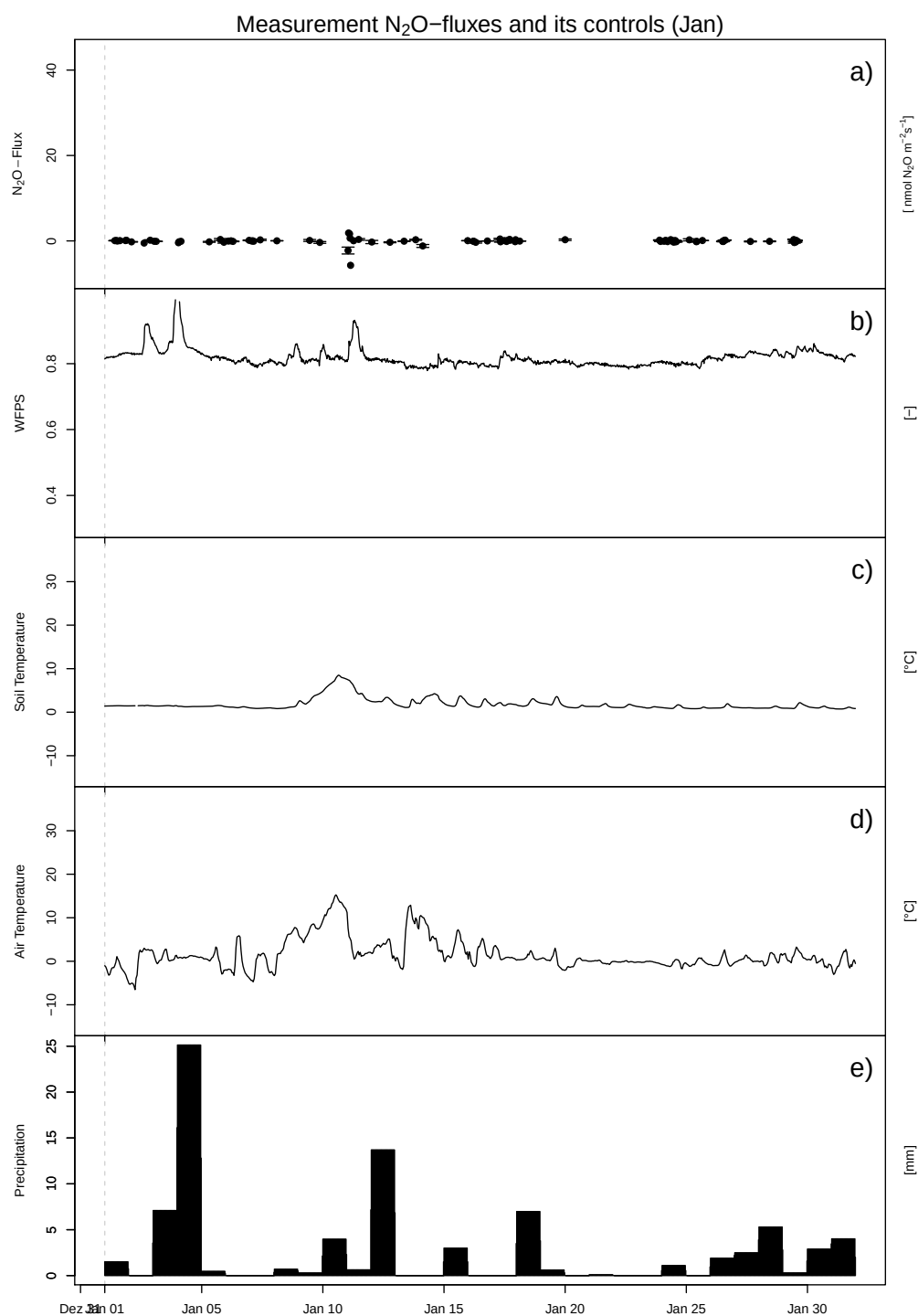


Fig. C.3 Also in January mostly low fluxes were observed. The time periods with 0°C are due to snow cover on wet soil at the same time.

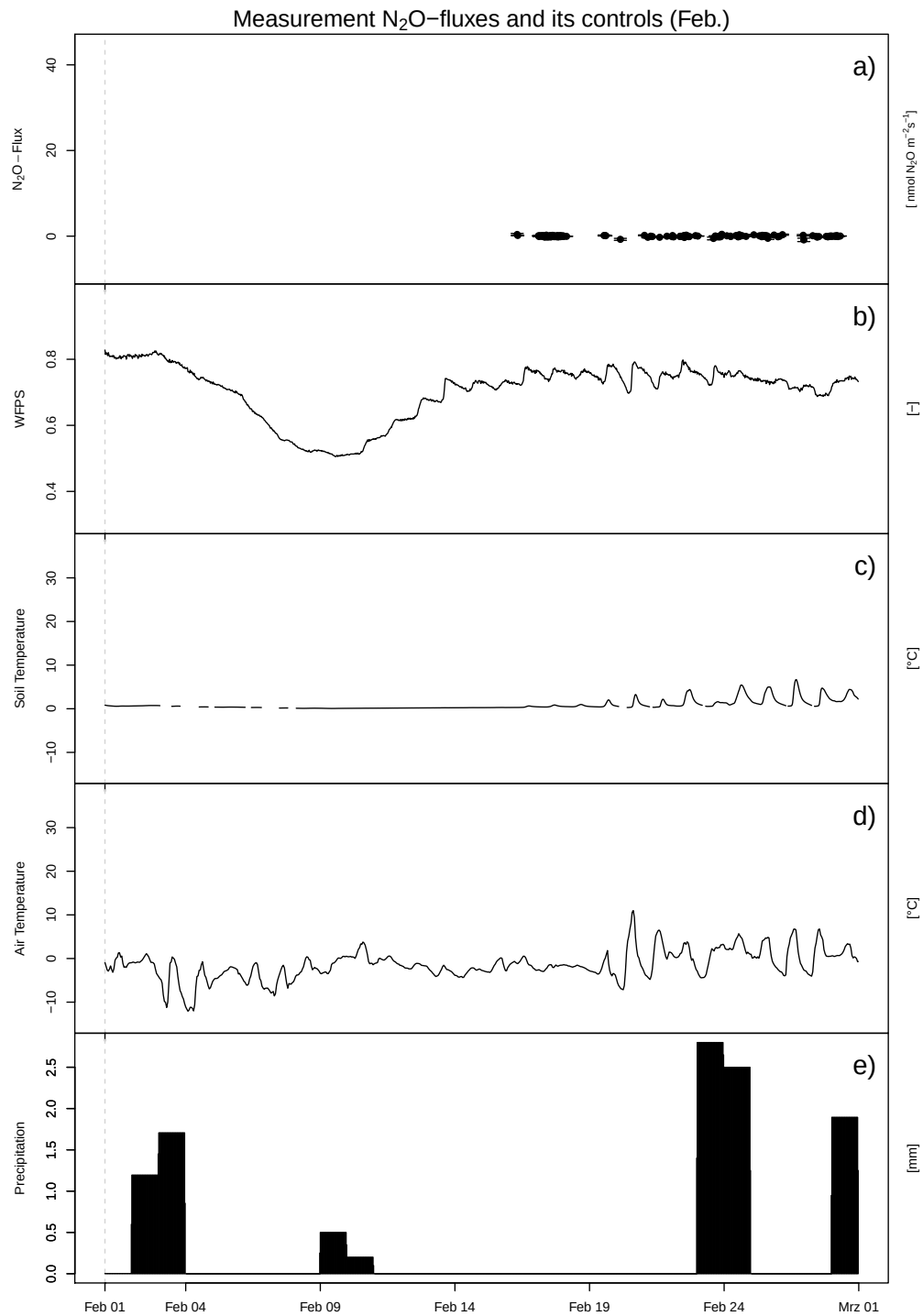


Fig. C.4 In February no fluxes were measured. The existence of N₂O-fluxes in the beginning of February when no measurements exist is speculative as we know from soil gas measurements show that N₂O is formed in all depths (see Fig. E.3 in the Appendix)

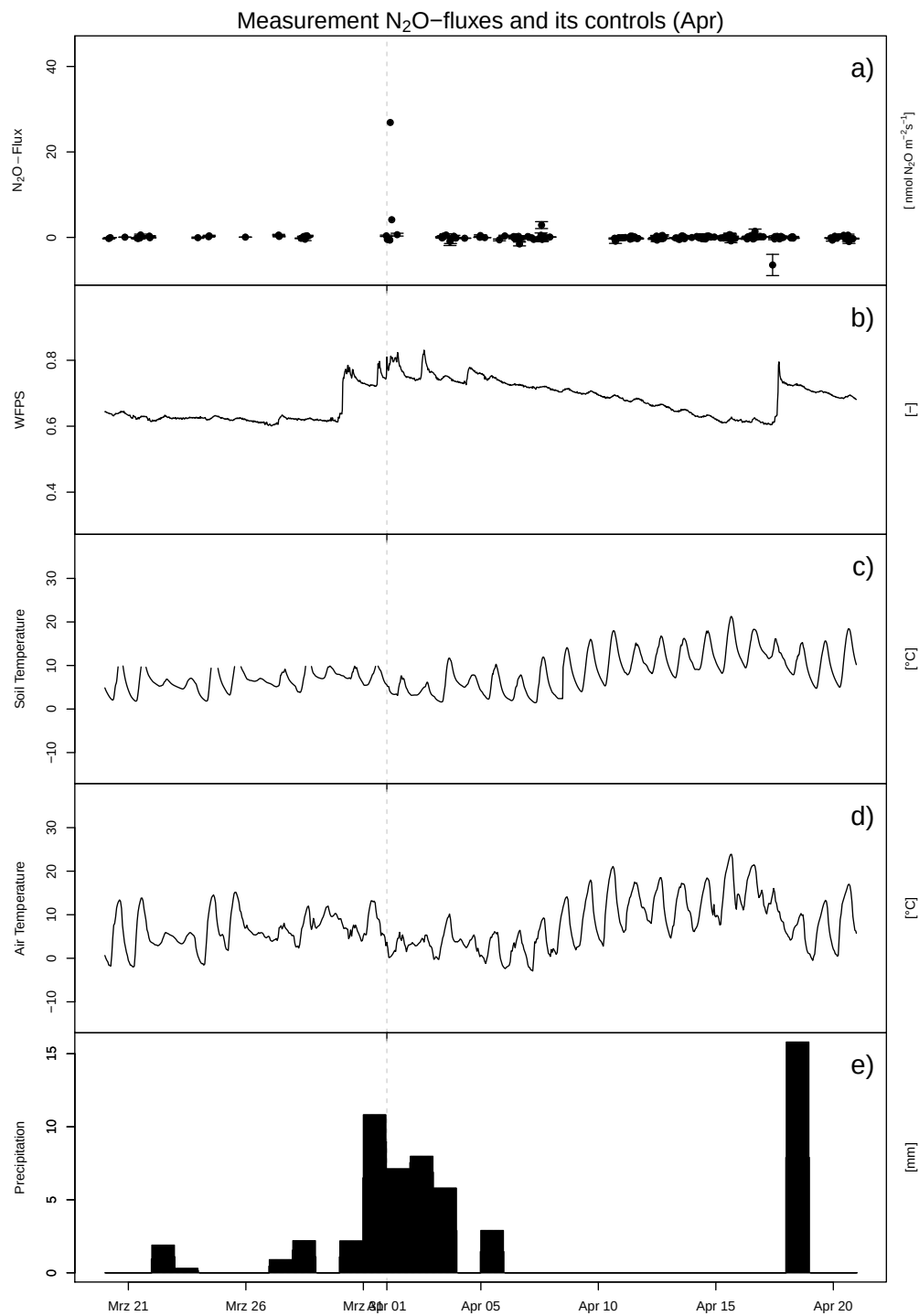


Fig. C.5 In April two high fluxes of N_2O are measured. Rapid change of water content and 0 $^{\circ}\text{C}$ air temperature are seen as the responsible drivers.

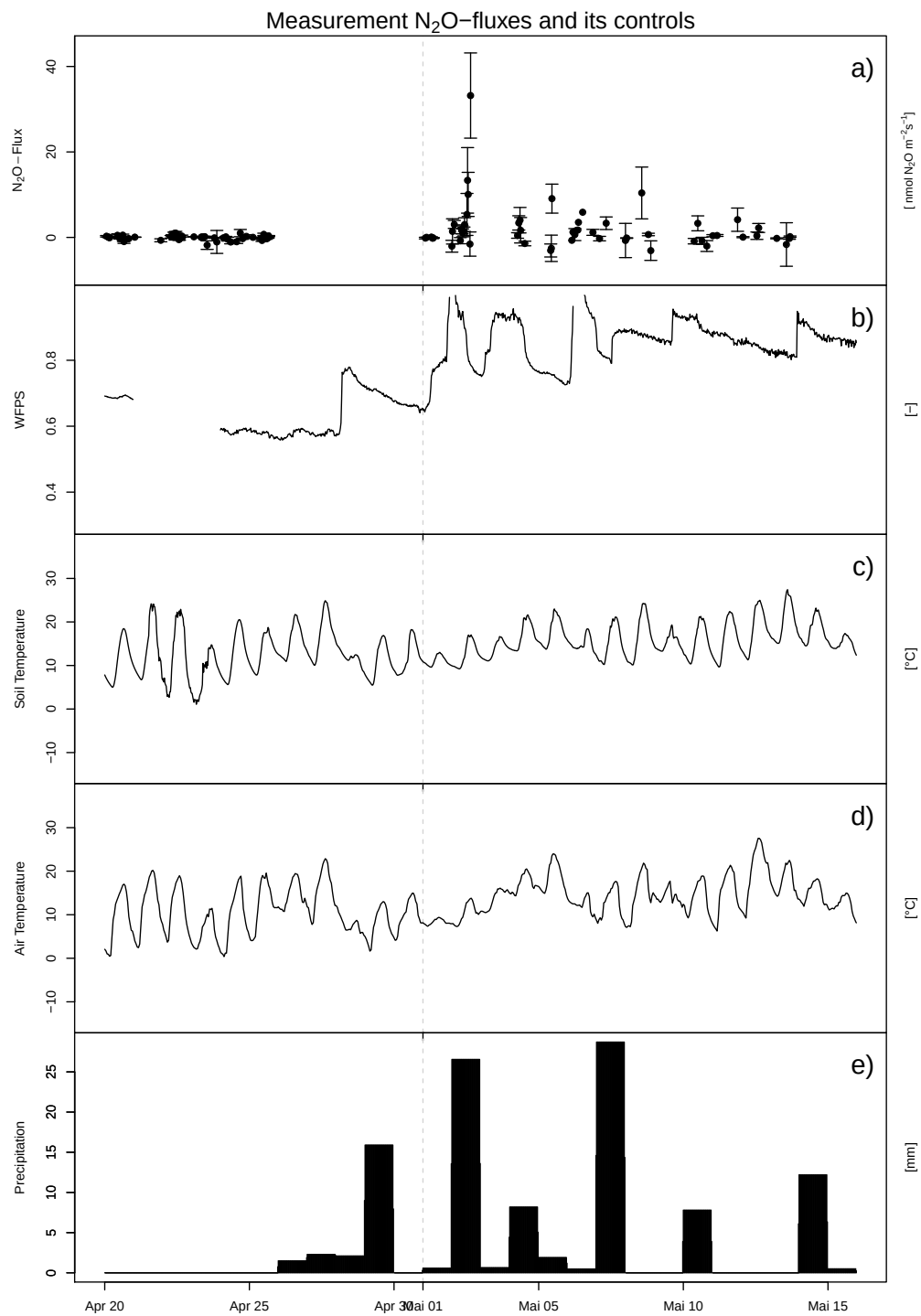


Fig. C.6 The highest N₂O-flux peaks were measured after the 1. fertilisation in the vegetation period (93 kg, NPK-fertiliser, 2015-04-15). The highest values occurred during daytime.

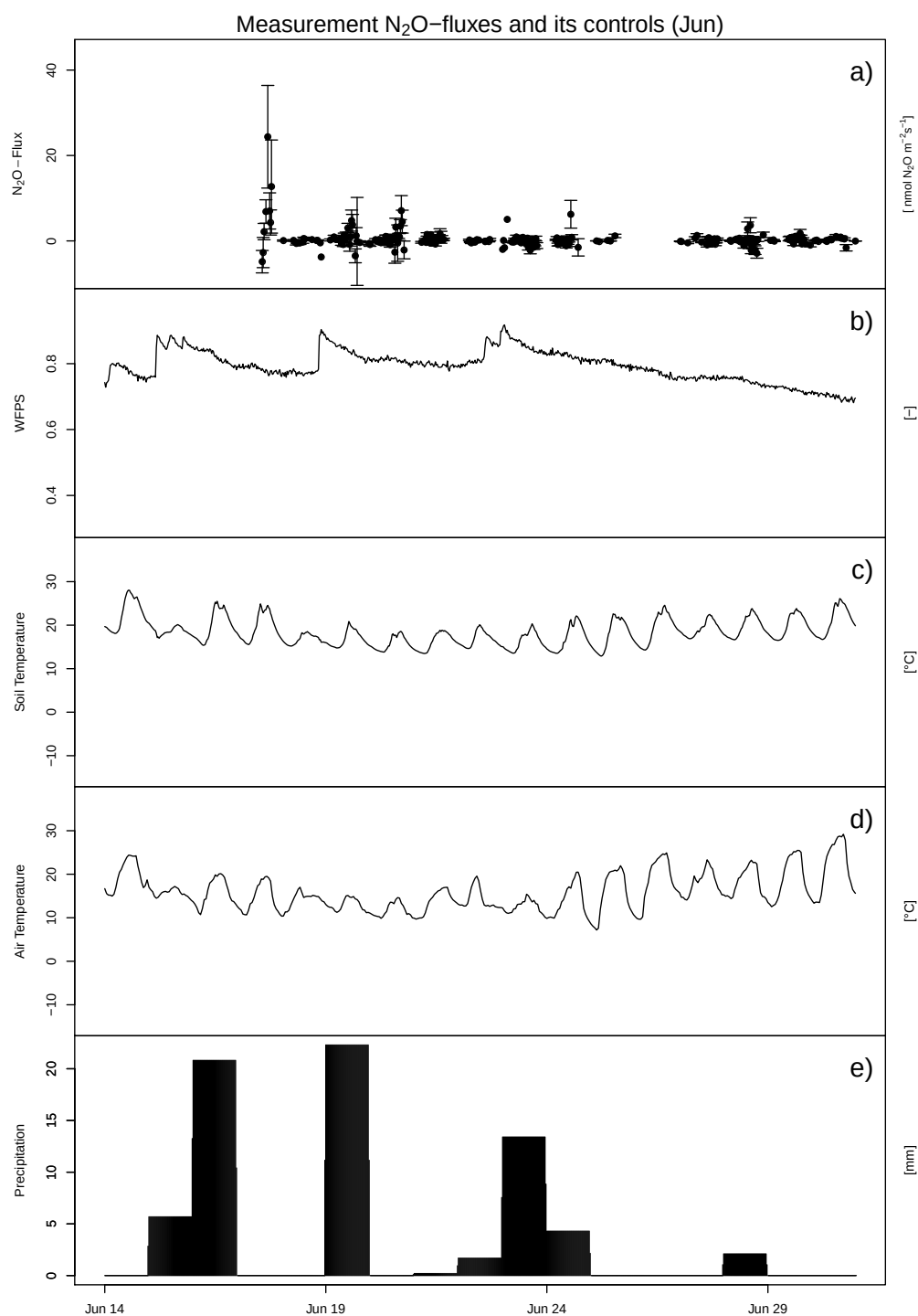


Fig. C.7 N_2O -fluxes in the beginning of June were not measured, as east wind dominated during the first two weeks.

Appendix D

Histogramm of N₂O-fluxes measured by the eddy covariance technique

In Fig. D.1, a histogram of the 1758 measurements is depicted. The picture clearly shows that most of the fluxes measured with the eddy covariance method are very small.

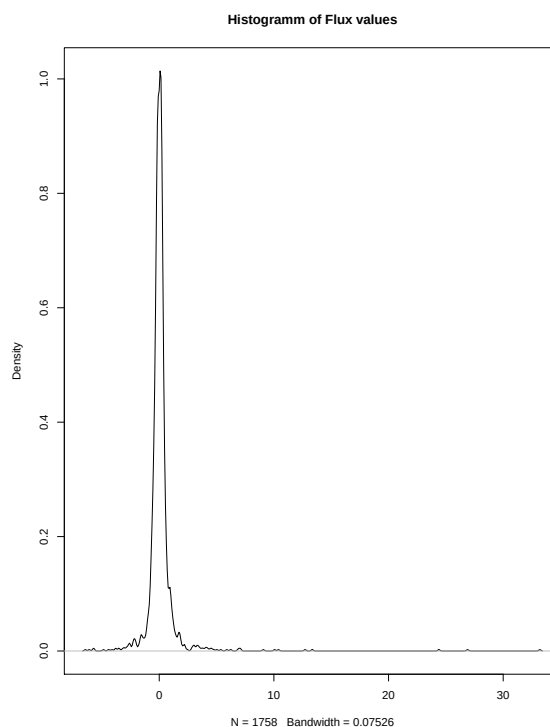


Fig. D.1 Histogramm of the distribution of N₂O-fluxes.

Appendix E

Soil air measurements of N₂O from A17

Soil air measurements were taken along an elevational gradient at field A17 in 2015. The measurement method was conducted according to Kiese et al. (2005). The samples taken in Scheyern were measured at the "Institute of Meteorology and Climate Research, Atmospheric Environmental Research, Karlsruhe Institute of Technology".

The first measurement (#1) is taken at the hilltop, the second and the third measurements are taken at the hillslope (#2 and #3) and the fourth measurement (#4) in the colluvium of the field. During winter the measurement depth was chosen as 15 cm, 30 cm, and 45 cm. During summer the measurements were taken in 5 cm and 10 cm.

Samples were taken maximum once a week due to the measurement method. Repetitions were not conducted, therefore the measurements have no error bar.

During winter the sampling devices were left in the soil until the field was harrowed. The sampling devices could be reinstalled after the field was prepared for sowing. Samples were not taken during the first fertilisation period. However, they were reinstalled after the second fertilisation period. In Fig. E.4 a decrease of N₂O could be detected with time after the second fertilisation event.



Fig. E.1 Shown are the septa, which are connected to GORE-TEX tubes (Fig. E.2)



Fig. E.2 GORE-TEX tubes in 50 cm soil depth

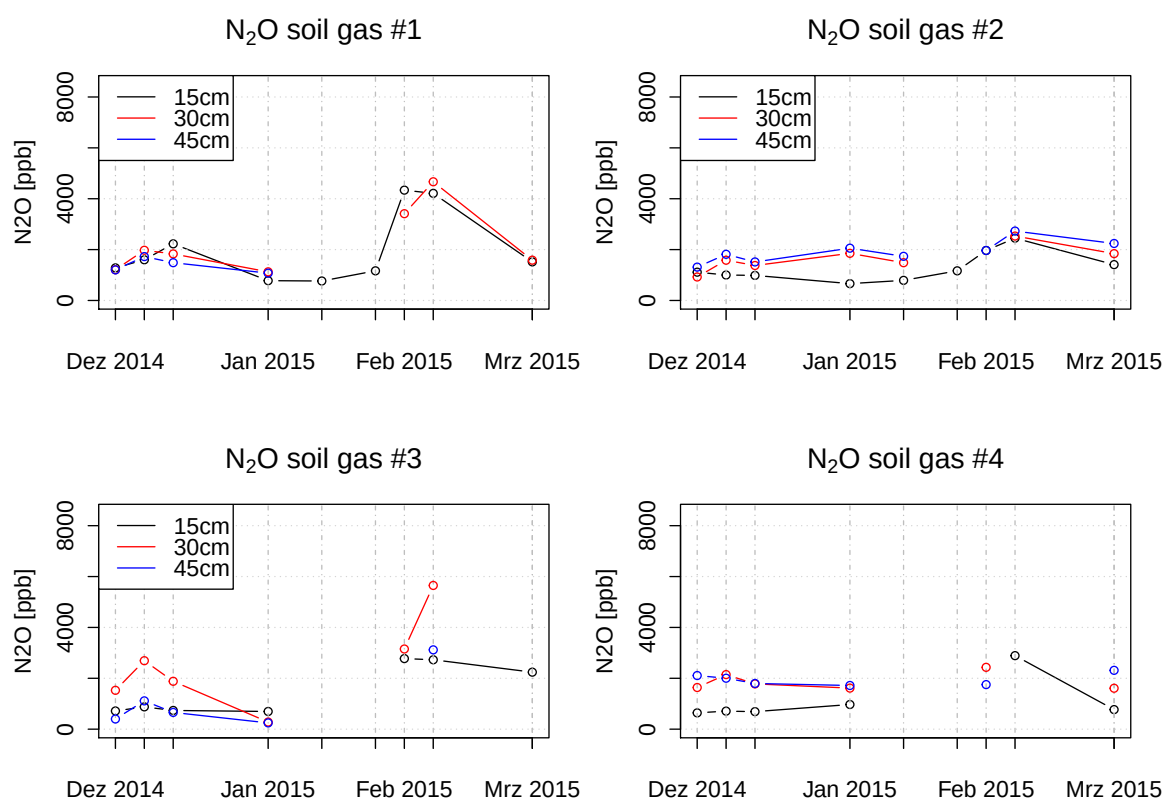


Fig. E.3 Soil gas measurements of N_2O during the winter 2014/2015 on A17. In case of missing measurements, no diffusion happened from the surrounding soil into the GORE-TEX tube which was due to very wet soil limiting diffusion into the GORE-Tex tubes. Interestingly, high N_2O -measurements appear in the beginning of February when the soil was freezing.

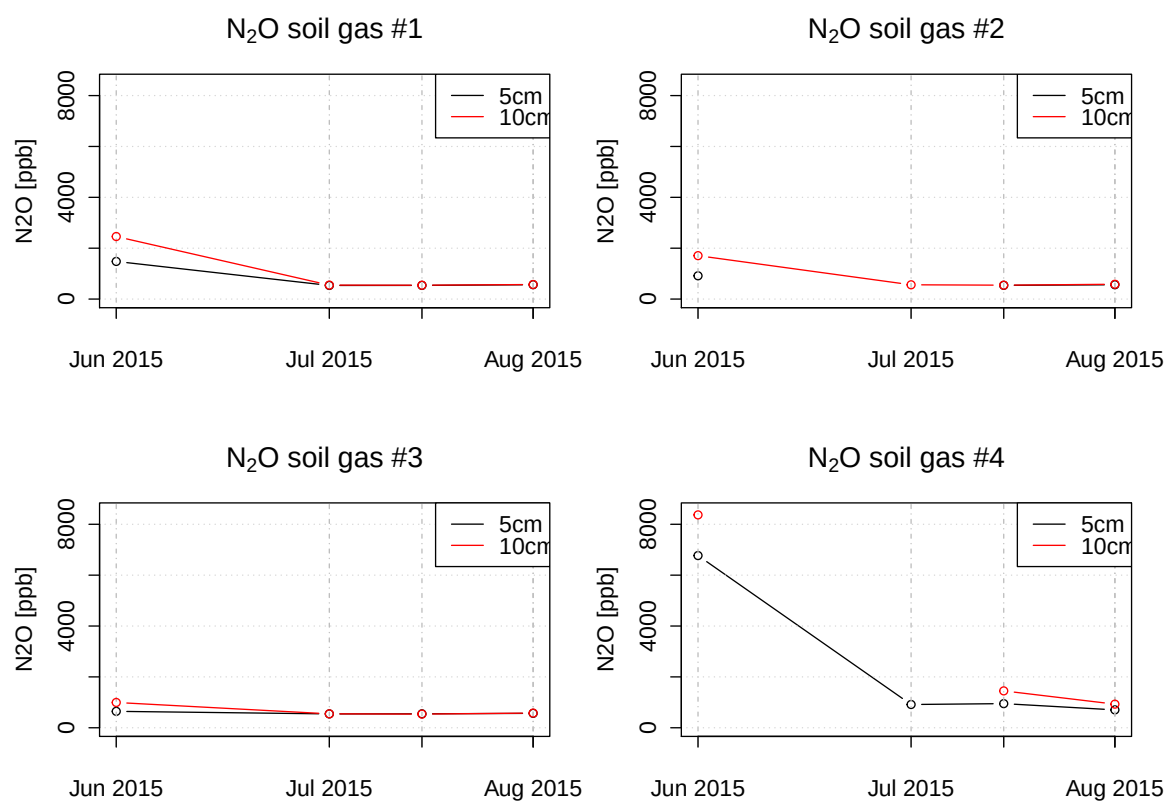


Fig. E.4 Soil gas measurements of N₂O during summer of 2015. In case of missing measurements, no diffusion happened from the surrounding soil into the GORE-TEX tube.

Appendix F

Expert-N simulations

Table F.1 Model configuration of Expert-N 5.0:

Model type	processes	Name	Reference
Nitrogen cycle	nitrification	LeachN	Hutson and Wagenet (1992)
	Denitrification		Johnsson et al. (1987)
	Mineralization		
	Urea hydrolysis		
soil water	soil water transport	HYDRUS 1D	Šimunek et al. (1998)
soil heat	soil heat flux	DAISY	Hansen et al. (1991)
	soil freezing		
plant growth	LAI	SPASS	Wang and Engel (1998)
	Plant height		Wang (1997)
	Root water uptake		Wang and Engel (2000)
			Gayler et al. (2002)
management	fertilization	Schaaf	(Schaaf and Engel, 1997)
	tillage	Schaaf	

Table F.2 Management data of automated chamber site, the variant with high fertilization. The used fertilizer was UAN. The depth of tillage was 30 cm. Water content of winter wheat and maize was 14 % for both crops.

Date	crop	management	$N_{\min-tot}$ kg – Nha ⁻¹	NO ₃ – N kg – Nha ⁻¹	NH ₄ ⁺ -N kgNha ⁻¹	Urea kgNha ⁻¹	yield [dry mass] dtha ⁻¹
2006-10-27	winter	sowing					
2007-03-12	wheat	fertilization	50.0	12.5	12.5	25.0	
2007-04-23		fertilization	40.0	10.0	10.0	20.0	
2007-05-26		fertilization	40.0	10.0	10.0	20.0	
2007-08-02		harvest					62.83
2008-05-08	potato	sowing/fert.	50.0	12.5	12.5	25.0	
2008-05-14		fertilization	150.0	37.5	37.5	75.0	
2008-10-01		harvest					73
2008-10-18		tillage					
2008-10-18	winter	sowing					
2009-04-07	wheat	fertilization	50.0	12.5	12.5	25.0	
2009-04-30		fertilization	45.0	11.25	11.25	22.5	
2009-05-22		fertilization	90.0	22.5	22.5	45.0	
2009-08-07		harvest					55.39
2009-08-07		tillage					
2010-04-23	maize	sowing					
2010-05-01		fertilization	135	33.75	33.75	67.5	
2010-10-05		harvest					99.33
2010-10-17		tillage					
2010-11-06	winter	sowing					
2011-02-27	wheat	fertilization	50	12.5	12.5	25.0	
2011-03-31		fertilization	40	10	10	20.0	
2011-05-20		fertilization	45	11.25	11.25	22.5	
2011-05-22		fertilization	45	11.25	11.25	22.5	
2011-xx-xx		harvest					59.28
2012-05-13	potato	sowing					
2012-05-20		fertilization	50	12.5	12.5	25.0	
2012-05-24		fertilization	150	37.5	37.5	75.0	
2012-10-03		harvest					68
2009-10-16		tillage					
2012-10-23	winter	sowing					
2013-03-30	wheat	fertilization	50	12.5	12.5	25.0	
2013-04-05		fertilization	40	10.0	10.0	20.0	
2013-05-15		fertilization	45	11.25	11.25	22.5	
2013-05-19		fertilization	45	11.25	11.25	22.5	
2012-10-23		harvest					60.27
2014-04-14	maize	sowing					
2014-04-21		fertilization	135	33.75	33.75	67.5	
2014-10-17		harvest					91.52

crop	date	patch of A17	management	N_{min} [$kg\ ha^{-1}$]	NO_3^- [$kg\ ha^{-1}$]	NH_4^+ [$kg\ ha^{-1}$]	Urea [$kg\ ha^{-1}$]	BBCH	yield [dt ha^{-1}]	LAI[-] (green)
Potato	2013-04-29	a,b,c	sowing					0		
		a,b,c	rotor harrow					0		
	2013-05-16	a,b,c	fertilization (NPK)	93	31	62	0	9		
	2013-07-01	a,b,c	fertilization (Urea)	10	0	0	10	33		
	2013-07-06	a,b,c	fertilization (Urea)	10	0	0	10	40		
	2013-07-15	a,b,c	fertilization (Urea)	10	0	0	10	60		
	2013-08-29	b,c	desiccation					93		
	2013-09-04	a	desiccation					93		
	2013-09-23/24	c	harvest					99	47.9	
	2013-09-23/24	b	harvest					99	51.9	
	2013-09-25	a	harvest					99	95.2	
Winter Wheat	2013-10-22	a,b,c	sowing					0		
		a,b,c	rotor harrow					0		
	2013-10-22	a,b,c	fertilization (NPK)	73	29.5	43.8	0	13		
	2014-03-13	a,b,c						23		
	2014-04-04	a,b,c						23		
	2014-04-12	a,b,c	fertilization (UAN)	65	16.25	16.25	32.5	23		
	2014-04-26	a,b,c	fertilization (NH ₄ SO ₄)	5				24		
	2014-05-19	a,b,c	fertilization (UAN)	70				30		
	2014-05-19	a,b,c						39		
	2014-06-11	a,b,c						61		
	2014-08-06	a,b,c	harvest					92	87	
	2015-04-14	a,b,c	sowing					0		0
		a,b,c	fertilization (NPK)	88	35.2	52.8	0			
Maize	2015-04-22	a,b,c	fertilization (NP)	33	13.635	19.635	0			
	2015-04-22	a,b,c	fertilization (Urea)	105	0	0	105			
	2015-05-19	a,b,c						13		0.05
	2015-05-28	a,b,c						17		0.19
	2015-06-09	a,b,c						31		
	2015-06-19	a,b,c						-		1.63
	2015-06-29	a,b,c						65		2.47
	2015-07-16	a,b,c						71		2.25
	2015-07-22	a,b,c						89		1.4
	2015-08-27	a,b,c	harvest					92	80.6	0.8

Table F.3 Management of field A17 from the year 2013 to 2015. Shown are

crop	date	patch of	management	N_{min} [kg ha ⁻¹]	NO_3 [kg ha ⁻¹]	NH_4 [kg ha ⁻¹]	Urea [kg ha ⁻¹]	BBCH	yield [dt ha ⁻¹]	LAI[-] (green)
Winter Wheat	2012-10-11	a,b	sowing, cultivating					0		
	2012-10-11	a,b	rotor harrow					0		
	2013-03-15	a,b	fertilization (NPK)	76	31	62	0	9		
	2013-04-24	a,b	fertilization	36.5	0	0	36.5	33		
	2013-05-09	a,b	fertilization	40	10	10	20	40		
	2013-05-15	a,b	fertilization	10	0	0	10	60		
	2013-08-11	a,b	harvest	66	0	0	66	60	80.5	
Potato	2014-01-05	a,b	dam shaping					0		
	2014-03-21	a,b	fertilization (NH_4SO_4)					0		
	2014-03-21	a,b	rotor harrow					0		
	2014-04-17	a,b	fertilization (NPK)	73	29.5	43.8	0	0		
	2014-04-18	a,b						0		
	2014-04-18/17	a,b	planting					0		
	2014-04-28	a,b	fertilization (UAN)	65	16.25	16.25	32.5	23		
	2014-05-06	a,b	fertilization (NH_4SO_4)	5	0	5	0	24		
	2014-05-23	a,b	fertilization (UAN)	70	17.5	17.5	35	30		
	2014-08-14	a,b	siccation, Reglone							
Winter Wheat	2014-08-19	a,b	siccation, Shark							
	2014-09-16	b	harvest (Krone)					80-89	74.7	
	2014-09-20	a	harvest (Burana)					80-89	60.9	
	2014-11-03	a,b	sowing							
	2015-04-29	a,b								
	2015-04-22	a,b	fertilization (in vert)	65	21.125	43.875	-	00		
	2015-05-07	a,b								
	2015-05-19	a,b	fertilization (urea)	52			52			
	2015-05-28	a,b								
	2015-06-05	a,b	fertilization (UAN)	45	11.25	11.25	22.5			0.93
	2015-06-09	a,b								
	2015-06-15	a,b	fertilization (urea)	60	0	0	60			1.16
	2015-06-19	a,b						65		0.46
	2015-06-29	a,b								
	2015-07-16	a,b								0
	2015-07-22	a,b								0
	2015-07-27	a,b	harvest						80.6	0

Table F.4 Management at field A18 from the year 2013 to 2015. Dry mass of potato results from water contents for the potato sorts Krone and Burana. For Krone water content is 82% for Burana water content is 79 %. The time frames for catch crops can be looked up in Fig. 3.14

Appendix G

Footprint weighted simulations of Q_H and Q_E

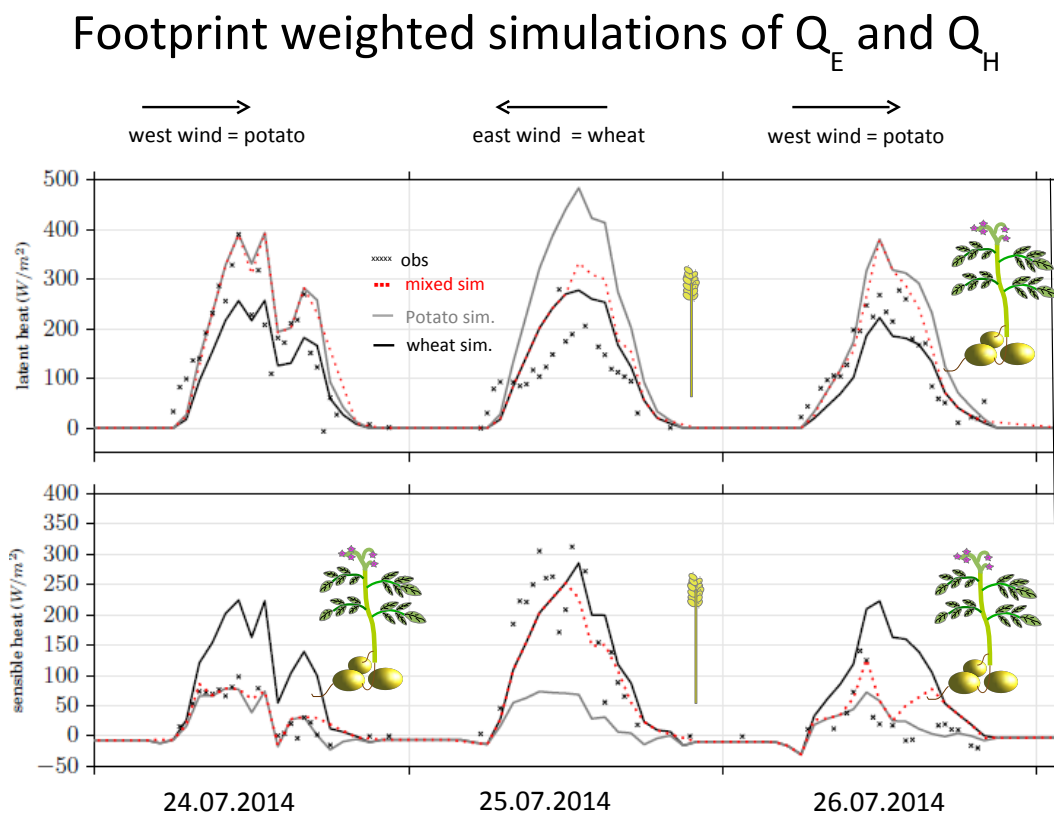


Fig. G.1 The performance of a footprint weighted modelling study is shown. The graph is made based on simulation results of Christian Klein (Klein, 2018). The mentioned model study was conducted driver data and evaluation data measured in this study.

Appendix H

6 years of N₂O-simulations (automated chambers)

Shown are the 6 years of N₂O simulations during wintertime that are not shown in the main part of the PhD-thesis.

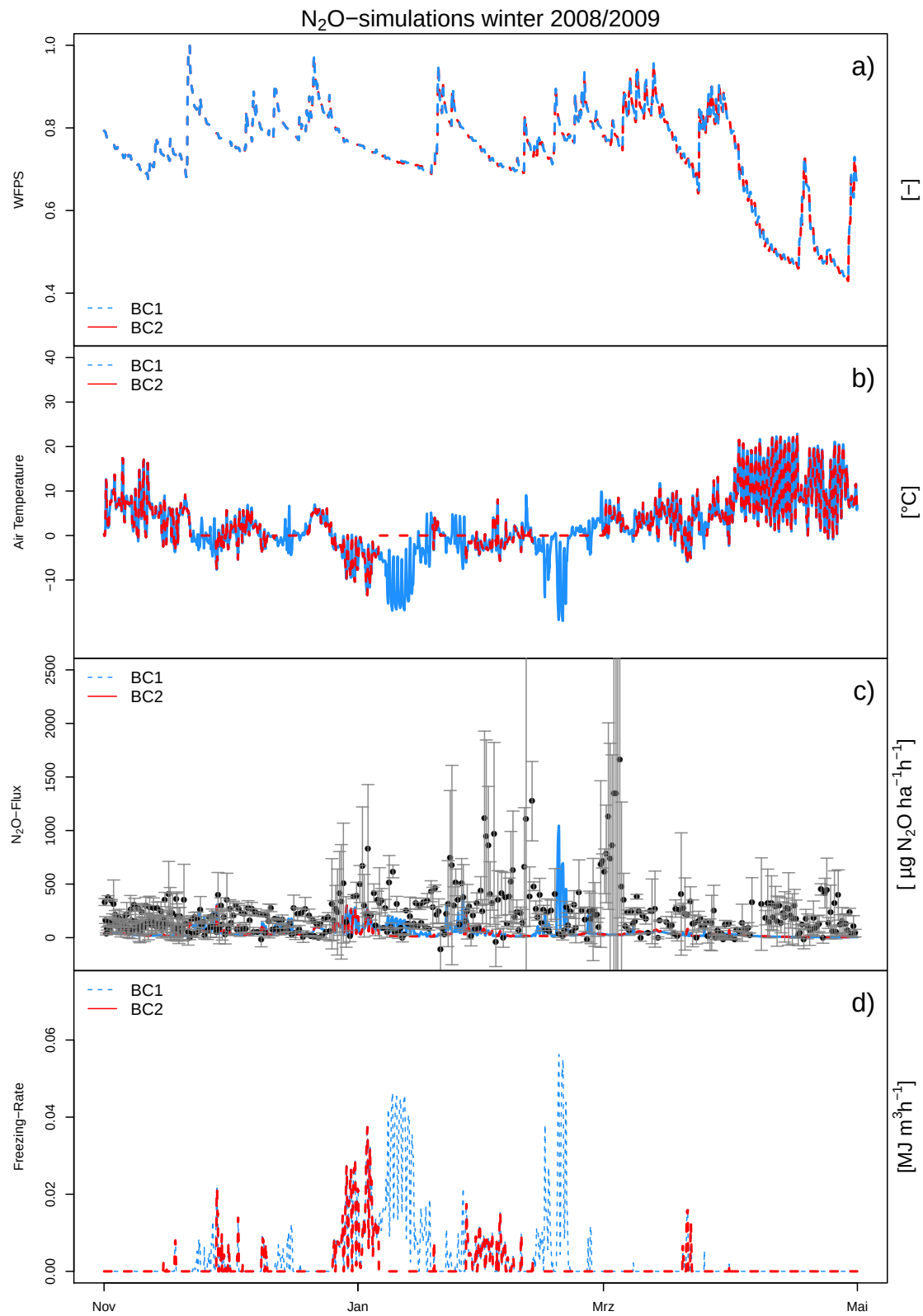


Fig. H.1 N₂O simulation during winter 2008/2009. Water filled pore space (WFPS) in subfigure a) air temperature in b) N₂O-flux in c) and the simulated soil freezing rate in 10 cm

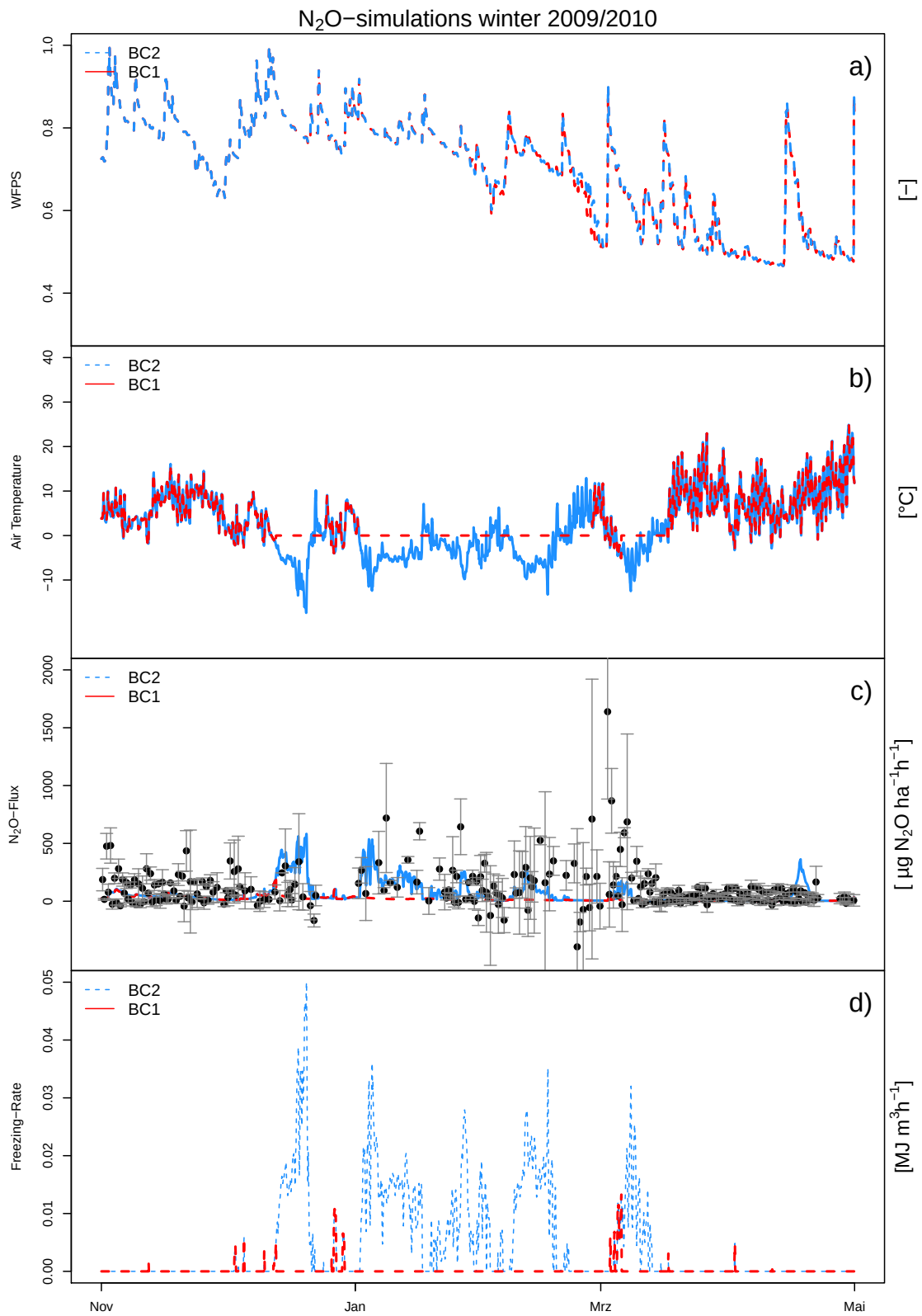


Fig. H.2 N₂O simulation during winter 2009/2010. Water filled pore space (WFPS) in subfigure a) air temperature in b) N₂O-flux in c) and the simulated soil freezing rate in 10 cm

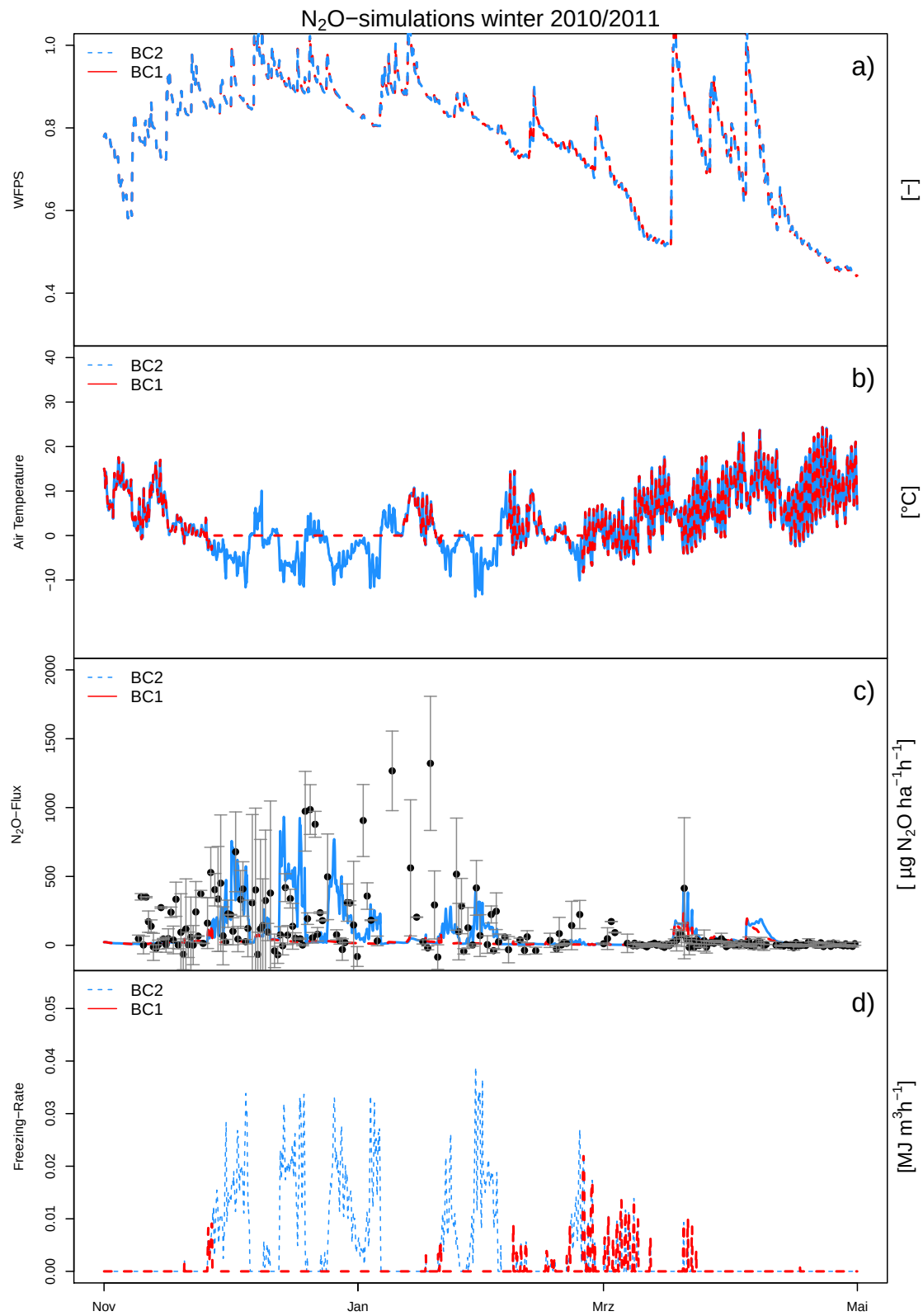


Fig. H.3 N₂O simulation during winter 2010/2011. Water filled pore space (WFPS) in subfigure a) air temperature in b) N₂O-flux in c) and the simulated soil freezing rate in 10 cm

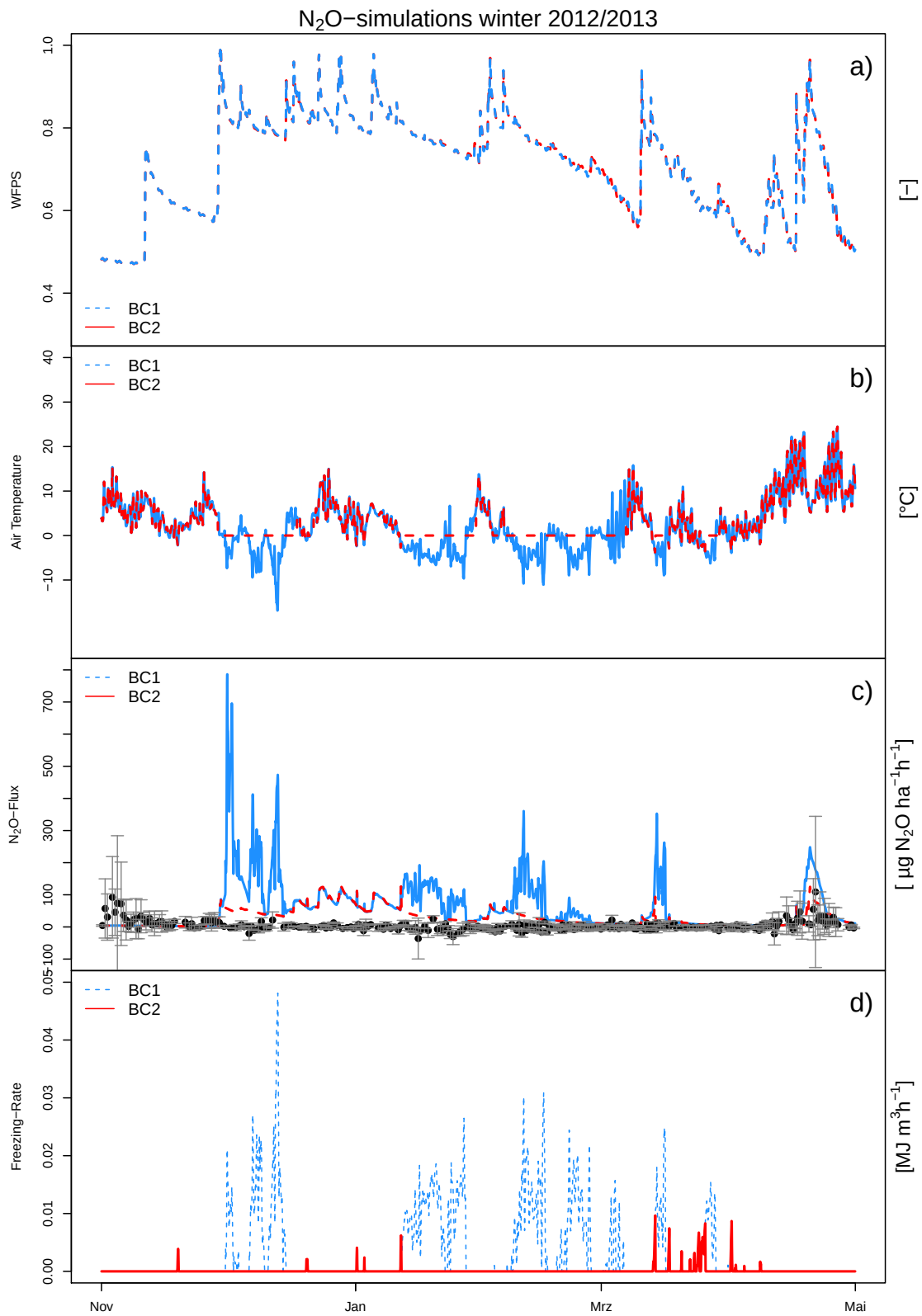


Fig. H.4 N₂O simulation during winter 2012/2013. Water filled pore space (WFPS) in subfigure a) air temperature in b) N₂O-flux in c) and the simulated soil freezing rate in 10 cm

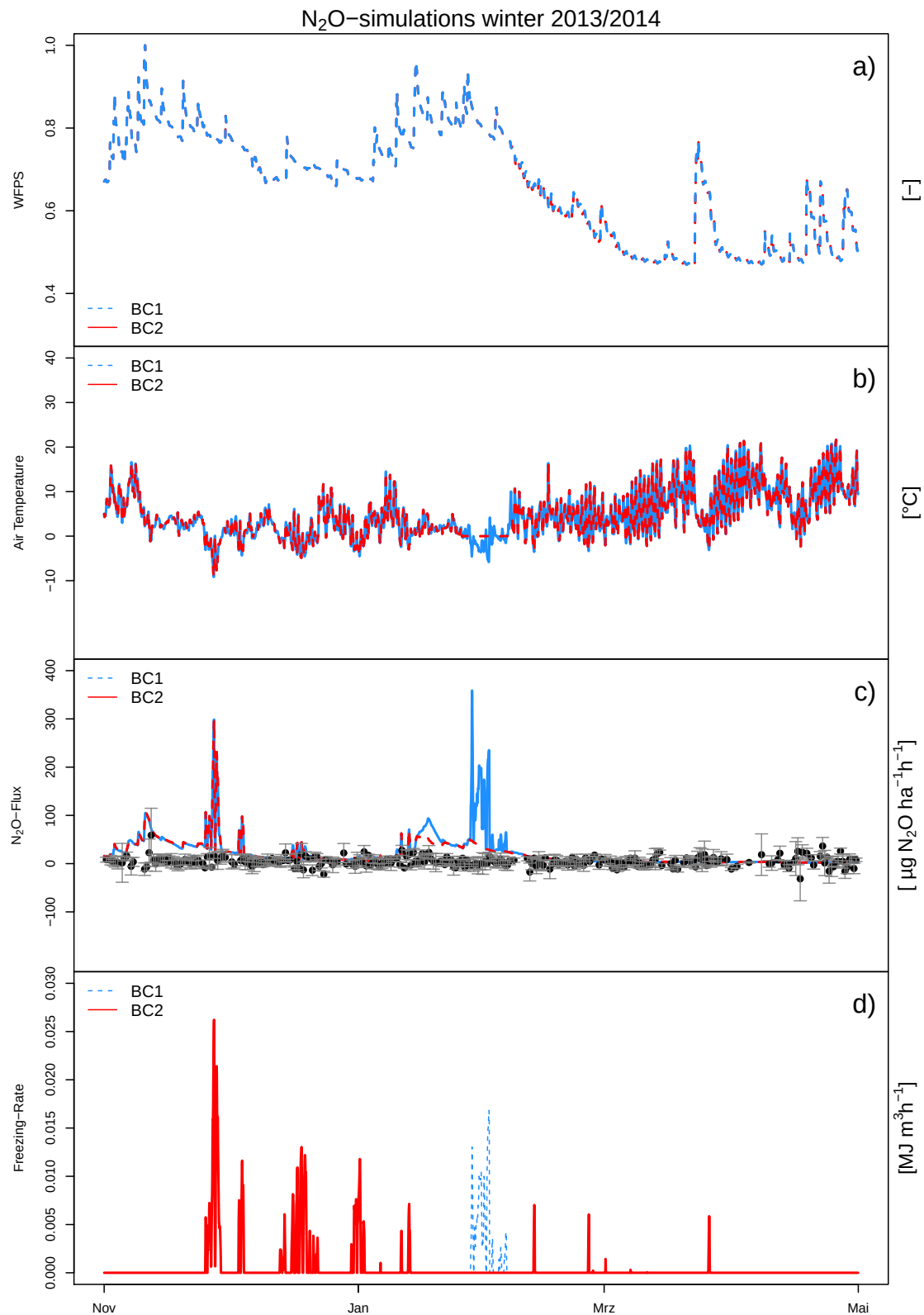


Fig. H.5 N₂O simulation during winter 2013/2014. Water filled pore space (WFPS) in subfigure a) air temperature in b) N₂O-flux in c) and the simulated soil freezing rate in 10 cm

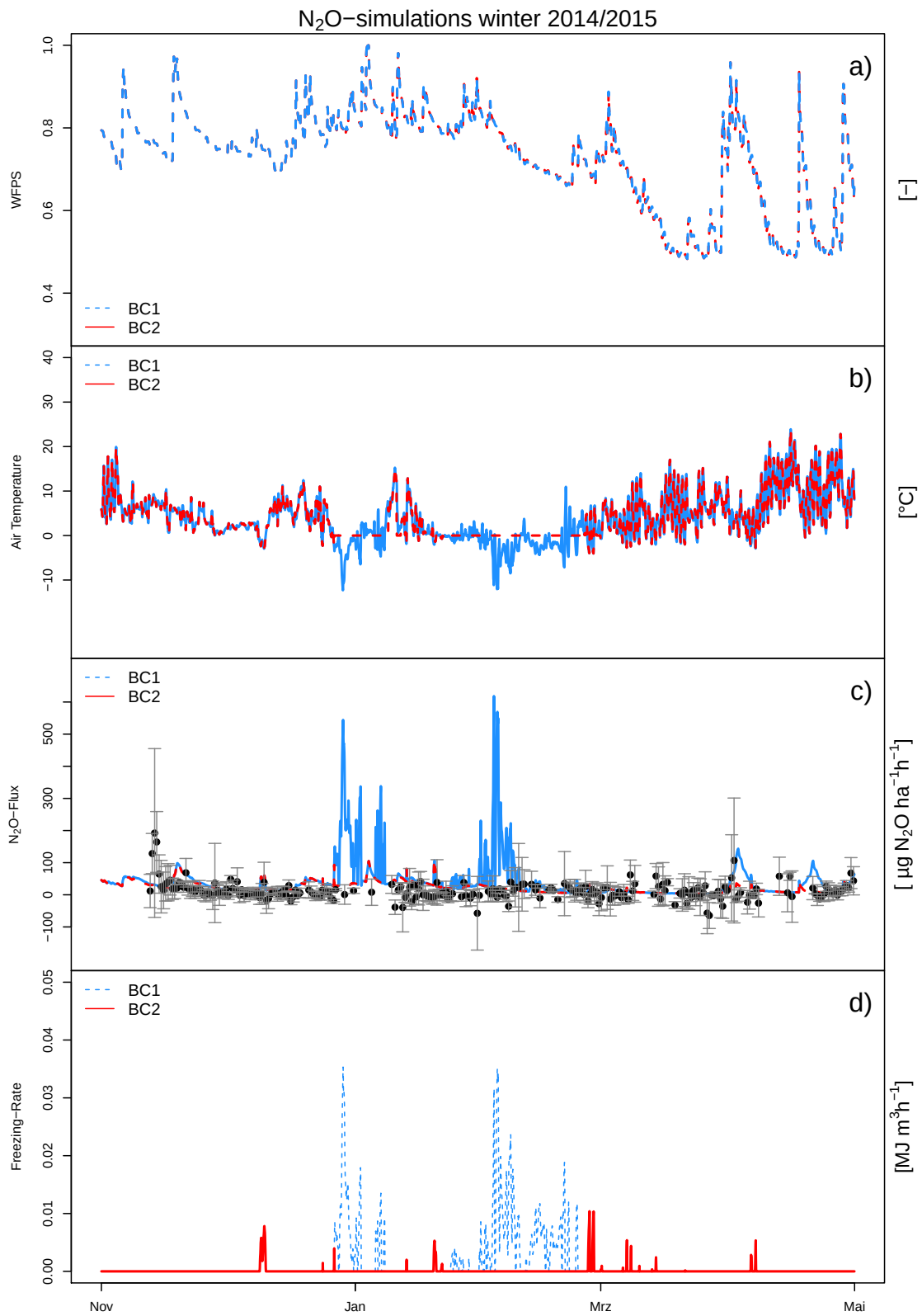


Fig. H.6 N₂O simulation during winter 2014/2015. Water filled pore space (WFPS) in subfigure a) air temperature in b) N₂O-flux in c) and the simulated soil freezing rate in 10 cm

H.1 Sums of all 7 winter half-years

Table H.1 Half-yearly amounts of winter emissions over 7 years. Emitted amounts of N₂O for one half year are shown and two simulations with two different boundary conditions for the upper soil layer.

kg N ₂ O-N per halfyear in winter	08/09 kg N ₂ O – N ha ⁻¹	09/10 kg N ₂ O – N ha ⁻¹	10/11 kg N ₂ O – N ha ⁻¹	11/12 kg N ₂ O – N ha ⁻¹	12/13 kg N ₂ O – N ha ⁻¹	13/14 kg N ₂ O – N ha ⁻¹	14/15 kg N ₂ O – N ha ⁻¹
measurements	9.9	4.7	5.0	0.1	0.2	0.2	0.5
BC 1	2.5	3.0	3.6	1.5	2.6	1.0	1.8
BC 2	1.7	0.9	1.1	0.7	1.3	0.8	1.0

H.2 Evaluation volumetric water content

Shown are the NSE values we obtained by evaluating simulations of Expert-N against gravimetric water content measurements was lower than zero in all cases. In that case the goodness of fit is comparable to the values that are reported by Liang et al. (2016), who obtained an NSE of -0.51 for an evaluation of Expert-N simulations against gravimetric soil water measurements.

Comparing the simulations of chapter 3.7.3 and the simulations of (Klein, 2018) which had clearly positive NSE values (>0.3) to the evaluations against gravimetric measurements of this study and the study of (Liang et al., 2016) one can also conclude that gravimetric measurements give worse results than measurements from TDR sondes.

Table H.2 NSE [-], NRMSE [%] for both boundary condition 1 and 2. The implementation of the upper boundary condition doesn't change the goodness of fit of the simulations of volumetric water content.

	NSE θ winter	NSE θ summer	NRMSE θ winter	NRMSE θ summer
08/09	- 2.24	- 4.82	164.3	208.9
09/10	- 1.68	- 0.07	151.5	89.4
10/11	- 1.89	- 5.36	159.0	225.6
11/12	- 1.03	- 1.07	131.9	136.5
12/13	- 1.64	- 3.56	154.8	197.8
13/14	- 0.37	- 3.62	112.6	206.4
14/15	- 0.37	0.237	113.5	71.3

Glossary

sign	description	unit
δ^2	Allan Variance	
I_0	intensity of light from detector	Wm^{-2}
I	intensity of light after measurement	Wm^{-2}
L_P	path length	m
NO_3	nitrate	
N_2	di-nitrogen	
ν	nu	cm^{-1}
σ	optical cross section of measurement cell	m^2sr^{-1}
τ	integration time	s
θ_{ice}	ice content	
ξ	stability parameter	m m^{-1}
n_s	ns	mol^{-1}
$\bar{x}$	mean of scalar	
ρ	density	kgm^3
λ	evaporation heat	Jkg^{-1}
A	area	m^2
A17	field number of western field	
A18	field number of eastern field	
ANN	artificial neural net	
β	nitrification rate	—
Bo	bowen ratio	—
cp	specific heat with constant pressure	$\text{Wm}^{-1}\text{K}^{-1}$
CO_2	carbon dioxide	
CH_4	methane	
C_{frost}	Amplification factor for frost	
CV	coefficient of variation	

sign	description	unit
DOY	Day of the year	
DWD	Deutscher Wetter Dienst	
E	evaporation	$\text{Wm}^{-2}\text{s}^{-1}$
EBC	energy balance closure	
EC	eddy covariance	
EC _{plant}	development stage after BBCH	
f _{freeze}	correction function for freezing	
f _{rew}	correction function for rewetting	
f _{NO3}	correction function for nitrate availability	
f _{thaw}	correction function for thawing	
f _{theta}	correction function for temperature	
GC	gas chromatography	
Hz	frequency	s^{-1}
IR	infrared wavelet range of light	
K _{sat}	half saturation constant	kg N
L	Obhukov-Length	m
LAI	leaf area index	m^2m^{-2}
MT	mustard	
MZ	maize	
N	number of observations	
NH ₄	ammonia	
N ₂ O	nitrous oxide	
NEE	Net ecosystem exchange	$\mu\text{molCO}_2 \text{ m}^{-2}\text{s}^{-1}$
NSE	Nash-Sutcliffe (model efficiency)	
O	Observation	
$\bar{O}$	observation	
P ₀	Power of laser light (initial)	mW
P	Power of laser light (after cell)	mW
P	prediction of simulation	
$\bar{P}$	mean of prediction of simulation	
PT	Potato	
Q _E	latent heat	$\text{Wm}^{-2}\text{s}^{-1}$
Q _H	sensible heat	$\text{Wm}^{-2}\text{s}^{-1}$
QCL	Quantum Cascade Laser	

sign	description	unit
R^2	coefficient of determination	—
R_n	net radiation	$\text{Wm}^{-2}\text{s}^{-1}$
RH	relative humidity of water vapour	%
SPASS	Soil-plant-atmosphere System Simulation	
T	transpiration	$\text{Wm}^{-2}\text{s}^{-1}$
TDL	Tunable diode laser	
T_{air}	air temperature	$^{\circ}\text{C}$
T_s	sonic temperature	K
TERENO	Terrestrial network of environmental observatories	
TK3	Turbulenzknecht	
UAN	urea ammonium nitrate	
w'	fluctuation of vertical wind speed	ms^{-1}
WFPS	Water filled pore space	—
$\bar{w}$	mean vertical wind speed	ms^{-1}
WPL	Webb-Pearman-Leuning (correction)	
WRB	World reference base of soil classification	
WS	wind speed	ms^{-1}
WW	winter wheat	
X	scalar	
z_0	roughness length	m