- Our reply to the comments in four referee reports are included.
- All the changes in the manuscript are made in track-change mode.

Suggestions for revision in Report #1

I have reviewed the subject manuscript and the comments of two earlier reviewers. The authors provide management strategies for reducing nitrogen leaching, using the grey water footprint as the metric for nitrogen pollution. The estimates of nitrogen leaching in response to management strategies are predicted using an un-calibrated model (APEX). I'm afraid I have to agree with the spirit of the first two reviewers' criticism that it is unlikely that an un-calibrated is unlikely to provide any new insight on the well-known tradeoffs between nitrogen application, nitrogen leaching, and crop yield. While the authors can provide numerical results with the APEX model, as long as it's unclear what the uncertainty in those results are, I don't think the authors' recommendations on optimal management strategies are worthwhile. While exploring various model tiers could be interesting, it seems to me that we could have easily predicted that different results would be found for the simple tier-1 versus the more complex tier 3 approach. In addition, because we don't have any data to calibrate to or any idea of the uncertainty in the two models, I don't think the authors can be prescriptive about when the simple tier 1 approach "suffices and when it doesn't."

We acknowledge that we did not calibrate the model with field experiment data for the specific site, but it would have been difficult to measure nutrient fluxes for a large range of soil, water and nutrient management strategies. However, we put efforts to validate our simulation results i.e. N-response curve, yield and net irrigation requirement with previous studies. Our simulated N-response curve, yields and net irrigation requirement are consistent with the results presented by Godard et al. (2008), Berenguer et al. (2009) and Chukalla et al. (2015), respectively. Other researchers who compared APEX simulated results with values from field experimental studies in similar conditions as that of our site in Spain also reported that APEX can adequately simulate maize yield and leached nitrate-N. Cavero et al. (2012) show that the leached nitrate-N simulated using APEX is equivalent with the observed value. Berenguer et al. (2009) showed a satisfactory agreement of maize yields simulated using APEX to the maize yield observed in a field experimental study for six N-application rates. We think that such consistency in the APEX model makes the model suitable to compare the leaching-runoff fractions estimated with tier-1 and tier-3 approaches. The result that shows that the tier-1 approach underestimates the leaching-runoff fraction beyond an N application rate of 150 kg ha^{-1} is understandable in that for larger N application rates, N uptake by the crop is stabilizing and N surplus increase exponentially, which should increase the N leaching - runoff fraction beyond the proportion to N application. Being able to estimate grey WFs at tier-3 level is a great advancement compared to the reliance of earlier studies on the tier-1 level approach.

Nevertheless, we acknowledge the need of validating APEX simulated results with field experiments, also conduct sensitivity analysis for input data and uncertainty analysis for the APEX model. In the discussion section, we already highlighted in line 516-523 the limitation of the research.

A few other comments:

Much of the English grammar was improved in the revision, but the whole manuscript still needs to be edited by a person whose first language is English.

Move Table 2 to appendix.

The two panels in Figure 3 seem repetitive.

Based on the suggestion, we moved Table 2 into an appendix. The two panels in Figure 3 are not repetitive: the one in the left is grey WF in m3 per ton, an indicator of pollution per unit of production, and the panel in the right (grey WF in m3 per ha) is an indicator of pollution per unit area. These are complementary indicators.

Suggestions for revision in Report #2

The authors tried to show the trade-off between crop yield, nutrient application rates, and nutrient loading to downstream waterbodies. However, I do not think the findings are new to the literature (please read Journal of Soil and Water Conservation and other relevant journals). In addition, the methodology including APEX model preparation and leaching-runoff fraction definition is unclear and questionable. Furthermore, the results are confusing, and they are not appropriately presented and explained in the manuscript. My specific comments are provided below.

We do not claim the finding of the current study is entirely new. Yet, we believe that the current paper gave the first insights on the combined effect N application rate, N form, tillage practice and irrigation strategy on the pollution load per unit of crop (or grey WF per tonne).

In the manuscript, the leaching-runoff fraction is defined in two ways. The first definition: the leaching-runoff fraction, called α, is the percentage of the amount of chemical applied to the field as fertilizer that is lost to groundwater through leaching or to surface water through runoff. The second definition: the leaching-runoff fraction, now called β, is the percentage of the amount of 'surplus nitrogen' (= input - crop uptake) in the soil that is transported to groundwater by leaching or to surface water by runoff.

In the current research, we describe the APEX model (section 2.1), the grey WF concept (2.2), th definition of leaching-runoff fractions (section 2.3) and simulation set-up (section 2.4). However, we did not describe the entire set of equations to simulate the water and nutrient processes and crop growth, which can be referred in the documentation of APEX (Williams et al., 2008).

Lines 21 to 22: Does this mean the crop yield decreases from 11.1 ton/ha to 3.7 ton/ha when the N application rate is reduced from 300 kg N/ha to 50 kg N/ha? Is so, I do not think this N application scenario is feasible and realistic since farmers will not apply this practice.

The yield reduces form 11.1 ton/ha to 3.7 ton/ha when the N application rate is reduced from 300 kg N/ha to 50 kg N/ha. This N application scenario is to show the grey WF reduction potential in crop production, which could be practiced by farmers if they are compensated for their yield loss. But anyway, we don't suggest that this is 'feasible', we just present the results.

Lines 28 to 30: Applying manure can cause another water quality (phosphorus) issues such as algal bloom and eutrophication.

It is true that applying manure can cause other water quality (phosphorus) issues such as algal bloom and eutrophication. The grey WF value would have been different if the grey WF of phosphorus or other chemicals in crop production are considered. The focus of the current study is on N-related grey WF, which is highlighted in the revised manuscript (line-96).

Lines 51 to 52: I do not follow this sentence. I do not understand why water pollution (or nutrient loads) is compared to the volume of crops produced. Is this a meaningful comparison?

The grey water footprint per tonne (the nutrient load per amount of crop produced) is an indicator that compares the pollution and yield per ha. Hence, the indicator can help to optimise pollution per unit of production.

Lines 49 to 73: What is the main idea of this paragraph?

The paragraph is a review of literature on the effect of N-application rate, N form, tillage and irrigation practices on yield, N fluxes and crop growth.

Lines 180 to 182: I wonder if the authors had a chance to evaluate the applicability of the maximum acceptable N concentration (of 50 N mg/L) and natural concentration (of 0.5 mg N/L) to the study watershed. They must be highly varying depending on many factors.

We adopted the maximum acceptable N concentration, Cmax, based on the EU nitrate directive; which applies for EU member countries including the case study area (Spain). The natural concentration is site specific, however we considered a conservative value (0.5 mg N/L).

Lines 204 to 220: I do not understand why the leaching-runoff fractions are less than 1.0. For instance, the N load to freshwater bodies can be greater than the N fertilizer applied or the N applied but not taken up by the plant. Please describe the mathematical relationship between the variables.

The leaching-runoff fraction, $\alpha = \frac{L}{Appl}$

L is pollutant load to freshwater bodies contributed by the amount of chemical applied (Appl) to the field. N is supplied to the soil through many paths including N anthropogenic application, N deposition and N fixation. However, the grey WF is an indicator to measure pollution due to anthropogenic chemical application (Total pollutant minus pollutant load caused by non-anthropogenic addition). Thus L is always less than Appl and the leaching-runoff fraction should be less than 1.

The description of L is improved in the manuscript (Line 213): "L (kg N ha-1 y-1) is the N load to freshwater bodies due to the anthropogenic N addition".

Lines 241 to 253: There is no information about the reliability of the assumptions made. I wonder if the authors had a chance to compare the assumptions with other reference values, statistics, and field observations. Lines 282 to 290: I could not find information about how the other parameters (for flow, N cycle and transport) were determined. I believe they might be calibrated to measurements, but there is no description about the parameter calibration.

We acknowledge the model was not calibrated with field experiment data. However, efforts have been put to validate our simulation results which is already explained in the reply to referee#1 and also discussed in the manuscript.

Line 361: Could you explain why the grey WF is minimized at the N application rate of 50 kg N/ha rather than 25 kg N/ha? In addition, the authors might be able to find an N application rate that minimizes grey WF between 50 and 100 kg N/ha. In addition, I wonder if these results can be applicable to other cases and watersheds.

While increasing the N-application rate from 25 to 50 kg N ha^{-1} ya^{-1}, crop yield increases at a slightly faster rate than N pollutant load (the nitrogen efficiency is high at lower N application rates); as a result, the grey WF per tonne slightly drops. At higher N application, the yield increases but at slower rate than the N load and thus the grey WF per tonne will increase.

In the manuscript, we reported results of simulation for the N application rates at 25, 50, 100, 150, 200, 250 or 300 kg N ha^{-1}y^{-1}. We did not simulate for all intermediate N application rates, however the simulation result at

N = 75kg N ha⁻¹ y⁻¹ under the reference management package (inorganic N fertilizer in combination with conventional tillage and full irrigation) is consistent with the results.

Lines 373 to 392 and Figure 5: In Figure 5b, the largest consumptive WF (blue and green WFs) is found at the lowest nitrogen application rates (of 25 kg N/ha), and it rapidly decreases with increases in the application rates. When nitrogen application rates low, however, crop yields are also low, and ETs are low as well, as demonstrated in Figure 5a. Thus, consumptive WF should be low when the nitrogen application rates are low (rather than high like 3000 m3/ton, compared to 700 m3/ton). Please explain why the consumptive WF is high even though ET is low when nitrogen application rate is low.

The consumptive WF at low N rate is high (3000 m3/ton) even though ET and yield are low. This is because the reduction in yield from the high N application to the low N application rate is faster (83.7%, 11.1 to 1.8 ton/ha) than the reduction in ET (23.6%, 762 to 582 mm).

Lines 402 to 447: I do not understand these descriptions and explanations.

This section describes the results of the side objective of the current study (line 116 - 118): "comparing the N leaching-runoff fractions that result from the APEX simulations with the leaching-runoff fractions estimated with the simpler tier-1 approach, in order to find out the added value of employing the advanced model approach."

Lines 464 to 464 and Table 2: I believe it is good to show three WFs separately rather than total WF so that the authors can effectively discuss the strengths and weaknesses of each scenario.
Lines 488 to 492: I think the findings mentioned are well known (not new to the literature). The authors just used different terms such as grey, blue, and green water footprint.

We believe that the current paper is the first to provide insight on the combined effect of N application rate, N form, tillage practice and irrigation strategy on the pollution load per unit of crop (or grey WF per tonne).

Suggestions for revision in Report #3
GENERAL COMMENTS
This manuscript details the results of a modeling exercise to assess the fate of nitrogen and grey water footprint size in agricultural systems under different management practices. The authors use the Agricultural Policy Environmental eXtender (APEX) model to assess crop yields and nutrient leaching/ runoff, and results are compared against a more simplistic, less-data intensive, expert-based approach for estimating N loads from agricultural areas. The assessments are based on climate and agricultural characteristics of a farming region in Spain. Results indicated that for low levels of nitrogen application, the simple approach yields approximately the same results as the more data-intensive modeling endeavor. At higher levels of nitrogen application, the simple method underestimates nitrogen leaching/runoff. The modeling results also explored multiple types and combinations of management practices, finding there are inevitable tradeoffs between crop yield and water pollution, and water pollution and water consumption.

SPECIFIC COMMENTS
This is an interesting paper with potential implications for applied agricultural management to reduce water pollution problems while minimizing negative impacts to crop yields. The following are a few comments that could help improve this work if incorporated.

- Lines 79-84 provide an overview of studies that have explored the impacts of crop yield and N management via various agricultural management practices. However, what would be more helpful to the reader is an overview of those study findings, and how these findings informed the present work.

The purpose of the section (Line 79-84) is to inform the current work on the number of management packages that are considered in the previous researches. The previous studies are for different environments and sometimes for different crop types than the current case study. Thus the effect of the management package on the yield, water productivity and leaching are not quantified for a comparison with the current study.

- I realize that validating model results with field experiments is difficult, and the authors clearly explain why this is so (Lines 90-94). I also appreciate the author's comparison of their model results with those of Berenguer et al 2009- particularly given that the APEX results are only really comparing Tier 1 and Tier 3 levels. Given the lack of field data available, this multi-model comparison is very important. However, I feel the discussion and comparison of model results is short and lacks depth. There is brief mention of modeling results based on EU studies, and research by Berenguer et al 2009, but digging in and really discussing the differences and similarities between these results would add greatly to this work.

In addition to showing the comparison of our study result with the research by Berenguer et al., (2009) in Figure 10; in the revised manuscript, the difference between our study and the study by Berenguer et al., (2009) is quantified to be 25% higher and this is highlighted in Line 489.

- At the beginning of Section 2.3, the authors state that part of the reason for evaluating Tier 3 vs Tier 1 is to see if "the simpler estimation approach (Tier 1) as applied to previous studies" is an accurate measure. I'm not sure what these "other studies" are in particular, maybe they're the ones I mention in the comment above, but either way, there could be much value added to explicitly showing the comparisons between Tier 1 results and Tier 3 results, if possible?

The previous studies that applied the Tier 1 approach are the studies by Mekonnen and Hoekstra (2011), and Brueck and Lammel (2016), which are mentioned in Line 110 of the manuscript. Section 3.4., Figures 7 to 9 and Lines 419 to 465 give explicit explanation and comparison of Tier 1 and Tier 3.

TECHNICAL COMMENTS

- In line 36, "fertilizer" should be "fertilizers".
Considered.

- The authors use the spelling "freshwater" and "fresh water" in this manuscript (see lines 38 and 39 for examples). One spelling version should be selected and used consistently throughout.
Fresh water is now consistently used in the revised manuscript.

- In line 157, I suspect the authors meant "Phenological", not "Phonological".
Yes we meant "Phenological", it is corrected.

- Equations 4 & 5 (Lines 220-223) reference work done by Franke et al 2013. In these equations, there is a variable s¬_i that is a "score for leaching runoff potential", while I realize this is information from another paper, it would be helpful to discuss how these values are developed, even if briefly.

The following description is added in the revised manuscript in the Line 226 to 229.

Corresponding to a certain state of factor, a score s is between 0 and 1: scores of 0, 0.33, 0.67 and 1 refer to a very low, low, high and a very high leaching-runoff potential, respectively. A weight w per factor i denotes the importance of the factor. The weights given to the separate influencing factors add up to a total of 100.

These values are developed by the Grey Water Footprint Expert Panel, who are formed to guide on how to best estimate the values of the leaching-runoff fraction at Tier-1 level.

- In Figs 8 & 9, I assume the "calculated, tier-1" numbers (in blue) are mean values? Please specify in the body of the manuscript for clarity.

The " calculated leaching-runoff fractions, Tier-1" (in blue) are not mean values; the line looks horizontal and thus the calculated Tier-1 values look equal due to that fact that the difference is small.

Suggestions for revision in Report #4

In the present study, the authors explore the extent to which fertilizer use and other agricultural management practices impact the agricultural Grey Water Footprint (GWF). The results of the study show that the GWF, which is defined as the amount of freshwater required to assimilate pollutants to meet specific water quality standards, can be reduced by 91% with a decrease in fertilizer application to corn to 50 kg/ha-y. However, with this decrease in the GWF there is also an approximately 70% decrease in yields as well as increase in the blue and green water footprints of crop production. The authors find that the overall water footprint (grey + green + blue) can be minimized with an N application rate of 150 kg/ha-y, with N being applied to the crops as manure and with changes in other management practices (no-till, deficit irrigation). Under this water-optimized scenario, crop yields decrease by 20%. Importantly, the paper shows that there are clear, quantifiable tradeoffs between environmental costs and the human benefits of crop production, and also tradeoffs between avoiding water pollution and reducing water consumption (green and blue water).

General Comments/Suggestions

Lines 49-50 How does phosphorus play into your assumptions here? Obviously the P content of runoff also contributes to the GWF. In particular, if you are using manure to meet the N requirement, you are (based on typical N:P ratios in manure) almost surely applying excess P, which would increase the GWF of the farming system. You should be explicit about your assumptions here and make clear that, even if P pollution is outside the scope of your analysis, you are likely underestimating the GWF under these scenarios.

The focus of the current study is on N-related grey WF, which is highlighted in the revised manuscript (line-96). Line 529-531 also reflect on the focus of the current study.

Lines 49-73 Very nice discussion of the complex tradeoffs among various agricultural management practices. Lines 94-96 One of the strengths of the paper is that you explore tradeoffs associated with optimizing for multiple objectives (grey water footprint, blue/green water footprint, crop yield). I think it would be useful to more explicitly include this larger goal here when you state your objectives.

Lines 99-101 Why is Badajoz, Spain a relevant site for your purposes?

Badajoz is located in the water-scarce Guadiana river basin, where reducing the green, blue and grey WF has a positive impact in managing water scarcity.

Lines 110-114 You are using a model-based approach that would also allow you to estimate losses of N to the atmosphere. Although you are specifically interested in water footprint effects here, it is also worth mentioning that managing N use also has impacts on greenhouse gas production. Optimizing for minimal pollution to the atmosphere would add additional complexity to your discussion of tradeoff. Although this is certainly beyond the scope of the present study, it would be valuable to mention this part of the agricultural management puzzle.

The focus of the current study is highlighted in the objective (introduction section) and in the discussion section.

Figure 1 The labeling on the figure is messed up—maybe this is just a function of the pdf creation, but please check.

The comment is addressed in the revised version.

Line 205 How is the beta-value defined here different from the Tier-2 mass balance approach? It seems that beta is also based on a mass balance.

The calculation of N load (beta, leaching-runoff fraction) to fresh water in Tier-2 ignores soil organic matter build-up and decomposition, and nitrogen transformations such as mineralization, immobilization and nitrification, which all affect the N uptake and N load to fresh water. We already discussed the comparison between Tier-1, Tier-2 and Tier-3 approaches in lines 105 to 118 of the manuscript.

Section 3.2 What about soil health under the low-fertilizer scenarios? Do yields decrease over time at low fertilizer application rates?

Yes, soil fertility decreases under low-fertilizer scenarios due to nutrient mining.

Section 3.2 How do things vary from year to year? How do calculated GWF rates vary under different temperatures and rainfall quantities?

The inter-annual grey WF variation is not significant, as irrigation is applied even if the rainfall quantity varies year after year.

Figure 2 This is a good figure, but it might be easier to understand if the bars were all the same height (0-100%), so we could see the proportions of the different fluxes varying under the different application rates. As it is, it is very difficult to see or understand the flux magnitudes at the lower application rates.

Presenting Figure 2 with all bars at the same height (in %) can show the proportions of the different fluxes under the different N application rates, however this option hides the magnitude of the total N load to fresh water at different N application rates.

Figure 3 Nice figure—the portrayal of the GWF under the normalized and nonnormalized conditions is very useful. Lines 332-333 It is not clear in your discussion how the use of manure N compares to that of commercial N fertilizer in terms of runoff/leaching. It has been shown that N leaching is usually greater with manure application (Edmeades, 2003, "Long-term effects of manures and fertilisers on soil productivity and quality: a review"), but your results do not seem to support this. Do the specific conditions of your simulations have an impact on these results?

In our simulation, N leaching is shown to be greater from N fertilizer than N in manure. This is in line with other studies explained in Line 57 to 61 of the manuscript. Inorganic N is readily available for uptake by crops (Haynes, 2012), whereas the organic-N contained in manure becomes available only gradually, as it should first be

converted (mineralized) to inorganic form (Ketterings et al., 2005). The mobile nature of nitrate makes it susceptible for higher risk of leaching (Yanan et al., 1997), while the slow disappearance of manure makes it susceptible to N losses through runoff before being taken up by the crop (Withers and Lord, 2002).

Line 485 Your statement here again goes back to the issue of why this study site was selected. It may not be feasible to represent, in this study, a range of climatic conditions to represent all of Europe. On the other hand, your model results should provide some information regarding how your estimate of GWF effects could vary across varying climates. Would the GWF be larger or smaller in a more humid climate? How might the recommended regime for optimizing GWF/BWF/GrWF values change across a distribution of climates and landscapes? As your stated objective is to explore how management practices and N application rates impact the water footprint (not just the water footprint in a semiarid region of Spain), it would be beneficial to include some comments regarding the wider applicability of your findings.

Exploring the validity of the findings at Badajoz at a range of climatic conditions that represent all Europe is interesting, which is however beyond the scope of the current study.

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Grey water footprint reduction in irrigated crop production: effect of nitrogen application rate, nitrogen form, tillage practice and irrigation strategy

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Abstract

Grey water footprint (WF) reduction is essential given the increasing water pollution associated with food production and the limited assimilation capacity of fresh water. Fertilizer application can contribute significantly to the grey WF as a result of nutrient leaching to groundwater and runoff to streams. The objective of this study is to explore the effect of the nitrogen application rate (from 25 to 300 kg N ha^{-1}), nitrogen form (inorganic-N or manure-N), tillage practice (conventional or no-tillage) and irrigation strategy (full or deficit irrigation) on the nitrogen load to groundwater and surface water, crop yield and the N-related grey water footprint of crop production by a systematic model-based assessment. As a case study, we consider irrigated maize grown in Spain on loam soil in a semi-arid environment, whereby we simulate the twenty-years period 1993-2012. The water and nitrogen balances of the soil and plant growth at field scale were simulated with the APEX model. As a reference management package, we assume the use of inorganic-N (nitrate), conventional tillage and full irrigation. For this reference, the grey WF at a usual N application rate of 300 kg N ha^{-1} (with crop yield of 11.1 t ha^{-1}) is 1100 m^3 t^{-1}, which can be reduced by 91% towards 95 m^3 t^{-1} when the N application rate is reduced to 50 kg N ha^{-1} (with a yield of 3.7 t ha^{-1}). The grey WF can be further reduced to 75 m^3 t^{-1} by shifting the management package to manure-N and deficit irrigation (with crop yield of 3.5 t ha^{-1}). Although water pollution can thus be reduced dramatically, this comes together with a great yield reduction, and a much lower water productivity (larger green plus blue WF) as well. The overall (green, blue plus grey) WF per tonne is found to be minimal at an N application rate of 150 kg N ha^{-1}, with manure, no-tillage and deficit irrigation (with crop yield of 9.3 t ha^{-1}). The paper shows that there is a trade-off between grey WF and crop yield, as well as a trade-off between reducing water pollution (grey WF) and water consumption (green and blue WF). Applying manure instead of inorganic-N and deficit instead of full irrigation are measures that reduce both water pollution and water consumption with a 16% loss in yield.

Key words: grey water footprint, nitrogen balance, water balance, deficit irrigation, tillage, crop growth, APEX

1. Introduction

Crop yields depend on anthropogenic addition of nitrogen (N). But using N fertilizers inevitably result in some N leaching and runoff, which result in the pollution of groundwater and surface water. Fresh water dilutes pollutant

loads entering a water body, which can be interpreted as an appropriation of fresh water (Postel et al., 1996; Falkenmark and Lindh, 1974; Chapagain et al., 2006; Hoekstra, 2008). The amount of fresh water appropriated to assimilate the load of pollutants in order to meet ambient water quality standards is called the grey water footprint (WF) (Hoekstra et al., 2011). For crop production, the grey WF can be expressed as the volume of water per hectare or per tonne [m^3 ha^{-1} or m^3 ton^{-1}]. Global crop production makes three quarters of the total N-related grey WF in the world (Mekonnen and Hoekstra, 2015). Anthropogenic N application in agriculture and the resulting fresh water pollution is expected to increase with the growing production of food, feed, fibre, and biofuel in the world, driven by population growth and improving living standards. The assimilation capacity of fresh water, however, is limited, which calls for appropriate management practices that limit the grey WF per tonne of crop production.

Factors that influence the grey WF include the N application rate, the form of N applied (particularly inorganic-N versus manure or organic-N), and the tillage and irrigation practice. A low N-application rate will hamper plant growth and reduce crop yield (Raun et al., 2002). The low N-application rate will result in relatively little water pollution per hectare, but, because of the low yield per hectare, it may cause relatively much water pollution per unit of crop produced. A high N-application rate will result in a high crop yield, but with high water pollution per hectare and per tonne of crop as well. The reason for the high water pollution per tonne of crop is that there is a threshold for the N application rate beyond which yield does not respond (Zhou et al., 2011), while the surplus N contributes to pollution (Carpenter et al., 1998; Vitousek et al., 2009). The form of N applied is another important factor affecting N losses. Inorganic N is readily available for uptake by crops (Haynes, 2012), whereas the organic-N contained in manure becomes available only gradually, as it should first be converted (mineralized) to inorganic form (Ketterings et al., 2005). The mobile nature of nitrate makes it susceptible for higher risk of leaching (Yanan et al., 1997), while the slow disappearance of manure makes it susceptible to N losses through runoff before being taken up by the crop (Withers and Lord, 2002). Field operation practices such as tillage affect the water holding capacity of the soil, the movement of moisture and nutrients in the soil, surface runoff, and eventually crop yield and nutrient load to fresh water. There are various good reasons why conventional tillage is being practiced: it mixes fertilizer, organic matter and oxygen in the soil, breaks up surface soil crusts and reduces weeds (Horowitz, 2011). However, conventional tillage disrupts aggregates within the soil and life cycles of beneficial organisms, increases soil erodability, and results in soil compaction and tillage pan formation (Triplett and Dick, 2008); tillage-pan is a formation of compacted soil layer caused by repeated ploughing using heavy weight tillage machineries (Podder et al., 2012). Alternatively, no-tillage maintains the crop residue that serves as mulch cover, improves the soil water holding capacity (Dangolani and Narob, 2013) and increases hydraulic conductivity (Azooz and Arshad, 1996; Triplett and Dick, 2008). The irrigation practice primarily influences the water balance of the soil, but as a side effect it influences nutrient movement in the soil. The advantage of deficit irrigation compared to full irrigation is that there may be less leaching and runoff of nutrients (Withers and Lord, 2002), but the disadvantage is that it may result in reduced N demand as crop growth diminished and reduced N supply as N transporting agent is reduced and thus reduction in water pollution per unit of crop produced (Gonzalez-Dugo et al., 2010).

Various studies show how increasing N-application rates result in both increased crop yield and N leaching (Berenguer et al., 2009; Rong and Xuefeng, 2011; Valero et al., 2005; Zhou et al., 2011; Cooper et al., 2012; Good and Beatty, 2011). Pittelkow et al. (2015) analysed the effect of tillage practices on crop yield; Yu et al. (2016) explored the effect of different combinations of tillage practice and N fertilizer form on crop yield; Huang et al. (2017) and Yanan et al. (1997) considered the effect of manure versus inorganic N fertilizer application on nitrate leaching; and Huang et al. (2015) analysed the effect of different tillage practices and N application rates on yield and N leaching. Furthermore, there are quite some studies on the relation between rates of irrigation and N application and crop yield (Yin et al., 2014; Al-Kaisi and Yin, 2003; Rimski-Korsakov et al., 2009). These earlier studies provide insight in the effects of individual management practices on yield, water productivity, or leaching, however most of the studies vary only one or two management practices, not considering the combined effect of N application rate, N form, tillage practice and irrigation strategy. Besides, none of these studies consider the effect on the pollutant load per unit of crop obtained or the effect on the grey WF per tonne.

It is challenging to conduct field experimental studies and even more laborious and expensive to study the effects of a comprehensive list of different combinations of management practices. Besides, leaching and runoff of N from fields is difficult to determine through field experiments; N that can be measured in groundwater and streams originates from different sources and cannot easily be attributed to an experimental field. An alternative approach avoiding these downsides is to use modelling (Chukalla et al., 2015; Ragab, 2015).

The objective of this study is to explore the effect of nitrogen application rate, nitrogen form, tillage practice and irrigation strategy on the nitrogen load to groundwater and surface water, crop yield and the N-related grey water footprint of crop production by a systematic model-based assessment. We apply the Agricultural Policy Environmental eXtender (APEX) model, which simulates nutrient and water balances of the soil and plant growth, is able to simulate the effect of a wide variety of agricultural management practices, and has been applied for a wide variety of cases (Wang et al., 2012; Gassman et al., 2010; Liu et al., 2016; Clarke et al., 2017; Chen et al., 2017). As a case study, we simulate irrigated-maize growth for twenty-years (1993-2012) at Badajoz in Spain on loam soil in a semi-arid environment.

Franke et al. (2013) distinguish three tiers to estimate grey WFs from diffuse pollution, from tier-1 to tier-3, ordered in the direction of increasing level of advancement. The tier-1 approach, simplest but also least data demanding, is based on expert-based assumptions on which fractions of applied or surplus N in the soil will leach or run off given contextual factors. It provides a first rough estimate of the N load without describing the interaction and transformation of different chemical substances in the soil or along its flow pathways (see for instance Mekonnen and Hoekstra (2011), and Brueck and Lammel (2016)). The more advanced tier-2 approach for estimating grey WFs from diffuse pollution is based on an annual N mass balance approach (see for example Mekonnen and Hoekstra (2015), and Liu et al. (2012)). This approach ignores soil organic matter build-up and decomposition, and nitrogen transformations such as mineralization, immobilization and nitrification, which all

affect the N uptake and N load to fresh water. The current study is the first one to apply the tier-3 approach, which explicitly considers daily physical and biochemical processes using an advanced water and nutrient balance model (the APEX model). As an additional component of the current study, we will compare the N leaching-runoff fractions that result from the APEX simulations with the leaching-runoff fractions estimated with the simpler tier-1 approach, in order to find out the added value of employing the advanced model approach.

2. Method and data

2.1. Modelling the soil water & nitrogen balances and crop growth

The effect of various combinations of management practices on water flows (like soil evaporation, crop transpiration, percolation and runoff), N flows (like N uptake by plants, leaching and runoff) and crop growth are simulated using the APEX model, a dynamic, deterministic and process-based model with a daily time step (Williams and Izaurralde, 2006). Below we briefly summarise the processes simulated in the model. More detailed descriptions of the processes and the equations to simulate these processes can be found in the documentation of APEX (Williams et al., 2008).

The water balance component of APEX encompasses key processes that impact the soil water compartment in the hydrologic cycle. Initially, incoming inputs such as precipitation, snowmelt, or irrigation is partitioned between surface runoff and infiltration. Surface runoff volume is simulated using a modified Soil Conservation Service curve number technique described by Williams (1995). Infiltrated water can be stored in the soil profile, be lost via evapotranspiration (ET), percolate vertically to groundwater, or flow laterally as subsurface flow, with a quick and slow component. Reference ET is calculated using the Penman-Monteith method. The actual ET, an important variable in estimating green and blue WF of crop production, is computed by simulating evaporation from the soil and transpiration from plants separately, considering the soil moisture status and how agricultural management practices affect the root zone. Percolation and lateral flow are computed using storage routing and pipe flow equations described by Gassman et al. (2010). A deep groundwater table is assumed and thus capillary rise, which APEX would simulate using storage routing (Gassman et al., 2010), is not considered in the water balance.

The N balance of the soil in APEX is computed based on inputs and outputs and conversion processes (Figure 1). N is added to the soil-plant system through natural and anthropogenic pathways. Natural N inputs include wet and dry deposition (Anderson and Downing, 2006) and N fixation, through lightning and through biological fixation by legume plants (Carpenter et al., 1998). Anthropogenic input occurs when inorganic or organic N fertilizers are applied (Vitousek et al., 2009). N outputs include N uptake by crops (partly harvested and removed later on), denitrification, volatilization, nitrate-N losses through leaching, horizontal losses of organic N with eroded sediments, and horizontal losses of inorganic N through surface runoff, or lateral subsurface flow. N transformation includes mineralization, immobilization and nitrification.
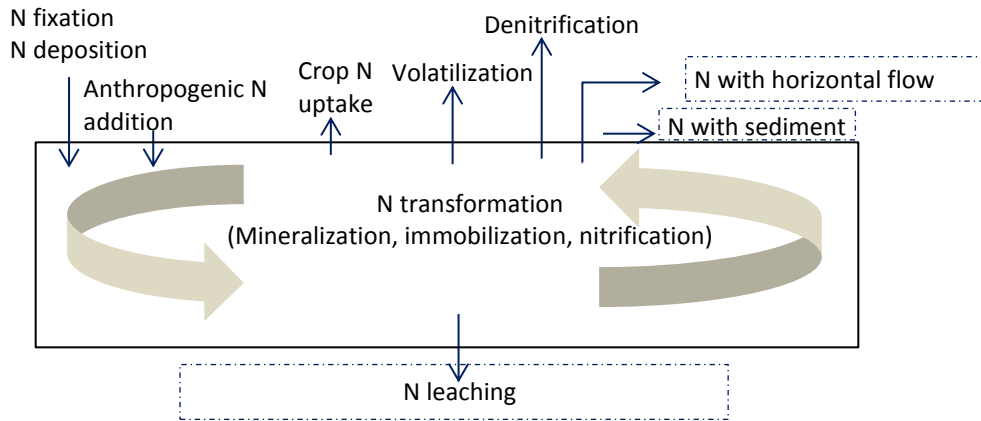
Figure 1. Nitrogen fluxes into and from the root zone, and N transformation.

APEX simulates the growth of annual and perennial crops based on the EPIC model (Williams et al., 1989), an energy-driven crop growth model using a radiation-efficiency approach to simulate the generation of biomass. Potential biomass production is derived as function of leaf area index and climatic variables (solar radiation, CO_2, air humidity and temperature). Pheenological development of the crop is based on heat unit accumulation measured in growing degree days. Annual crops grow from planting date to harvest date or until the accumulated heat units equal the potential heat units for the crop (Steduto, 1997). Daily potential growth is lowered to actual growth using the most limiting stress factor, considering stresses caused by water, nutrients (N and P), temperature and aeration, which are evaluated by assigning stress factors (from 0, high stress, to 1, no stress). Root growth is constrained based on the most limiting stress caused by soil strength and temperature. Total biomass is partitioned to root and above ground biomass, and from the above-ground biomass is the economic yield is partitioned using harvest index.

2.2. The grey water footprint of growing crops

The grey water footprint (WF), an indicator of appropriated pollution assimilation capacity, is calculated following the Global Water Footprint Standard (Hoekstra et al., 2011), which means that the total pollutant load entering fresh water (groundwater or surface water) is divided by the difference between the maximum acceptable concentration for that pollutant and the natural background concentration for that pollutant. The grey WF can be expressed in two different ways, either as a water volume per ha, or as a water volume per tonne of crop:

$$Grey\ WF\ per\ hectare\ = \frac{L}{C_{max}-C_{nat}}\ [m^3\ ha^{-1}\ y^{-1}] \tag{1a}$$

$$Grey\ WF\ per\ tonne\ = \frac{Grey\ WF\ per\ hectare}{Y}\ [m^3\ t^{-1}] \tag{1b}$$

13

where L (kg ha^{-1} y^{-1}) is the pollutant load to surface water and groundwater, C_{max} and C_{nat} are the maximum acceptable and natural concentrations (kg m^{-3}), and Y the crop yield (t ha^{-1} y^{-1}).

The total N load to fresh water (L, in kg N ha^{-1} y^{-1}) is calculated as the sum of the N load in surface runoff, the N in quick subsurface flow, the N in slow subsurface flow, the N adsorbed to eroded sediments and the N in percolation. Each of these N loads are simulated separately in APEX.

A maximum acceptable N concentration of 50 mg nitrate-N L^{-1} (or 11.3 mg N L^{-1}) is adopted, based on the EU Nitrates Directive (Monteny, 2001). The natural concentration was considered to be 0.5 mg N L^{-1}, following for example (de Miguel et al., 2015).

Next to the grey WF, the green and blue WF of crop production are calculated as well, again using the Global WF standard (Hoekstra et al., 2011). The green WF refers to the rainwater consumed (water evaporated or incorporated into the crop), while the blue WF refers to the irrigation water consumed (which comes from surface water or groundwater). Together, the green and blue WF are called the consumptive WF. The consumptive WF per tonne of crop is calculated by dividing the ET over the growing period by the crop yield.

2.3. Leaching-runoff fraction

As an additional component of the current study, we will compare the N leaching-runoff fraction simulated through APEX (tier-3 level estimation) with the leaching-runoff fraction estimated with the simpler estimation approach (tier-1) as applied in previous studies, in order to find out when the simple tier-1 approach suffices and when it doesn't.

The leaching-runoff fraction can be defined in two ways (Franke et al., 2013). In the first definition, the leaching-runoff fraction, called α, is defined as the percentage of the amount of chemical applied to the field as fertilizer that is lost to groundwater through leaching or to surface water through runoff. In the second definition, the leaching-runoff fraction, now called β, is defined as the percentage of the amount of 'surplus chemical' in the soil that is transported to groundwater by leaching or to surface water by runoff. The 'surplus chemical' in the soil is defined as the amount of chemical applied minus the uptake of the chemical by the crop.

$$\alpha = \frac{L}{Appl} \qquad (2)$$

$$\beta = \frac{L}{Surplus} \qquad (3)$$

where α and β are the leaching-runoff fractions, and where L (kg N ha^{-1} y^{-1}) is the N load to fresh water bodies due to the anthropogenic N addition, Appl (kg N ha^{-1} y^{-1}) the N fertilizer applied, and Surplus (kg N ha^{-1} y^{-1}) the N applied but not taken up by the plant.

At the tier-3 level, the fractions α and β are not used in the calculations, but they can easily be calculated afterwards, based on the outputs of the model. At the tier-1 level, α and β can be estimated using equation 4 and 5 following the guidelines of Franke et al. (2013). According to these guidelines, the leaching-runoff fractions lie between a minimum and a maximum value (0.01 to 0.25 for α and 0.08 to 0.8 for β). The precise value is estimated based context-specific environmental and management factors, using the following equations:

$$\alpha = \alpha_{min} + \left[\frac{\sum_i s_i * w_i}{\sum_i w_i}\right] * (\alpha_{max} - \alpha_{min}) \tag{4}$$

$$\beta = \beta_{min} + \left[\frac{\sum_i s_i * w_i}{\sum_i w_i}\right] * (\beta_{max} - \beta_{min}) \tag{5}$$

where s_i is the score for the leaching-runoff potential for environmental or management factor i, and w_i is the weight of that factor. Corresponding to a certain state of factor, i, a score s is assigned between 0 and 1: scores of 0, 0.33, 0.67 and 1 refer to a very low, low, high and a very high leaching-runoff potential, respectively. A weight w per factor i denotes the importance of the factor. The weights given to the separate influencing factors add up to a total of 100.

2.4. Simulation set-up

We carry out model simulations with APEX for 56 management packages, whereby each management package consists of a certain combination of management practices. We consider all possible combinations of seven N application rates, two N forms, two tillage practices, and two irrigation strategies (Table 1). As a reference management package, we assume the use of inorganic N fertilizer (nitrate) in combination with conventional tillage and full irrigation. Conventional tillage is the most wide-spread tillage practice in the EU (EUROSTAT, 2013) and full irrigation is the most common irrigation practice, aimed at achieving maximum yield.

Table 1. Research set-up: the APEX model is used to simulate the effect of 56 management packages (combinations of different management practices) on ET, crop yield, nitrogen load to fresh water, and green, blue and grey WF.

Management practices	Modelling	Effects
• Nitrogen application rates: 25, 50, 100, 150, 200, 250 or 300 kg N ha^{-1} y^{-1} • Nitrogen forms: inorganic-N (nitrate) or organic-N (manure)	Soil water & nutrient balances and crop growth model (APEX)	- ET - Yield - N load

• Tillage practices: no-tillage or conventional tillage • Irrigation strategies: full or deficit irrigation	- Green, blue, grey WF

The EU Nitrate Directive legally restricts annual farm application of manure in EU member states to 170 kg N ha^{-1} y^{-1}, or in case of derogation up to 250 kg N ha^{-1} y^{-1} (Amery and Schoumans, 2014; Van Grinsven et al., 2012). Surveys in Spain, however, show that application rates of 300-350 kg N ha^{-1} y^{-1} are common to cultivate maize in the Ebro Valley (Berenguer et al., 2009) and up to 300 kg N ha^{-1} y^{-1} in La Mancha (Valero et al., 2005). As the upper value for the N application rate in our simulations we apply 300 kg N ha^{-1} y^{-1}.

The fertilization is assumed to be performed in two splits (30% in a first round, at planting for mineral fertilizer and 15 days before planting for manure; 70% in a second round, one month after planting). In the first round of application, inorganic fertilizer is assumed to be nitrate-N and applied through broadcasting while manure is assumed to be injected. Manure injection is getting recognition in the EU and in the world due to its many advantages, including reduction of N losses to fresh water and to the atmosphere and bad odour (Van Dijk et al., 2015; van den Pol-van Dasselaar et al., 2015). In the second round, both the manure and nitrate-N fertilizers are added as side-dressing.

As for the inorganic N applied, we assume that the N is 100% in the form of nitrate. Manure is generally contained of mostly organic N, and a smaller amount of inorganic N (Ketterings et al., 2005; Pratt and Castellanos, 1981). In this study, we assume the manure composition as in the APEX database: 91.67% organic N, 8.33% inorganic N (0.23% nitrate and 8.10% ammonium N). In addition, the current study assumes that other nutrients (P, K and micro nutrients) do not to constrain crop production.

We simulate conventional tillage in APEX as two times ploughing to a depth of 20 cm at thirty and fifteen days before sowing date and one time harrowing following the emergence of the seed. The two times ploughing is the average of what is most common, namely one to three times tilling (Nagy and Rátonyi, 2013; FAO, 2016). With the tillage depth of 20 cm we follow the average estimate reported by Townsend et al. (2015) and FAO (2016). No-tillage, a form of conservation tillage that is strongly encouraged by the EU agricultural policy (De Vita et al., 2007), is simulated as no soil disturbance; the stubble of the previous crop is kept on the field.

We simulate full irrigation in APEX by irrigating up to field capacity as soon as the soil water content would otherwise drop below a level at which water stress occurs. Deficit irrigation is simulated to allow for 20% plant water stress, a deficit level that can achieve 61-100% of full ET (Fereres and Soriano, 2007). With this irrigation strategy, average water productivity is higher than in case of full irrigation (Chukalla et al., 2015). We assume the

use of furrow irrigation, the irrigation technique that covered the largest irrigated area in the EU in 2010, particularly in the Eastern and Mediterranean regions of Europe (EUROSTAT, 2016).

2.5. Data

The model experiment is carried out at field scale for a place near Badajoz in Spain, in the Guadiana river basin, which has a semi-arid climate and faces water scarcity during part of the year, particularly in summer when water is needed for irrigation (Hoekstra et al., 2012).

The following climatic and soil data have been collected for Badajoz in Spain (38.88° N, -6.83° E; 185 m above mean sea level). Daily observed rainfall and temperature data (for the period 1993-2012) are extracted from the European Climate Assessment and Dataset (Klein Tank et al., 2002). These data have been subject to homogeneity testing and missing data have been filled with observations from nearby stations (Klein Tank, 2007). Mean monthly solar radiation, relative humidity and wind speed data are taken from the FAO CLIMAWAT database (Smith, 1993). Daily reference evapotranspiration is calculated using the Penman-Montheith equation, as implemented in APEX (Williams et al., 2008). The average monthly climatic and reference evapotranspiration data are shown in Table A.1 in Appendix~~Table 2~~.

~~**Table 2.** The average monthly climatic data of Badajoz in Spain.~~

~~Climatic variables~~	~~Jan~~	~~Feb~~	~~Mar~~	~~Apr~~	~~May~~	~~Jun~~	~~Jul~~	~~Aug~~	~~Sep~~	~~Oct~~	~~Nov~~	~~Dec~~
~~Temperature max, °C~~	~~14.1~~	~~16.5~~	~~20.4~~	~~22.2~~	~~26.1~~	~~31.9~~	~~34.9~~	~~34.7~~	~~30.0~~	~~24.4~~	~~18.0~~	~~14.3~~
~~Temperature min, °C~~	~~3.6~~	~~4.2~~	~~6.7~~	~~9.0~~	~~12.2~~	~~15.8~~	~~17.3~~	~~17.6~~	~~15.2~~	~~11.9~~	~~7.3~~	~~4.9~~
~~Precipitation, mm~~	~~50.2~~	~~39.5~~	~~30.9~~	~~41.1~~	~~41.9~~	~~10.8~~	~~2.3~~	~~4.2~~	~~25.1~~	~~64.4~~	~~65.2~~	~~64.0~~
~~Solar radiation, MJ/M^2~~	~~7.4~~	~~10.5~~	~~12.9~~	~~19~~	~~21.9~~	~~25.7~~	~~26.9~~	~~23.9~~	~~17.8~~	~~12.3~~	~~8.1~~	~~6.4~~
~~Relative humidity, %~~	~~83~~	~~71~~	~~63~~	~~56~~	~~45~~	~~42~~	~~37~~	~~35~~	~~46~~	~~64~~	~~76~~	~~80~~
~~Wind speed, m/s~~	~~1.7~~	~~1.9~~	~~2.09~~	~~2.09~~	~~2.2~~	~~2.3~~	~~2.4~~	~~2.2~~	~~1.81~~	~~1.6~~	~~1.7~~	~~1.7~~
~~ET$_0$, mm~~	~~33.2~~	~~57.1~~	~~108.8~~	~~145.3~~	~~196.6~~	~~224.2~~	~~250.9~~	~~218.2~~	~~139.7~~	~~83.7~~	~~43.3~~	~~29.3~~

Using the Soil Texture Triangle Hydraulic Properties Calculator from (Saxton et al., 1986), we identified the soil at our location as loam soil. The physical and chemical characteristics of the soil, and nutrient content in the soil (nitrogen, phosphorus, carbon) that are used in APEX are extracted from the 1×1 km^2 resolution European Soil Database (Hannam et al., 2009). We use a soil albedo of 0.13 for a loam soil at its field capacity (Sumner, 1999).

Regarding crop parameters, we use the default values from the APEX model. The effect of stresses related to weed, pest and diseases on crop growth are not considered; we simulate the effect of stresses from excess and limitation of water, from limitation of nitrogen, and from very high or very low temperature.

17

Soil moisture content is initialised using the standard procedure in APEX, which is based on average annual rainfall within the period considered (1993-2012). We adjust initial organic-N content for each simulation so that the N build-up in the soil over the 20-year period is zero. We apply the graphical time-series inspection method (Robinson, 2002) to determine the warm-up period, i.e. the period in which simulation results are still affected by the model initialization. We find that we best exclude the first five years of the simulation, thus we show results for the period 1998-2012.

3. Results

3.1. Pollutant loads and grey WF for the reference management package

N out-fluxes from the soil for maize production under the reference management package (inorganic-N, conventional tillage, full irrigation) for different N application rates are shown in Figure 2. The N out-fluxes are denitrification and volatilization to the atmosphere, N harvested with the crop, and N loads to fresh_water adhered to sediment and dissolved in percolation and runoff. All of these N out-fluxes increase with the N application rate and with the N surplus in the root zone (N application minus crop uptake). For all N application rates the N harvested with the crop is the main share of the N out-flux. For larger N application rates, the share of N leaching increases substantially. For all application rates, N leaching to groundwater constitutes at least 95% of the total N load to fresh_water, and the N flux to surface water (N dissolved in runoff plus N in eroded sediments) 5% at most.

Crop yields increase with the N application rate as a result of reduced N stress. Yields stabilize at larger N application rates. The yield increase, however, comes at a price: the N load to fresh_water, through leaching, runoff and eroded sediment, increases exponentially. As a result, large N-application rates result in a large grey WF (Figure 3). At lower N-application rates, crop yields decline as a consequence of N stress. While the grey WF in m^3 ha^{-1} keeps on declining with lower N-application rates, the grey WF in m^3 t^{-1} starts increasing again at very low N-application rate (in our case when the N-application rate drops below 50 kg N ha^{-1}. The smallest grey WF per tonne can be found at an N-application rate of 50 kg N ha^{-1}, where yield is substantially lower than the maximum, but where additional N application goes along with increasing N load per unit of crop yield gain, thus with increasing grey WF per tonne.
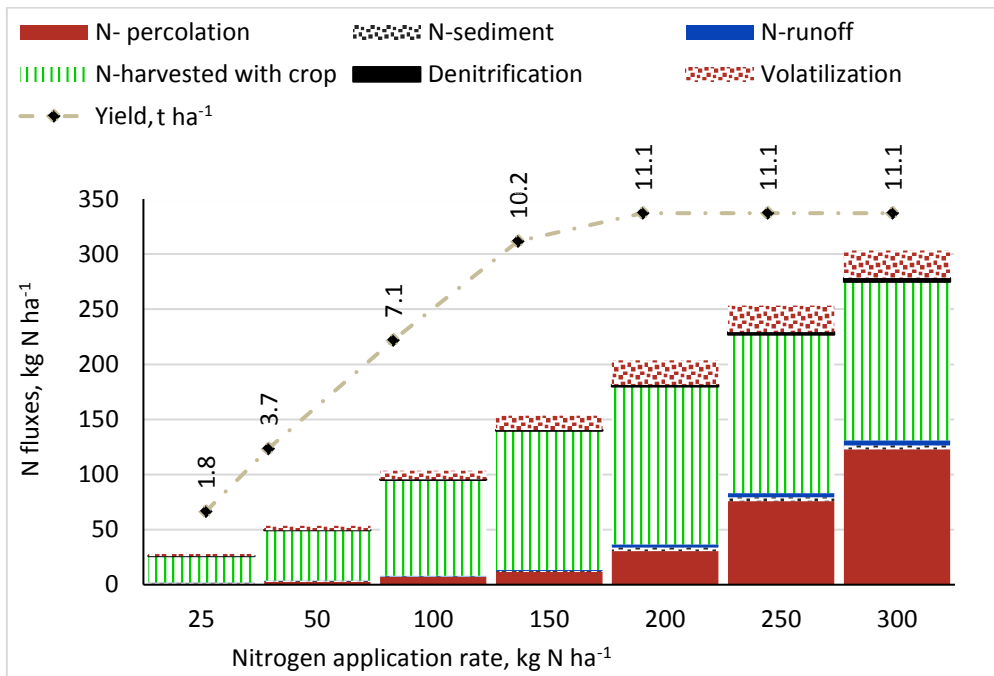
Figure 2. Nitrogen out-fluxes and yield for an irrigated maize field for a range of N-application rates under the reference management package (inorganic-N, conventional tillage, full irrigation).
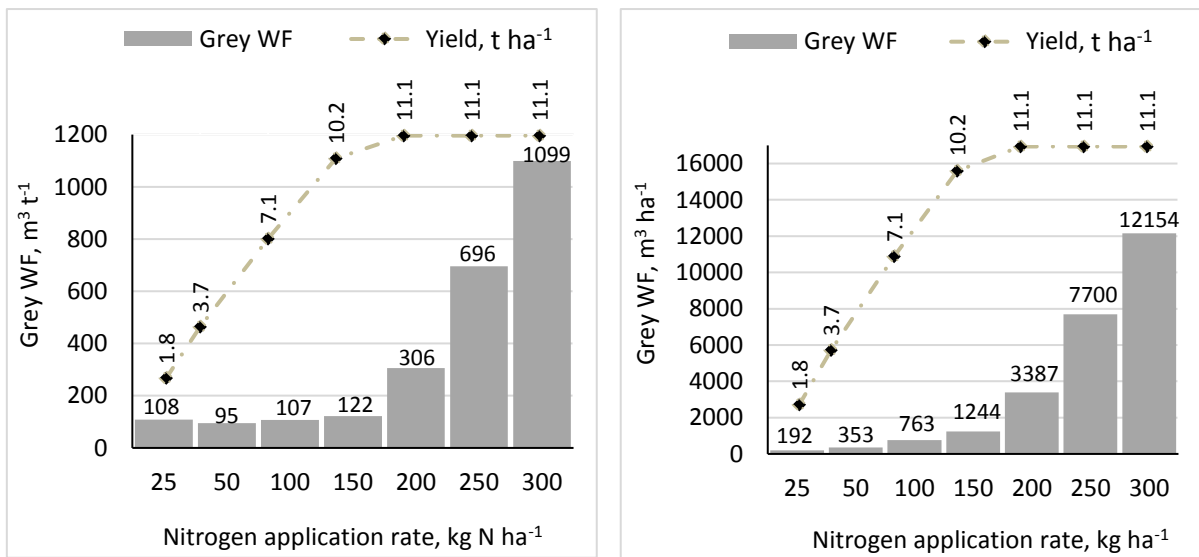

Figure 3. Grey WF of maize production in m^3 t^{-1} (left) and m^3 ha^{-1} (right) for a range of N-application rates under the reference management package.

3.2. Effect of fertilizer form, tillage practice and irrigation strategy on grey WF

Figure 4 shows that, at a given N-application rate, the grey WF in $m^3\ t^{-1}$ can be higher or lower than for reference management package, by changing to manure, no-tillage or deficit irrigation, or a combination of those. Across the whole range of N application rates, the use of manure results in a smaller grey WF per tonne than the use of nitrate fertilizer. The effect of the tillage practice and irrigation strategy on the grey WF depends on the N-application rate. We can identify three ranges for the application rate, each with a different management package resulting in the smallest grey WF per tonne:

I.   Application rates up to 125 kg N ha^{-1}: the grey WF is smallest for manure with conventional tillage and deficit irrigation;

II.   Application rates between 125 and 225 kg N ha^{-1}: the grey WF is smallest for manure with conventional tillage and full irrigation;

III. Application rates above 225 kg N ha^{-1}: the grey WF is smallest for manure with no-tillage and full irrigation.

At low and intermediate N-application rates (ranges I-II), the advantage of conventional tillage over no-tillage is that it decreases the hydraulic conductivity of the soil (because of the removal of fine cracks in the soil), which reduces percolation and thus N leaching. At high N-application rates (range III), no-tillage appears to be better. The disadvantage of increased hydraulic conductivity is now compensated by another effect: no-tillage results in improved soil texture: the soil remains intact, which in combination with the build-up of organic content creates favourable conditions for soil organisms that help to glue the soil particles and increase the number of micro-pores and macro-pores in the soil. This increases the soil water holding capacity and thus N holding capacity of the soil, resulting in lower N leaching (by 30%) and higher yield (by 3.6%).

At low application rates (ranges I), deficit irrigation decreases the amount of water available for percolation and thus reduces N leaching as well. At intermediate and higher N-application rates (ranges II-III), full irrigation has a smaller grey WF per tonne as compared to deficit irrigation because of the higher crop yield. With the absence of water stress and the higher yield, the N uptake by the crop is higher, resulting in a lower N surplus in the root zone and decreased N leaching.
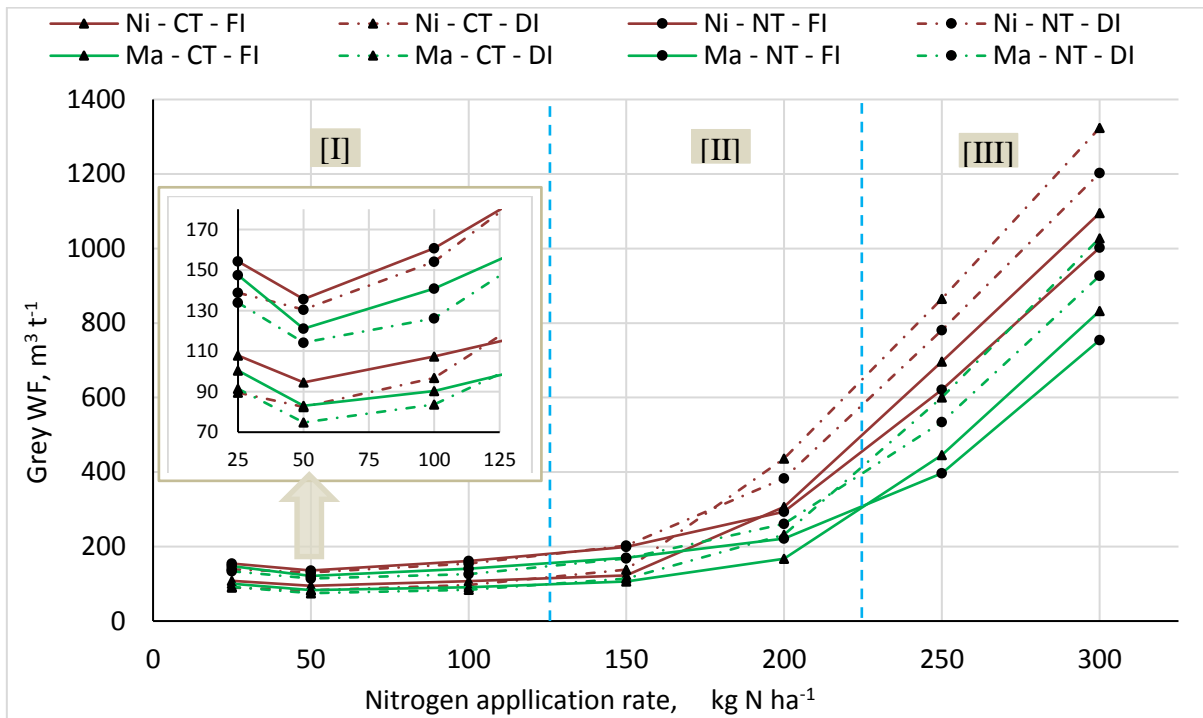
Figure 4. The effect of N application rate, N form, tillage practice and irrigation strategy on grey WF per tonne. Considering which management package gives the lowest grey WF, three ranges can be distinguished: [I] N application rates up to 125 kg N ha^{-1}, [II] N application rates between 125 and 225 kg N ha^{-1}, [III] N application rates above 225 kg N ha^{-1}. Red lines refer to nitrate (Ni); green lines refer to manure (Ma). Circular markers refer to no-tillage (NT); triangular markers refer to conventional tillage. Dashed lines refer to deficit irrigation (DI); solid lines refer to full irrigation (FI).

The smallest grey WFs per tonne are found for an N application rate of 50 kg N ha^{-1}. Taking the reference management package with an N application rate of 300 kg N ha^{-1} as a starting point, one can reduce the grey WF per tonne of crop production by reducing the N application rate while keeping the management package fixed, by shifting the management package to one with a smaller grey WF, or both (Table A.2~~1~~ in Appendix). Reducing the N application rate from 300 kg N ha^{-1} to the optimum of 50 kg N ha^{-1} under the reference management package will reduce the grey WF by 91% (from around 1100 to 95 m^3 t^{-1}), but the crop yield will reduce by two thirds (from 11.1 to 3.7 t ha^{-1}). When, at the application rate of 50 kg N ha^{-1}, shifting from the reference management package to organic N and deficit irrigation, once can further reduce the grey WF by 21% (from around 95 to 75 m^3 t^{-1}), with a yield reduction of 5% (from 3.7 to 3.5 t ha^{-1}).

3.3. Reducing grey WF vs consumptive WF

Both ET and yield increase with increasing N application rate, but level off at large N application rates (Figure 5a). Adding more N at relatively low application rates has a larger impact on Y increase than on ET increase. As a result, the consumptive WF per tonne, defined as ET over Y, decreases with increasing N application rate, levelling off at larger N application rate (Figure 5b). The grey WF per tonne, however, exponentially increases with increasing N application rate. As a result, the sum of grey and consumptive WF has a minimum somewhere at intermediate N application rate, at 150 N ha^{-1} in the case of our reference management package. The total WF is dominated by the consumptive WF for smaller N application rates and by the grey WF for larger N application rates.
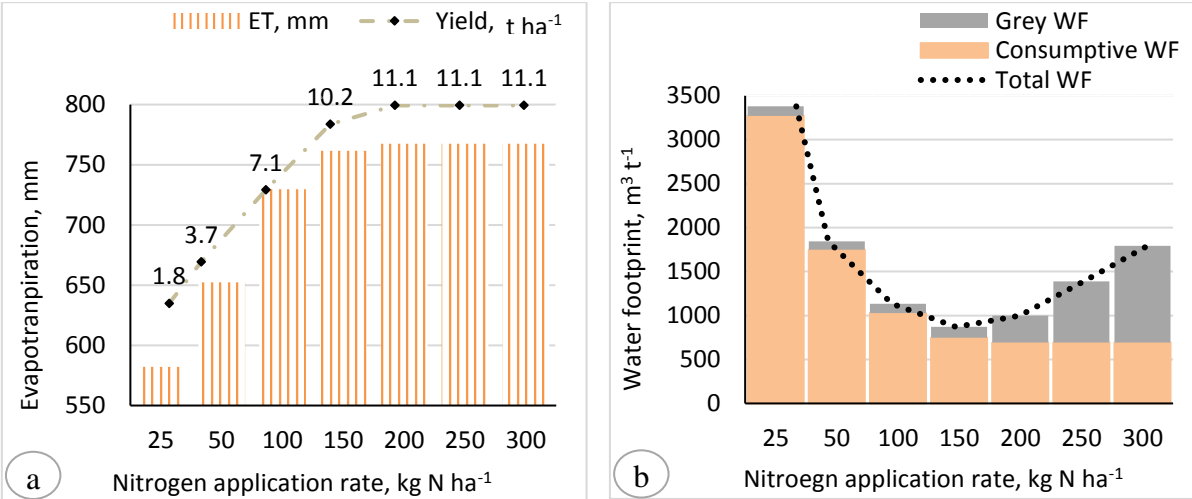

Figure 5. Evapotranspiration and yield (Fagard et al.) and consumptive WF and grey WF per tonne (b) for the reference management package.

Figure 6 shows the total (grey+consumptive) WF per tonne for the reference management package for different N application rates (the solid red line). For each given N application rate, shifting to another management package (the dashed red and green lines, and the solid green line) can reduce the total WF. Generally, the reduction in total WF is the result from reductions in both the grey WF and the consumptive WF (as indicated in the figure). At N application rates of 25, 50 and 100 kg N ha^{-1}, the total WF can be reduced by shifting towards no-tillage and deficit irrigation. At N application rates of 150 kg N ha^{-1}, the total WF can be reduced by shifting towards organic N, no-tillage and deficit irrigation. Finally, at N application rates of 200, 250 and 300 kg N ha^{-1}, the total WF can be reduced by shifting towards organic N and no-tillage. The total WF reductions shown in the figure are the net effect of changes in the consumptive WF and grey WF; in some cases, the total WF decrease is at the cost of some grey WF increase.
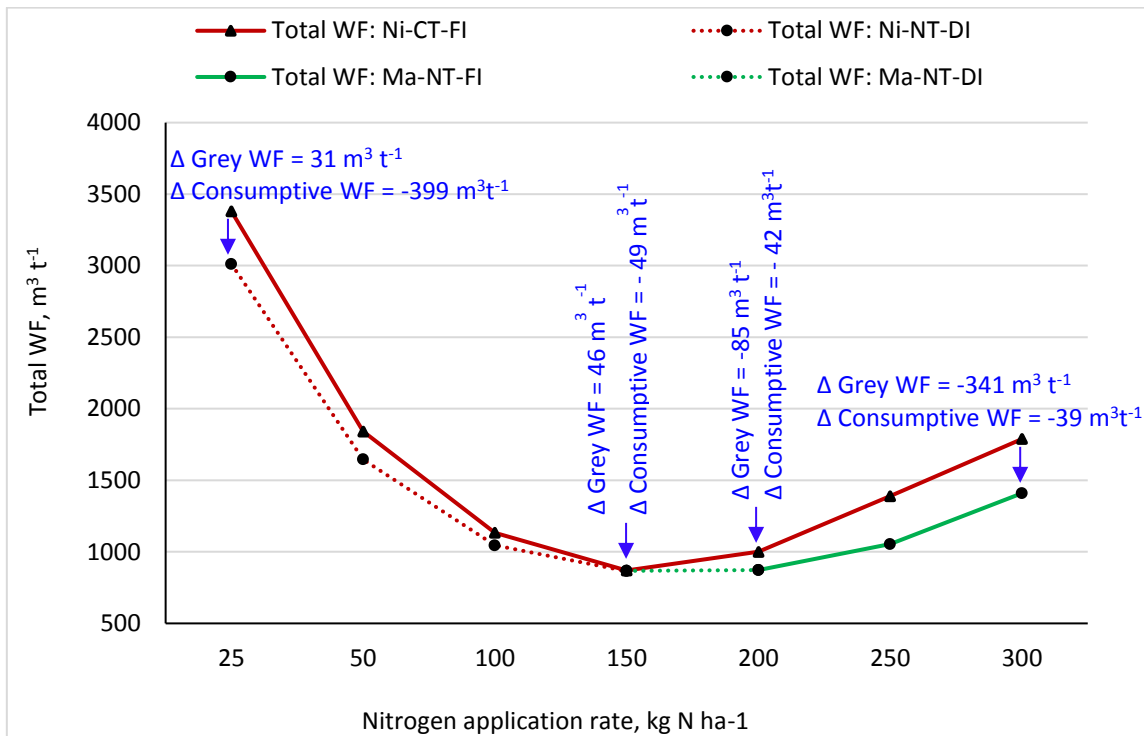
Figure 6. The total (green, blue plus grey) WF per tonne for the reference management package and for a management package with the largest total WF reduction potential. Red lines refer to nitrate (Ni); green lines refer to manure (Ma). Circular markers refer to no-tillage (NT); triangular markers refer to conventional tillage. Dashed lines refer to deficit irrigation (DI); solid lines refer to full irrigation (FI).

3.4. Resultant leaching-runoff fractions

The N leaching-runoff fractions α and β for different N application rates for the reference management package, as calculated here with the tier-3 approach, are shown in Figure 7. The α values, which show the ratio of the N load to fresh water to the N application rate are lower than the β values, which show the ratio of the N load to the N surplus in the soil. This can be logically understood, because the N load to fresh water (in the numerator of both ratios) is the same, while the α ratio has the total N application rate in the denominator, while the β ratio has the relatively smaller N surplus (which is only a fraction of the N applied) in the denominator.

With increasing N application rate, both N surplus in the soil and the N load to fresh water increase exponentially (Figure 2). The α values grow with increasing N application rate, because the N load to fresh water increases quicker with increasing N application rates than the application rate itself. The β values also grow with increasing N application rates, because denitrification and volatilization do not grow proportionally to the growth in N surplus, which leads to greater fractions of the surplus getting lost through leaching and runoff.
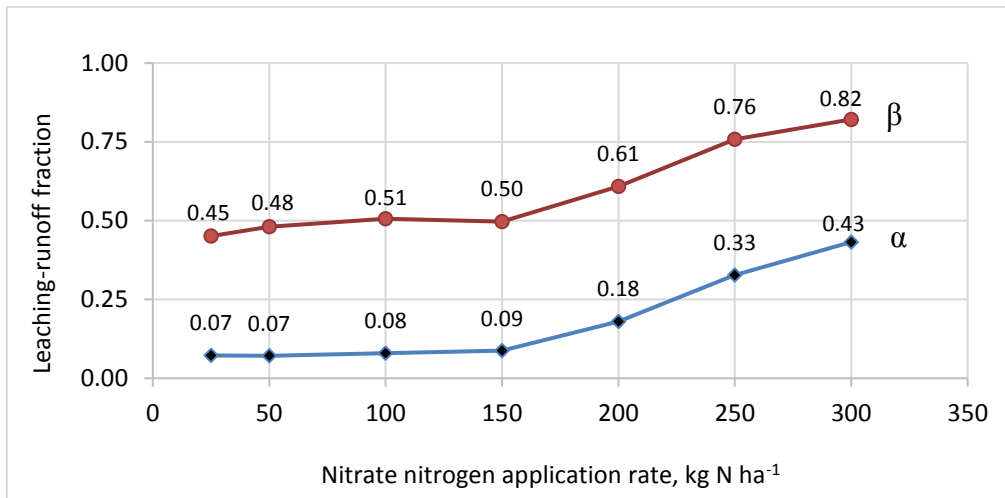
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Figure 7. The N leaching-runoff fractions α and β calculated per N application rate for the reference management package.

Figure 8 and Figure 9 show α and β values for different management packages and N application rates. For comparison, the figures also show the α and β values when estimated based on the simpler tier-1 approach (Tables A.32 and A.43 in Appendix), which estimates α and β within minimum and maximum values based on context-specific environmental and management factors (see section 2.3). The calculated leaching-runoff fractions based on the APEX model (tier-3 approach) for all management packages across the range of N application rates fall within the range set by the minimum and maximum leaching-runoff fractions margins as applied in the tier-1 approach (Franke et al., 2013), except for α for very high N application rates.

For N applications rates in the range up to 150 kg ha^{-1}, the tier-1 approach gives a good proxy for the α value. For the reference management package, the most common practice, the tier-1 approach even yields nearly the same α values as the more advanced tier-3 approach. For N applications rates exceeding about 150 kg ha^{-1}, the tier-1 approach underestimates the leaching-runoff fraction and thus the grey WF. The β values estimated based on the tier-1 approach are comparable to the ones calculated at the tier-3 level for the management packages with manure and conventional tillage. For the other management packages, β is underestimated with the tier-1 approach. Also for N application rates of 250 kg ha^{-1} and beyond, the tier-1 approach underestimates β.

The leaching-runoff fractions from the application of inorganic N (nitrate) calculated at the tier-3 level are larger than these for organic N (manure), a distinction that is not made in the tier-1 approach.
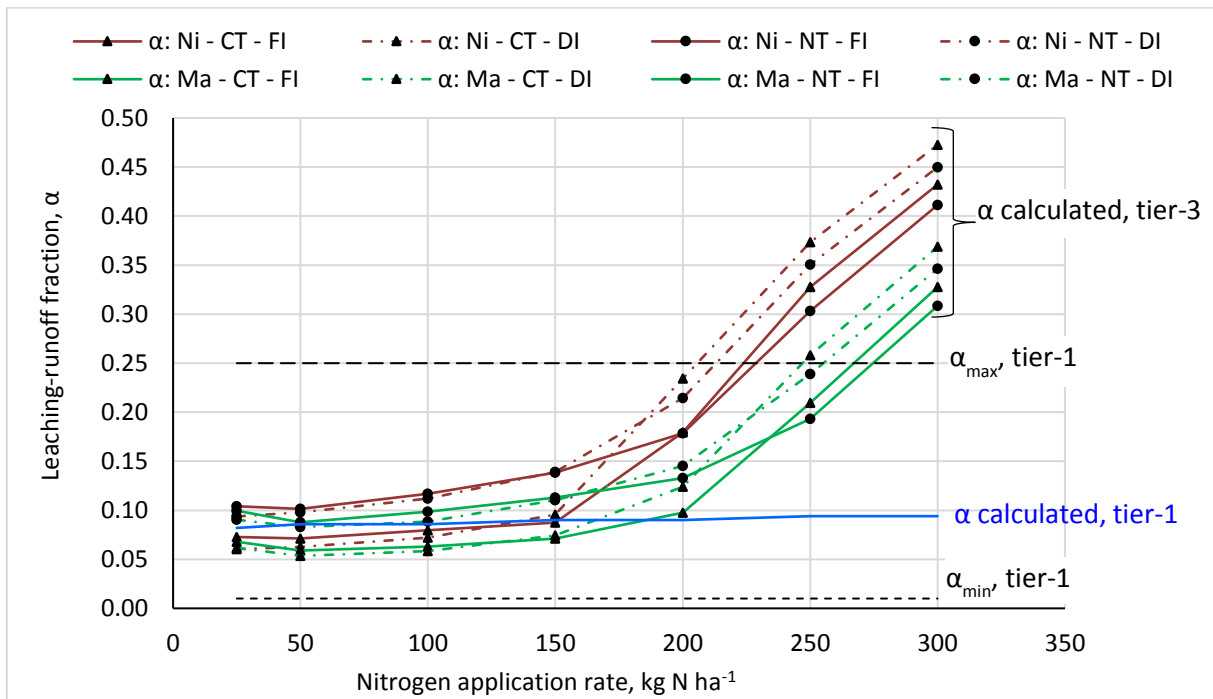
Figure 8. N leaching-runoff fractions α for different management packages and N application rates following from the tier-1 or tier-3 approach. Red lines refer to nitrate (Ni); green lines refer to manure (Ma). Circular markers refer to no-tillage (NT); triangular markers refer to conventional tillage. Dashed lines refer to deficit irrigation (DI); solid lines refer to full irrigation (FI).

Figure 9. N leaching-runoff fractions β for different management packages and N application rates following from the tier-1 or tier-3 approach. Red lines refer to nitrate (Ni); green lines refer to manure (Ma). Circular markers refer to no-tillage (NT); triangular markers refer to conventional tillage. Dashed lines refer to deficit irrigation (DI); solid lines refer to full irrigation (FI).
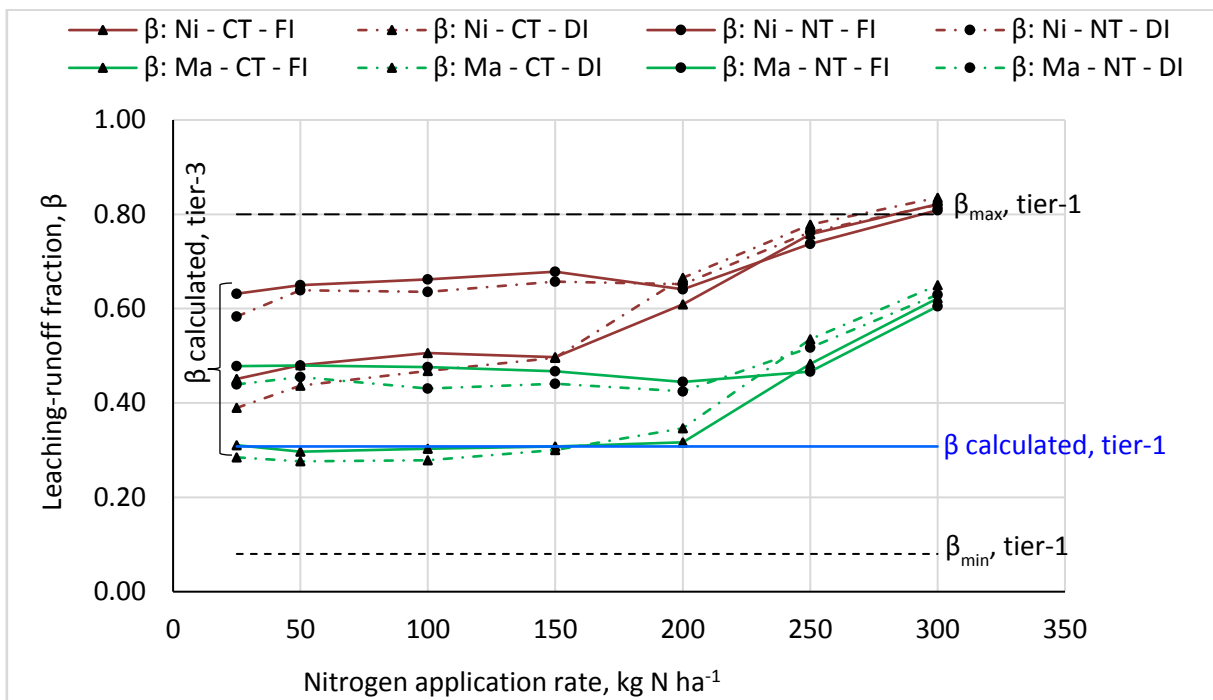
4. Discussion

The study shows that there is not one combination of management practices that minimises grey WF or overall WF and maximises crop yield at the same time. Table 23 shows that the best combination of practices depends on what variable is optimised. Yield is optimal when there is neither nitrogen stress nor water stress, so at high N application rate and full irrigation. The highest yield (11.5 t/ha) is found for when N is applied in the form of manure and the case of no-tillage. The total WF per tonne (the sum of the green, blue and grey WF) is smallest at 150 kg N ha^{-1}, manure application, no-tillage and deficit irrigation. The yield in this case, 9.3 t/ha, is below-optimum. There is both nitrogen and water stress, but the latter is more important. The grey WF per tonne is smallest at 50 kg N ha^{-1}, manure application, conventional tillage and deficit irrigation. This, however, reduces the yield to 3.5 t/ha because of nitrogen stress. Deficit irrigation gives some water stress as well, but at such high nitrogen stress, it is the latter that constrains crop yield. Our results confirm the finding by (Mekonnen and Hoekstra, 2014) that there is a trade-off between consumptive WF per tonne and grey WF per tonne, i.e. a trade-off between reducing water consumption and water pollution.

Table 23. The measures that give the optimum grey WF per tonne, total WF per tonne, or yield.

Indicator⟍ Management practice	Highest yield In t ha^{-1}	Smallest total WF* in m^3 t^{-1}	Smallest grey WF in m^3 t^{-1}
Nitrogen application rate	200 kg N ha^{-1}	150 kg N ha^{-1}	50 kg N ha^{-1}
Nitrogen form	Manure	Manure	Manure
Tillage practice	No-tillage	No-tillage	Conventional tillage
Irrigation strategy	Full irrigation	Deficit irrigation	Deficit irrigation

* Total WF refers to the sum of the green, blue and grey WF.

The response of maize yield to nitrogen input as simulated in this study with the APEX model is comparable with the shape of the N-response curves for a few crops, including maize, constructed for the EU based on field measurements from various earlier studies (Godard et al., 2008). Our finding is also consistent with the results presented by Berenguer et al. (2009), who carried out field experiments for maize for similar conditions in Spain (Figure 10). For every given N input, their yields are a bit25% higher than from our study, which may relate to the fact that Berenguer et al. (2009) used a high-yield maize variety.
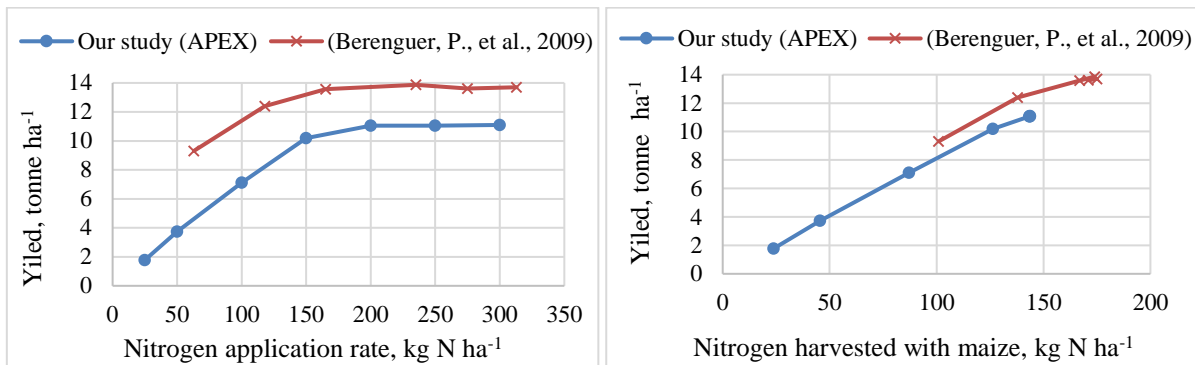
Figure 10. The maize yield simulated in our study in relation to N application rate (left) and N harvested with maize (right) in comparison to the maize yields from field experiments by Berenguer et al. (2009) when corrected for zero N build-up in the root zone.

An inter-model comparison for the case of no N stress and no water stress (taking optimal N application rate and full irrigation) for exactly the same growing conditions in Spain shows similar crop yields and net irrigation supply. The current study, using the APEX model, simulates a net irrigation supply of 638 mm and a maize yield of 11.1 t ha^{-1}, while in an earlier study, employing the AquaCrop model (Steduto et al., 2011), we simulate an irrigation supply of 630 mm and a maize yield of 11.9 t ha^{-1} (Chukalla et al., 2015). APEX is reported to adequately simulate evapotranspiration for different management practices with the Penman Monteith equation for semi-arid conditions in the Mediterranean, including Spain (Cavero et al., 2012). The study by Milly and Dunne (2016), however, reported that Penman Monteith overestimates evapotranspiration for non-water stress conditions, which suggests that ground-truthing with field experiments is necessary.

While acknowledging the need for further validation of our simulation results through field experiments, we need to be aware of the limitations attached to field measurements as well. The nitrogen that can be measured in groundwater and streams can originate from different sources and represents the N coming from an experimental field only partially, so that attribution of what can be measured in groundwater and streams to certain management practices can be very difficult. Besides, field experimental results from a few years have to be interpreted cautiously, because some management practices, such as no-tillage, become effective only after some several years (Grandy et al., 2006; Derpsch et al., 2010). A practical difficulty is that field experiments generally need to focus on varying just a few management practices as it is costly to experiment with a large number of combinations of practices.

Simulated yields, N loads to fresh water and grey WFs under different management packages are subject to the local environmental conditions of our case in Spain, which means that they cannot simply be transferred to other conditions. Besides, even for our specific case, the outcomes are subject to uncertainties inherent to any modelling effort (Kersebaum et al., 2016). We have also excluded other factors relevant in crop production, like the effects of weeds, pests and diseases. Therefore, the precise values presented should be taken with caution;

28

the value of our study rather lies in the understanding it provides on how different agricultural management practices can affect yield, N load and resultant grey WF of crop production, and how and why there are inevitable trade-offs between crop yield, water consumption and water pollution.

While the focus of the current study has been leaching and runoff of nitrogen, the effect of water pollution through phosphorous can be as important. The results from the current study cannot necessarily be transferred to the phosphorus-related grey WF of crop production, which requires additional study.

5.   Conclusion

This paper provides the first detailed study on potential N-related grey WF reduction of growing a crop by analysing the effect of a large number of combinations of different management practices. The paper shows that, when choosing a certain N application rate and when choosing between inorganic versus organic fertilizer, between conventional versus no tillage, and between full versus deficit irrigation, two inevitable trade-offs are made. The first trade-off is between crop yield and water pollution (grey WF). Whereas maximizing crop yields requires a relatively high N application rate and full irrigation, minimizing water pollution per unit of crop requires deficit irrigation and seeking a balance between N application rate (and associated water pollution) and the resultant yield. The second trade-off is between reducing water pollution (grey WF) and water consumption (green and blue WF). Minimizing consumptive water use per tonne requires a higher N application rate (150 kg N ha^{-1} in our case) than minimizing water pollution per tonne (50 kg N ha^{-1} in our case). Applying manure instead of inorganic-N and deficit instead of full irrigation are measures that reduce both water pollution and water consumption per tonne. However, for minimizing water pollution per tonne one can better choose for conventional tillage, because that reduces leaching, whereas for minimizing water consumption per tonne the no-tillage practice is to be preferred, because that reduces soil evaporation.

The study gives some support to the simple tier-1 approach of estimating the grey WF of applying N fertilizer as proposed by Franke et al. (2013), but only for N application rates below 150 kg ha^{-1}. Below that, the α value is estimated in the proper range (in our specific case), but the β value is underestimated. Beyond the N application rate of 150 kg ha^{-1}, the tier-1 approach underestimates the leaching-runoff fraction, by not accounting for the fact that N uptake by the crop is stabilizing and that denitrification and volatilization don't increase proportionally with growing N inputs, which results into an increasing fraction of the N surplus in the soil lost through leaching, runoff and erosion.

Acknowledgments

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Appendix

Table A.1. The average monthly climatic data of Badajoz in Spain.

Climatic variables	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Temperature max, ^{0}C	14.1	16.5	20.4	22.2	26.1	31.9	34.9	34.7	30.0	24.4	18.0	14.3
Temperature min, ^{0}C	3.6	4.2	6.7	9.0	12.2	15.8	17.3	17.6	15.2	11.9	7.3	4.9
Precipitation, mm	50.2	39.5	30.9	41.1	41.9	10.8	2.3	4.2	25.1	64.4	65.2	64.0
Solar radiation, MJ/M^2	7.4	10.5	12.9	19	21.9	25.7	26.9	23.9	17.8	12.3	8.1	6.4
Relative humidity, %	83	71	63	56	45	42	37	35	46	64	76	80
Wind speed, m/s	1.7	1.9	2.09	2.09	2.2	2.3	2.4	2.2	1.81	1.6	1.7	1.7
ET$_0$, mm	33.2	57.1	108.8	145.3	196.6	224.2	250.9	218.2	139.7	83.7	43.3	29.3

Table A.2. Grey WF per tonne of crop production for the different management packages.

Management packages									
Fertilizer form	Tillage practice	Irrigation strategy	Nitrogen application rate						
			25	50	100	150	200	250	300

Nitrate	Conventional	Full irrigation	108	95	107	122	306	696	1095
Nitrate	Conventional	Deficit irrigation	90	82	97	138	436	865	1324
Nitrate	No-tillage	Full irrigation	154	136	161	199	294	621	1002
Nitrate	No-tillage	Deficit irrigation	139	130	154	203	383	781	1202
Manure	Conventional	Full irrigation	100	83	90	106	167	445	832
Manure	Conventional	Deficit irrigation	91	75	84	114	231	600	1028
Manure	No-tillage	Full irrigation	148	121	141	170	221	397	754
Manure	No-tillage	Deficit irrigation	134	114	126	168	261	534	927

Table A.32. N leaching-runoff potential scores for environmental factors and agricultural practices, following the tier-1 approach (Franke et al., 2013).

Factors			Weight		Score	Remark
			α	β	(s)	
Environmental factors	Atmospheric	N-deposition	10	10	0	RFN=0.34 g m^{-2}y^{-1} less than 0.5
	Soil	Texture (for leaching)	15	15	0.67	Loam soil
		Texture (for runoff)	10	10	0.33	Loam soil
		Natural drainage (for leaching)	10	15	0.67	Assumed well drained
		Natural drainage (for runoff)	5	10	0.33	Assumed well drained
	Climate	Precipitation (mm)	15	15	0	0-600 very low precipitation (450mm)
	N-fixation (kg ha^{-1})		10	10	0	Non-legume crops
Agricultural practices	Application rate		10	0	*	
	Plant uptake (crop yield)		5	0	*	
	Management practice		10	15	0.33	Assumed good management practices

* See Table A.43.

Table A.43. N leaching-runoff potential scores based on fertilizer application rate and plant uptake, and calculated α and β values following the tier-1 approach.

Fertilizer application kg ha^{-1}	Categorized	Score for application rate	Score for plant uptake	Calculated α and β	
				α	β
25	Very low	0	1	0.08	0.308
50	Low	0.33	0.67	0.09	0.308
100	Low	0.33	0.67	0.09	0.308
150	High	0.67	0.33	0.09	0.308
200	High	0.67	0.33	0.09	0.308
250	Very high	1	0	0.09	0.308
300	Very high	1	0	0.09	0.308