

# 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<sup>-1</sup>), 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<sup>-1</sup> (with crop yield of 11.1 t ha<sup>-1</sup>) is 1100 m<sup>3</sup> t<sup>-1</sup>, which can be reduced by 91% towards 95 m<sup>3</sup> t<sup>-1</sup> when the N application rate is reduced to 50 kg N ha<sup>-1</sup> (with a yield of 3.7 t ha<sup>-1</sup>). The grey WF can be further reduced to 75 m<sup>3</sup> t<sup>-1</sup> by shifting the management package to manure-N and deficit irrigation (with crop yield of 3.5 t ha<sup>-1</sup>). 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<sup>-1</sup>, with manure, no-tillage and deficit irrigation (with crop yield of 9.3 t ha<sup>-1</sup>). 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

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

48  
49 Factors that influence the grey WF include the N application rate, the form of N applied (particularly inorganic-N  
50 versus manure or organic-N), and the tillage and irrigation practice. A low N-application rate will hamper plant  
51 growth and reduce crop yield (Raun et al., 2002). The low N-application rate will result in relatively little water  
52 pollution per hectare, but, because of the low yield per hectare, it may cause relatively much water pollution per  
53 unit of crop produced. A high N-application rate will result in a high crop yield, but with high water pollution per  
54 hectare and per tonne of crop as well. The reason for the high water pollution per tonne of crop is that there is a  
55 threshold for the N application rate beyond which yield does not respond (Zhou et al., 2011), while the surplus N  
56 contributes to pollution (Carpenter et al., 1998; Vitousek et al., 2009). The form of N applied is another important  
57 factor affecting N losses. Inorganic N is readily available for uptake by crops (Haynes, 2012), whereas the organic-  
58 N contained in manure becomes available only gradually, as it should first be converted (mineralized) to inorganic  
59 form (Ketterings et al., 2005). The mobile nature of nitrate makes it susceptible for higher risk of leaching (Yanan  
60 et al., 1997), while the slow disappearance of manure makes it susceptible to N losses through runoff before  
61 being taken up by the crop (Withers and Lord, 2002). Field operation practices such as tillage affect the water  
62 holding capacity of the soil, the movement of moisture and nutrients in the soil, surface runoff, and eventually  
63 crop yield and nutrient load to fresh water. There are various good reasons why conventional tillage is being  
64 practiced: it mixes fertilizer, organic matter and oxygen in the soil, breaks up surface soil crusts and reduces weeds  
65 (Horowitz, 2011). However, conventional tillage disrupts aggregates within the soil and life cycles of beneficial  
66 organisms, increases soil erodability, and results in soil compaction and tillage pan formation (Triplett and Dick,  
67 2008); tillage-pan is a formation of compacted soil layer caused by repeated ploughing using heavy weight tillage  
68 machineries (Podder et al., 2012). Alternatively, no-tillage maintains the crop residue that serves as mulch cover,  
69 improves the soil water holding capacity (Dangolani and Narob, 2013) and increases hydraulic conductivity (Azooz  
70 and Arshad, 1996; Triplett and Dick, 2008). The irrigation practice primarily influences the water balance of the  
71 soil, but as a side effect it influences nutrient movement in the soil. The advantage of deficit irrigation compared  
72 to full irrigation is that there may be less leaching and runoff of nutrients (Withers and Lord, 2002), but the  
73 disadvantage is that it may result in reduced N demand as crop growth diminished and reduced N supply as N  
74 transporting agent is reduced and thus reduction in water pollution per unit of crop produced (Gonzalez-Dugo et  
75 al., 2010).

76

77 Various studies show how increasing N-application rates result in both increased crop yield and N leaching  
78 (Berenguer et al., 2009; Rong and Xuefeng, 2011; Valero et al., 2005; Zhou et al., 2011; Cooper et al., 2012; Good  
79 and Beatty, 2011). Pittelkow et al. (2015) analysed the effect of tillage practices on crop yield; Yu et al. (2016)  
80 explored the effect of different combinations of tillage practice and N fertilizer form on crop yield; Huang et al.  
81 (2017) and Yanan et al. (1997) considered the effect of manure versus inorganic N fertilizer application on nitrate  
82 leaching; and Huang et al. (2015) analysed the effect of different tillage practices and N application rates on yield  
83 and N leaching. Furthermore, there are quite some studies on the relation between rates of irrigation and N  
84 application and crop yield (Yin et al., 2014; Al-Kaisi and Yin, 2003; Rimski-Korsakov et al., 2009). These earlier  
85 studies provide insight in the effects of individual management practices on yield, water productivity, or leaching,  
86 however most of the studies vary only one or two management practices, not considering the combined effect  
87 of N application rate, N form, tillage practice and irrigation strategy. Besides, none of these studies consider the  
88 effect on the pollutant load per unit of crop obtained or the effect on the grey WF per tonne.

89

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

95

96 The objective of this study is to explore the effect of nitrogen application rate, nitrogen form, tillage practice and  
97 irrigation strategy on the nitrogen load to groundwater and surface water, crop yield and the N-related grey water  
98 footprint of crop production by a systematic model-based assessment. We apply the Agricultural Policy  
99 Environmental eXtender (APEX) model, which simulates nutrient and water balances of the soil and plant growth,  
100 is able to simulate the effect of a wide variety of agricultural management practices, and has been applied for a  
101 wide variety of cases (Wang et al., 2012; Gassman et al., 2010; Liu et al., 2016; Clarke et al., 2017; Chen et al.,  
102 2017). As a case study, we simulate irrigated-maize growth for twenty-years (1993-2012) at Badajoz in Spain on  
103 loam soil in a semi-arid environment.

104

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

114 affect the N uptake and N load to fresh water. The current study is the first one to apply the tier-3 approach,  
115 which explicitly considers daily physical and biochemical processes using an advanced water and nutrient balance  
116 model (the APEX model). As an additional component of the current study, we will compare the N leaching-runoff  
117 fractions that result from the APEX simulations with the leaching-runoff fractions estimated with the simpler tier-  
118 1 approach, in order to find out the added value of employing the advanced model approach.  
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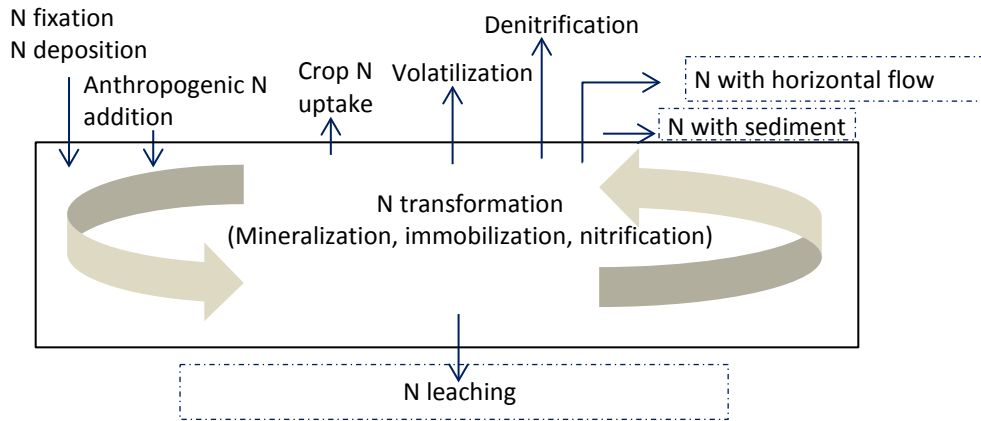
## 120 2. Method and data

### 121 2.1. Modelling the soil water & nitrogen balances and crop growth

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123 The effect of various combinations of management practices on water flows (like soil evaporation, crop  
124 transpiration, percolation and runoff), N flows (like N uptake by plants, leaching and runoff) and crop growth are  
125 simulated using the APEX model, a dynamic, deterministic and process-based model with a daily time step  
126 (Williams and Izaurralde, 2006). Below we briefly summarise the processes simulated in the model. More detailed  
127 descriptions of the processes and the equations to simulate these processes can be found in the documentation  
128 of APEX (Williams et al., 2008).  
129

130 The water balance component of APEX encompasses key processes that impact the soil water compartment in  
131 the hydrologic cycle. Initially, incoming inputs such as precipitation, snowmelt, or irrigation is partitioned between  
132 surface runoff and infiltration. Surface runoff volume is simulated using a modified Soil Conservation Service curve  
133 number technique described by Williams (1995). Infiltrated water can be stored in the soil profile, be lost via  
134 evapotranspiration (ET), percolate vertically to groundwater, or flow laterally as subsurface flow, with a quick and  
135 slow component. Reference ET is calculated using the Penman-Monteith method. The actual ET, an important  
136 variable in estimating green and blue WF of crop production, is computed by simulating evaporation from the soil  
137 and transpiration from plants separately, considering the soil moisture status and how agricultural management  
138 practices affect the root zone. Percolation and lateral flow are computed using storage routing and pipe flow  
139 equations described by Gassman et al. (2010). A deep groundwater table is assumed and thus capillary rise, which  
140 APEX would simulate using storage routing (Gassman et al., 2010), is not considered in the water balance.  
141

142 The N balance of the soil in APEX is computed based on inputs and outputs and conversion processes (Figure 1).  
143 N is added to the soil-plant system through natural and anthropogenic pathways. Natural N inputs include wet  
144 and dry deposition (Anderson and Downing, 2006) and N fixation, through lightning and through biological  
145 fixation by legume plants (Carpenter et al., 1998). Anthropogenic input occurs when inorganic or organic N  
146 fertilizers are applied (Vitousek et al., 2009). N outputs include N uptake by crops (partly harvested and removed  
147 later on), denitrification, volatilization, nitrate-N losses through leaching, horizontal losses of organic N with  
148 eroded sediments, and horizontal losses of inorganic N through surface runoff, or lateral subsurface flow. N  
149 transformation includes mineralization, immobilization and nitrification.  
150



151  
152 **Figure 1.** Nitrogen fluxes into and from the root zone, and N transformation.  
153

154 APEX simulates the growth of annual and perennial crops based on the EPIC model (Williams et al., 1989), an  
155 energy-driven crop growth model using a radiation-efficiency approach to simulate the generation of biomass.  
156 Potential biomass production is derived as function of leaf area index and climatic variables (solar radiation,  $\text{CO}_2$ ,  
157 air humidity and temperature). Phenological development of the crop is based on heat unit accumulation  
158 measured in growing degree days. Annual crops grow from planting date to harvest date or until the accumulated  
159 heat units equal the potential heat units for the crop (Steduto, 1997). Daily potential growth is lowered to actual  
160 growth using the most limiting stress factor, considering stresses caused by water, nutrients (N and P),  
161 temperature and aeration, which are evaluated by assigning stress factors (from 0, high stress, to 1, no stress).  
162 Root growth is constrained based on the most limiting stress caused by soil strength and temperature. Total  
163 biomass is partitioned to root and above ground biomass, and from the above-ground biomass is the economic  
164 yield is partitioned using harvest index.  
165

## 166 2.2. The grey water footprint of growing crops

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168 The grey water footprint (WF), an indicator of appropriated pollution assimilation capacity, is calculated following  
169 the Global Water Footprint Standard (Hoekstra et al., 2011), which means that the total pollutant load entering  
170 fresh water (groundwater or surface water) is divided by the difference between the maximum acceptable  
171 concentration for that pollutant and the natural background concentration for that pollutant. The grey WF can  
172 be expressed in two different ways, either as a water volume per ha, or as a water volume per tonne of crop:  
173

$$174 \text{ Grey WF per hectare} = \frac{L}{c_{\max} - c_{\text{nat}}} [m^3 \text{ ha}^{-1} \text{ y}^{-1}] \quad (1a)$$

$$176 \text{ Grey WF per tonne} = \frac{\text{Grey WF per hectare}}{Y} [m^3 \text{ t}^{-1}] \quad (1b)$$

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

The total N load to fresh water ( $L$ , in  $\text{kg N ha}^{-1} \text{y}^{-1}$ ) 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  $\text{L}^{-1}$  (or 11.3 mg N  $\text{L}^{-1}$ ) is adopted, based on the EU Nitrates Directive (Monteny, 2001). The natural concentration was considered to be 0.5 mg N  $\text{L}^{-1}$ , 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  $\alpha$ , 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  $\beta$ , 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.

$$\alpha = \frac{L}{\text{Appl}} \tag{2}$$

$$\beta = \frac{L}{\text{Surplus}} \tag{3}$$

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

215  
 216 At the tier-3 level, the fractions  $\alpha$  and  $\beta$  are not used in the calculations, but they can easily be calculated  
 217 afterwards, based on the outputs of the model. At the tier-1 level,  $\alpha$  and  $\beta$  can be estimated using equation 4 and  
 218 5 following the guidelines of Franke et al. (2013). According to these guidelines, the leaching-runoff fractions lie  
 219 between a minimum and a maximum value (0.01 to 0.25 for  $\alpha$  and 0.08 to 0.8 for  $\beta$ ). The precise value is estimated  
 220 based context-specific environmental and management factors, using the following equations:

$$222 \quad \alpha = \alpha_{min} + \left[ \frac{\sum_i s_i * w_i}{\sum_i w_i} \right] * (\alpha_{max} - \alpha_{min}) \quad (4)$$

$$223 \quad \beta = \beta_{min} + \left[ \frac{\sum_i s_i * w_i}{\sum_i w_i} \right] * (\beta_{max} - \beta_{min}) \quad (5)$$

224  
 225 where  $s_i$  is the score for the leaching-runoff potential for environmental or management factor  $i$ , and  $w_i$  is the  
 226 weight of that factor. Corresponding to a certain state of factor,  $i$ , a score  $s$  is assigned between 0 and 1: scores  
 227 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  
 228  $w$  per factor  $i$  denotes the importance of the factor. The weights given to the separate influencing factors add up  
 229 to a total of 100.

## 231 2.4. Simulation set-up

232  
 233 We carry out model simulations with APEX for 56 management packages, whereby each management package  
 234 consists of a certain combination of management practices. We consider all possible combinations of seven N  
 235 application rates, two N forms, two tillage practices, and two irrigation strategies (Table 1). As a reference  
 236 management package, we assume the use of inorganic N fertilizer (nitrate) in combination with conventional  
 237 tillage and full irrigation. Conventional tillage is the most wide-spread tillage practice in the EU (EUROSTAT, 2013)  
 238 and full irrigation is the most common irrigation practice, aimed at achieving maximum yield.

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

Management practices	Modelling	Effects
<ul style="list-style-type: none"> <li>Nitrogen application rates: 25, 50, 100, 150, 200, 250 or 300 <math>\text{kg N ha}^{-1} \text{y}^{-1}</math></li> </ul>	Soil water & nutrient balances and crop growth model (APEX)	- ET
<ul style="list-style-type: none"> <li>Nitrogen forms: inorganic-N (nitrate) or organic-N (manure)</li> </ul>		- Yield - N load

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

243

244 The EU Nitrate Directive legally restricts annual farm application of manure in EU member states to 170 kg N ha<sup>-1</sup> y<sup>-1</sup>, or in case of derogation up to 250 kg N ha<sup>-1</sup> y<sup>-1</sup> (Amery and Schoumans, 2014; Van Grinsven et al., 2012).  
245  
246 Surveys in Spain, however, show that application rates of 300-350 kg N ha<sup>-1</sup> y<sup>-1</sup> are common to cultivate maize in  
247 the Ebro Valley (Berenguer et al., 2009) and up to 300 kg N ha<sup>-1</sup> y<sup>-1</sup> in La Mancha (Valero et al., 2005). As the  
248 upper value for the N application rate in our simulations we apply 300 kg N ha<sup>-1</sup> y<sup>-1</sup>.

249

250 The fertilization is assumed to be performed in two splits (30% in a first round, at planting for mineral fertilizer  
251 and 15 days before planting for manure; 70% in a second round, one month after planting). In the first round of  
252 application, inorganic fertilizer is assumed to be nitrate-N and applied through broadcasting while manure is  
253 assumed to be injected. Manure injection is getting recognition in the EU and in the world due to its many  
254 advantages, including reduction of N losses to fresh water and to the atmosphere and bad odour (Van Dijk et al.,  
255 2015; van den Pol-van Dasselaar et al., 2015). In the second round, both the manure and nitrate-N fertilizers are  
256 added as side-dressing.

257

258 As for the inorganic N applied, we assume that the N is 100% in the form of nitrate. Manure is generally contained  
259 of mostly organic N, and a smaller amount of inorganic N (Ketterings et al., 2005; Pratt and Castellanos, 1981). In  
260 this study, we assume the manure composition as in the APEX database: 91.67% organic N, 8.33% inorganic N  
261 (0.23% nitrate and 8.10% ammonium N). In addition, the current study assumes that other nutrients (P, K and  
262 micro nutrients) do not to constrain crop production.

263

264 We simulate conventional tillage in APEX as two times ploughing to a depth of 20 cm at thirty and fifteen days  
265 before sowing date and one time harrowing following the emergence of the seed. The two times ploughing is the  
266 average of what is most common, namely one to three times tilling (Nagy and Rátonyi, 2013; FAO, 2016). With  
267 the tillage depth of 20 cm we follow the average estimate reported by Townsend et al. (2015) and FAO (2016).  
268 No-tillage, a form of conservation tillage that is strongly encouraged by the EU agricultural policy (De Vita et al.,  
269 2007), is simulated as no soil disturbance; the stubble of the previous crop is kept on the field.

270

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



275 use of furrow irrigation, the irrigation technique that covered the largest irrigated area in the EU in 2010,  
276 particularly in the Eastern and Mediterranean regions of Europe (EUROSTAT, 2016).  
277

## 278 2.5. Data

279

280 The model experiment is carried out at field scale for a place near Badajoz in Spain, in the Guadiana river basin,  
281 which has a semi-arid climate and faces water scarcity during part of the year, particularly in summer when water  
282 is needed for irrigation (Hoekstra et al., 2012).  
283

284 The following climatic and soil data have been collected for Badajoz in Spain (38.88° N, -6.83° E; 185 m above  
285 mean sea level). Daily observed rainfall and temperature data (for the period 1993-2012) are extracted from the  
286 European Climate Assessment and Dataset (Klein Tank et al., 2002). These data have been subject to homogeneity  
287 testing and missing data have been filled with observations from nearby stations (Klein Tank, 2007). Mean  
288 monthly solar radiation, relative humidity and wind speed data are taken from the FAO CLIMAWAT database  
289 (Smith, 1993). Daily reference evapotranspiration is calculated using the Penman-Montheith equation, as  
290 implemented in APEX (Williams et al., 2008). The average monthly climatic and reference evapotranspiration data  
291 are shown in Table A.1 in Appendix.  
292

293  
294 Using the Soil Texture Triangle Hydraulic Properties Calculator from (Saxton et al., 1986), we identified the soil at  
295 our location as loam soil. The physical and chemical characteristics of the soil, and nutrient content in the soil  
296 (nitrogen, phosphorus, carbon) that are used in APEX are extracted from the 1×1 km<sup>2</sup> resolution European Soil  
297 Database (Hannam et al., 2009). We use a soil albedo of 0.13 for a loam soil at its field capacity (Sumner, 1999).  
298

299 Regarding crop parameters, we use the default values from the APEX model. The effect of stresses related to  
300 weed, pest and diseases on crop growth are not considered; we simulate the effect of stresses from excess and  
301 limitation of water, from limitation of nitrogen, and from very high or very low temperature.  
302

303 Soil moisture content is initialised using the standard procedure in APEX, which is based on average annual rainfall  
304 within the period considered (1993-2012). We adjust initial organic-N content for each simulation so that the N  
305 build-up in the soil over the 20-year period is zero. We apply the graphical time-series inspection method  
306 (Robinson, 2002) to determine the warm-up period, i.e. the period in which simulation results are still affected  
307 by the model initialization. We find that we best exclude the first five years of the simulation, thus we show results  
308 for the period 1998-2012.  
309

### 310 3. Results

#### 311 3.1. Pollutant loads and grey WF for the reference management package

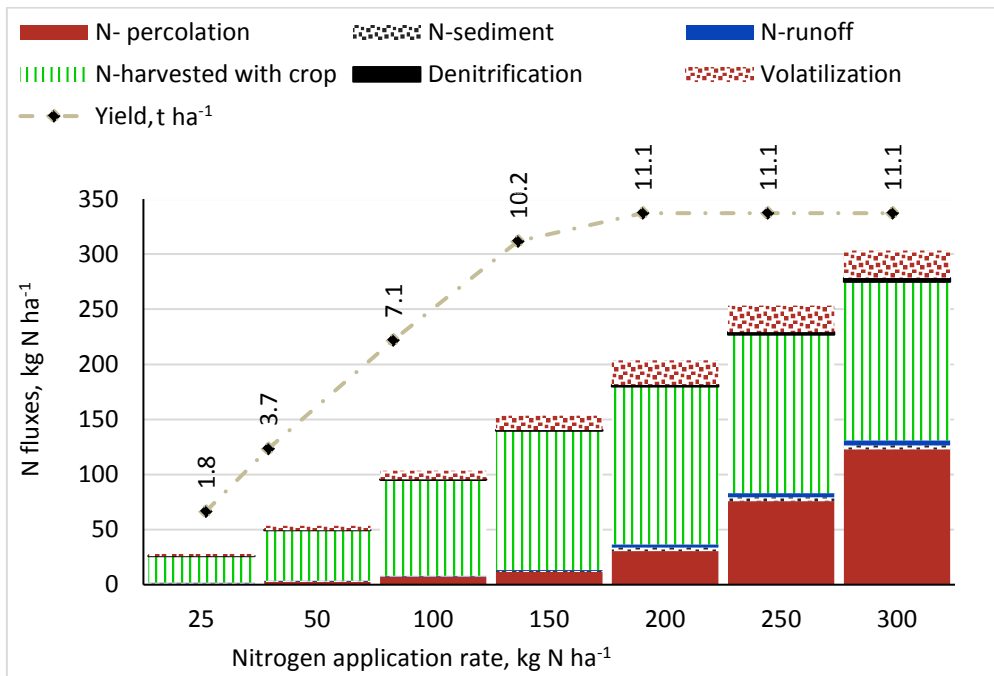
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313 N out-fluxes from the soil for maize production under the reference management package (inorganic-N,  
314 conventional tillage, full irrigation) for different N application rates are shown in Figure 2. The N out-fluxes are  
315 denitrification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

322

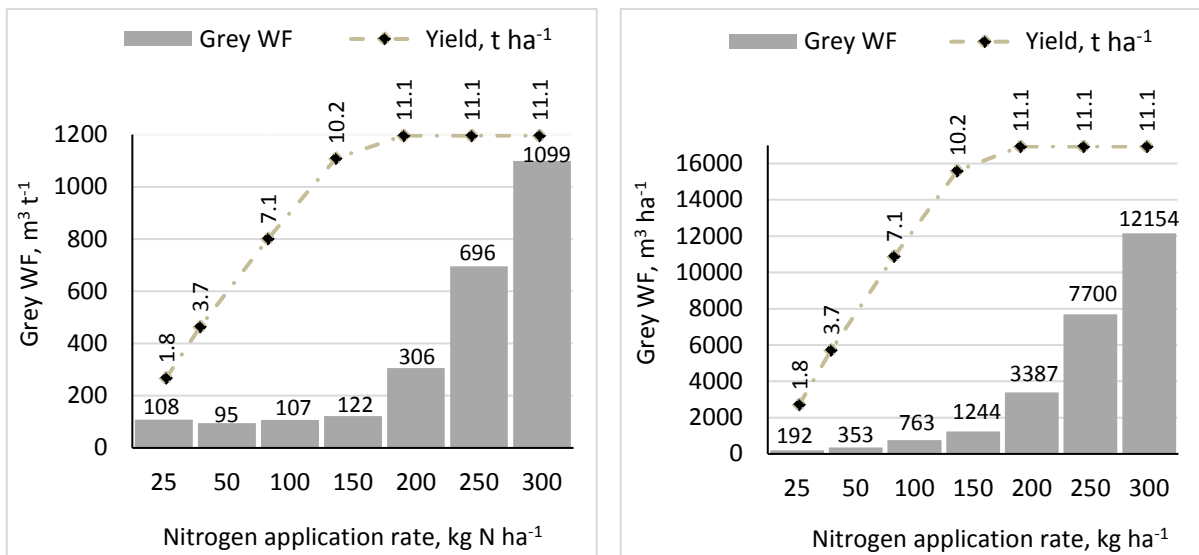
323 Crop yields increase with the N application rate as a result of reduced N stress. Yields stabilize at larger N  
324 application rates. The yield increase, however, comes at a price: the N load to fresh water, through leaching,  
325 runoff and eroded sediment, increases exponentially. As a result, large N-application rates result in a large grey  
326 WF (Figure 3). At lower N-application rates, crop yields decline as a consequence of N stress. While the grey WF  
327 in  $\text{m}^3 \text{ha}^{-1}$  keeps on declining with lower N-application rates, the grey WF in  $\text{m}^3 \text{t}^{-1}$  starts increasing again at very  
328 low N-application rate (in our case when the N-application rate drops below  $50 \text{ kg N ha}^{-1}$ ). The smallest grey WF  
329 per tonne can be found at an N-application rate of  $50 \text{ kg N ha}^{-1}$ , where yield is substantially lower than the  
330 maximum, but where additional N application goes along with increasing N load per unit of crop yield gain, thus  
331 with increasing grey WF per tonne.

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**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).



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**Figure 3.** Grey WF of maize production in m³ t⁻¹ (left) and m³ ha⁻¹ (right) for a range of N-application rates under the reference management package.

### 341 3.2. Effect of fertilizer form, tillage practice and irrigation strategy on grey WF

342

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

349

- 350 I. Application rates up to  $125 \text{ kg N ha}^{-1}$ : the grey WF is smallest for manure with conventional tillage and  
351 deficit irrigation;
- 352 II. Application rates between  $125$  and  $225 \text{ kg N ha}^{-1}$ : the grey WF is smallest for manure with conventional  
353 tillage and full irrigation;
- 354 III. Application rates above  $225 \text{ kg N ha}^{-1}$ : the grey WF is smallest for manure with no-tillage and full irrigation.

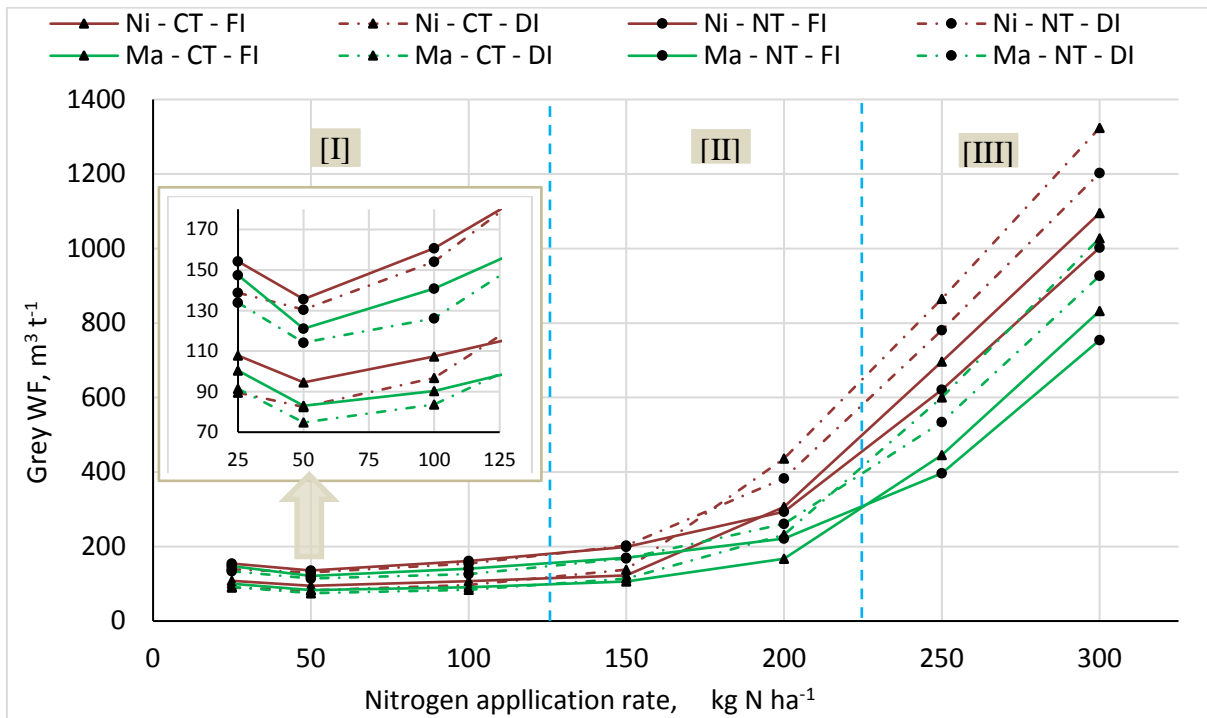
355

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

364

365 At low application rates (ranges I), deficit irrigation decreases the amount of water available for percolation and  
366 thus reduces N leaching as well. At intermediate and higher N-application rates (ranges II-III), full irrigation has a  
367 smaller grey WF per tonne as compared to deficit irrigation because of the higher crop yield. With the absence of  
368 water stress and the higher yield, the N uptake by the crop is higher, resulting in a lower N surplus in the root  
369 zone and decreased N leaching.

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**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<sup>-1</sup>, [II] N application rates between 125 and 225 kg N ha<sup>-1</sup>, [III] N application rates above 225 kg N ha<sup>-1</sup>. 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).

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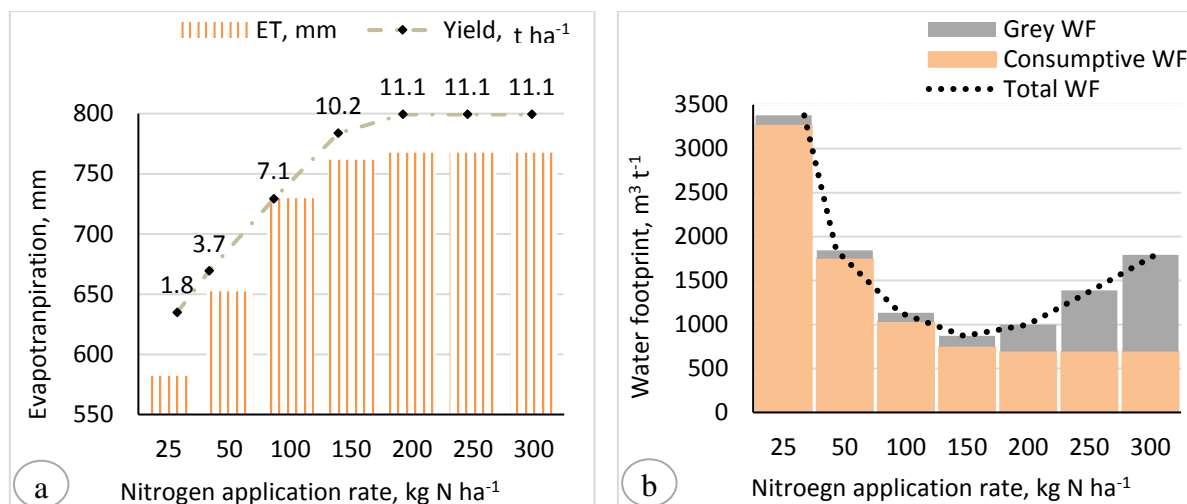
The smallest grey WFs per tonne are found for an N application rate of 50 kg N ha<sup>-1</sup>. Taking the reference management package with an N application rate of 300 kg N ha<sup>-1</sup> as a starting point, one can reduce the grey WF per tonne of crop production by reducing the N application rate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

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### 389 3.3. Reducing grey WF vs consumptive WF

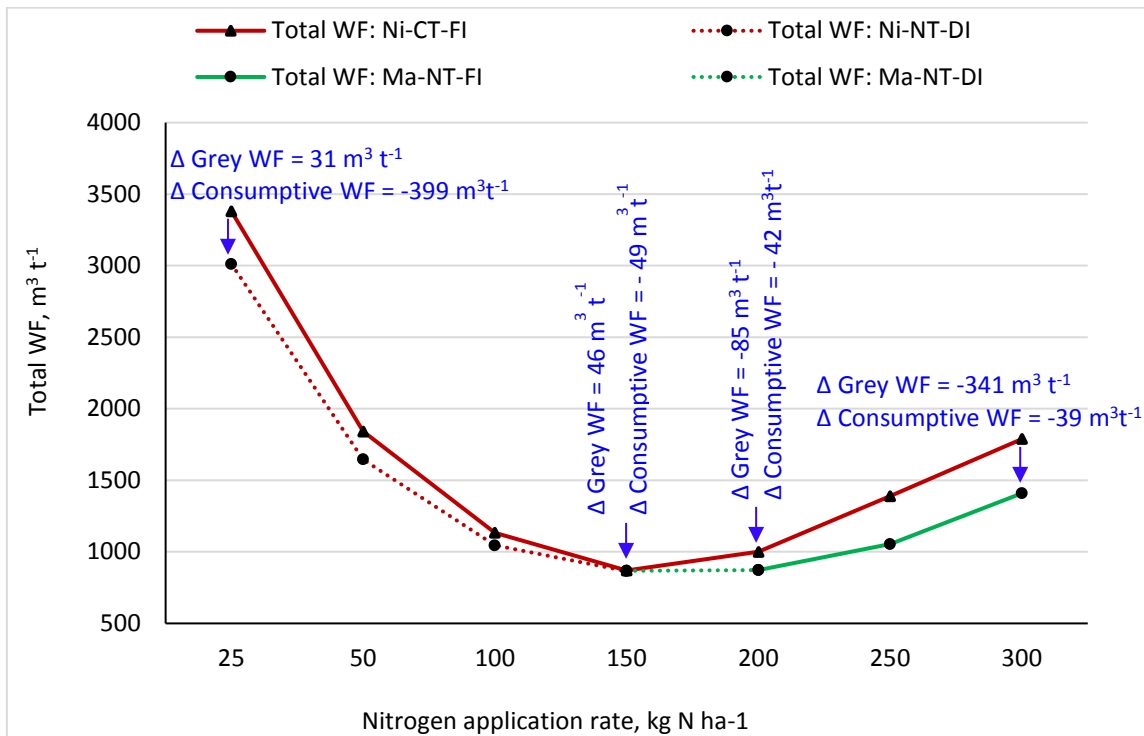
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391 Both ET and yield increase with increasing N application rate, but level off at large N application rates (Figure 5a).  
 392 Adding more N at relatively low application rates has a larger impact on Y increase than on ET increase. As a result,  
 393 the consumptive WF per tonne, defined as ET over Y, decreases with increasing N application rate, levelling off at  
 394 larger N application rate (Figure 5b). The grey WF per tonne, however, exponentially increases with increasing N  
 395 application rate. As a result, the sum of grey and consumptive WF has a minimum somewhere at intermediate N  
 396 application rate, at 150 N ha<sup>-1</sup> in the case of our reference management package. The total WF is dominated by  
 397 the consumptive WF for smaller N application rates and by the grey WF for larger N application rates.  
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399 **Figure 5.** Evapotranspiration and yield (a) and consumptive WF and grey WF per tonne (b) for the reference  
 400 management package.  
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403 Figure 6 shows the total (grey+consumptive) WF per tonne for the reference management package for different  
 404 N application rates (the solid red line). For each given N application rate, shifting to another management package  
 405 (the dashed red and green lines, and the solid green line) can reduce the total WF. Generally, the reduction in  
 406 total WF is the result from reductions in both the grey WF and the consumptive WF (as indicated in the figure).  
 407 At N application rates of 25, 50 and 100 kg N ha<sup>-1</sup>, the total WF can be reduced by shifting towards no-tillage and  
 408 deficit irrigation. At N application rates of 150 kg N ha<sup>-1</sup>, the total WF can be reduced by shifting towards organic  
 409 N, no-tillage and deficit irrigation. Finally, at N application rates of 200, 250 and 300 kg N ha<sup>-1</sup>, the total WF can  
 410 be reduced by shifting towards organic N and no-tillage. The total WF reductions shown in the figure are the net  
 411 effect of changes in the consumptive WF and grey WF; in some cases, the total WF decrease is at the cost of some  
 412 grey WF increase.

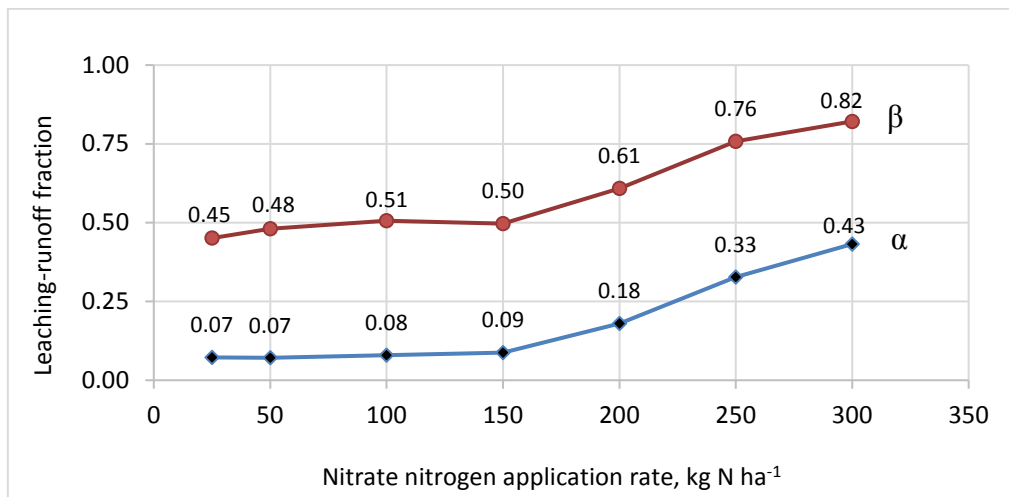


413  
 414 **Figure 6.** The total (green, blue plus grey) WF per tonne for the reference management package and for a  
 415 management package with the largest total WF reduction potential. Red lines refer to nitrate (Ni); green lines  
 416 refer to manure (Ma). Circular markers refer to no-tillage (NT); triangular markers refer to conventional tillage.  
 417 Dashed lines refer to deficit irrigation (DI); solid lines refer to full irrigation (FI).  
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### 419 3.4. Resultant leaching-runoff fractions

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 421 The N leaching-runoff fractions  $\alpha$  and  $\beta$  for different N application rates for the reference management package,  
 422 as calculated here with the tier-3 approach, are shown in Figure 7. The  $\alpha$  values, which show the ratio of the N  
 423 load to fresh water to the N application rate are lower than the  $\beta$  values, which show the ratio of the N load to  
 424 the N surplus in the soil. This can be logically understood, because the N load to fresh water (in the numerator of  
 425 both ratios) is the same, while the  $\alpha$  ratio has the total N application rate in the denominator, while the  $\beta$  ratio  
 426 has the relatively smaller N surplus (which is only a fraction of the N applied) in the denominator.  
 427

428 With increasing N application rate, both N surplus in the soil and the N load to fresh water increase exponentially  
 429 (Figure 2). The  $\alpha$  values grow with increasing N application rate, because the N load to fresh water increases  
 430 quicker with increasing N application rates than the application rate itself. The  $\beta$  values also grow with increasing  
 431 N application rates, because denitrification and volatilization do not grow proportionally to the growth in N  
 432 surplus, which leads to greater fractions of the surplus getting lost through leaching and runoff.



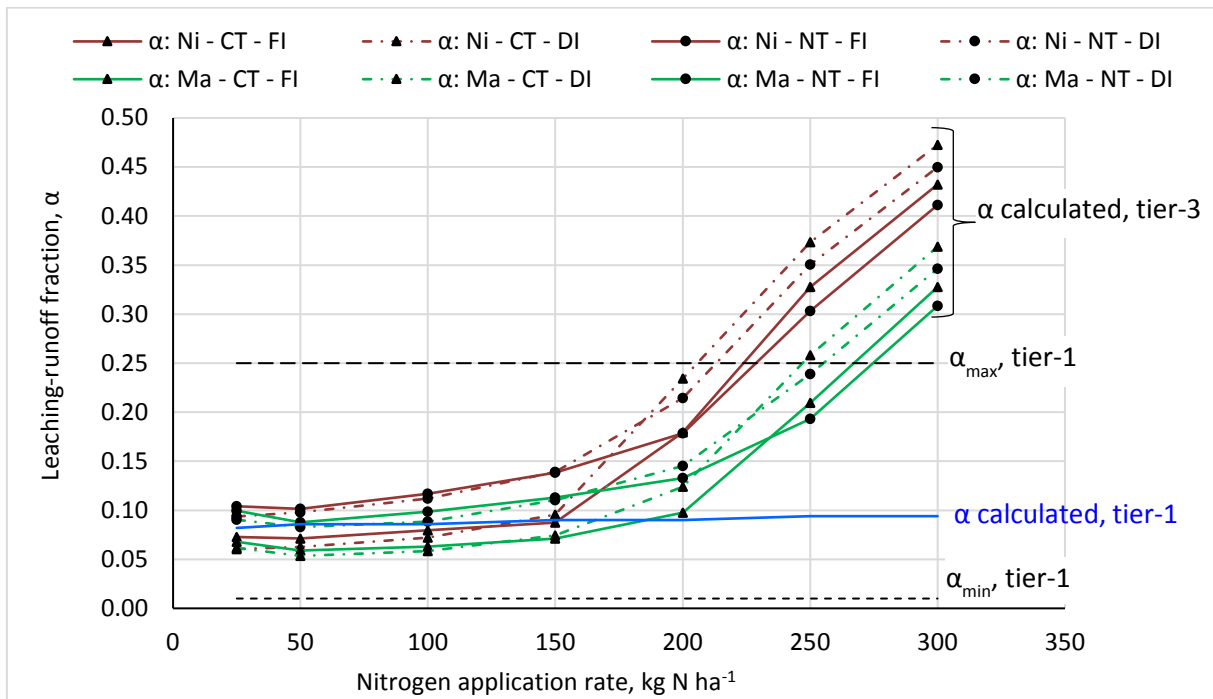
**Figure 7.** The N leaching-runoff fractions  $\alpha$  and  $\beta$  calculated per N application rate for the reference management package.

Figure 8 and Figure 9 show  $\alpha$  and  $\beta$  values for different management packages and N application rates. For comparison, the figures also show the  $\alpha$  and  $\beta$  values when estimated based on the simpler tier-1 approach (Tables A.3 and A.4 in Appendix), which estimates  $\alpha$  and  $\beta$  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  $\alpha$  for very high N application rates.

For N applications rates in the range up to 150 kg ha<sup>-1</sup>, the tier-1 approach gives a good proxy for the  $\alpha$  value. For the reference management package, the most common practice, the tier-1 approach even yields nearly the same  $\alpha$  values as the more advanced tier-3 approach. For N applications rates exceeding about 150 kg ha<sup>-1</sup>, the tier-1 approach underestimates the leaching-runoff fraction and thus the grey WF. The  $\beta$  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,  $\beta$  is underestimated with the tier-1 approach. Also for N application rates of 250 kg ha<sup>-1</sup> and beyond, the tier-1 approach underestimates  $\beta$ .

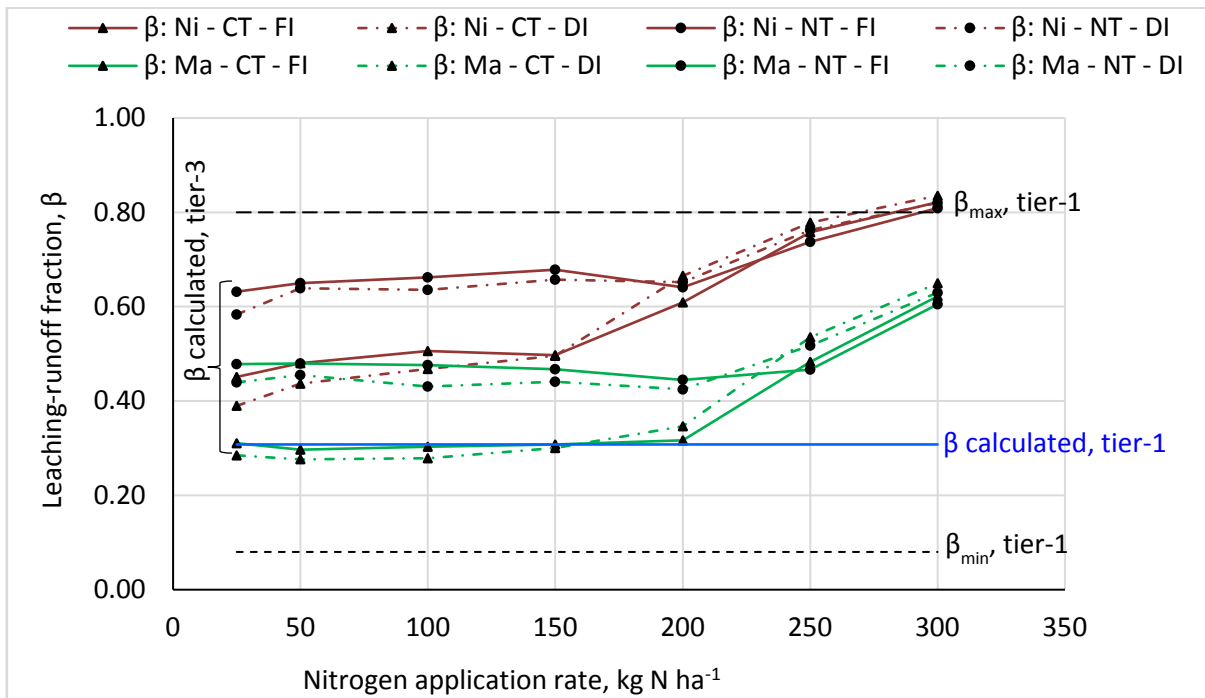
The leaching-runoff fractions from the application of inorganic N (nitrate) calculated at the tier-3 level are larger than these for organic N (manure), a distinction that is not made in the tier-1 approach.





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**Figure 8.** N leaching-runoff fractions  $\alpha$  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).



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**Figure 9.** N leaching-runoff fractions  $\beta$  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).

469 4. Discussion

470

471 The study shows that there is not one combination of management practices that minimises grey WF or overall  
 472 WF and maximises crop yield at the same time. Table 2 shows that the best combination of practices depends on  
 473 what variable is optimised. Yield is optimal when there is neither nitrogen stress nor water stress, so at high N  
 474 application rate and full irrigation. The highest yield (11.5 t/ha) is found for when N is applied in the form of  
 475 manure and the case of no-tillage. The total WF per tonne (the sum of the green, blue and grey WF) is smallest at  
 476 150 kg N ha<sup>-1</sup>, manure application, no-tillage and deficit irrigation. The yield in this case, 9.3 t/ha, is below-  
 477 optimum. There is both nitrogen and water stress, but the latter is more important. The grey WF per tonne is  
 478 smallest at 50 kg N ha<sup>-1</sup>, manure application, conventional tillage and deficit irrigation. This, however, reduces the  
 479 yield to 3.5 t/ha because of nitrogen stress. Deficit irrigation gives some water stress as well, but at such high  
 480 nitrogen stress, it is the latter that constrains crop yield. Our results confirm the finding by (Mekonnen and  
 481 Hoekstra, 2014) that there is a trade-off between consumptive WF per tonne and grey WF per tonne, i.e. a trade-  
 482 off between reducing water consumption and water pollution.

483

484 **Table 2.** The measures that give the optimum grey WF per tonne, total WF per tonne, or yield.

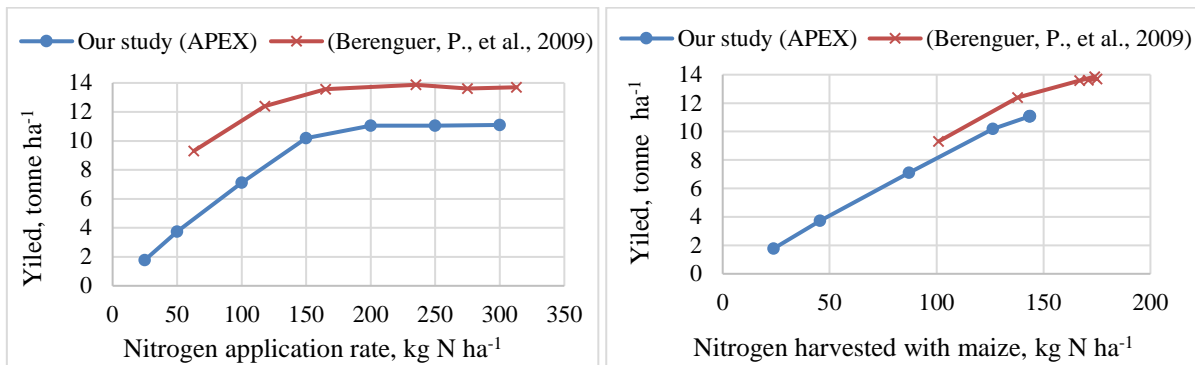
Indicator	Highest yield In t ha <sup>-1</sup>	Smallest total WF* in m <sup>3</sup> t <sup>-1</sup>	Smallest grey WF in m <sup>3</sup> t <sup>-1</sup>
Management practice			
Nitrogen application rate	200 kg N ha <sup>-1</sup>	150 kg N ha <sup>-1</sup>	50 kg N ha <sup>-1</sup>
Nitrogen form	Manure	Manure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

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

486

487 The response of maize yield to nitrogen input as simulated in this study with the APEX model is comparable with  
 488 the shape of the N-response curves for a few crops, including maize, constructed for the EU based on field  
 489 measurements from various earlier studies (Godard et al., 2008). Our finding is also consistent with the results  
 490 presented by Berenguer et al. (2009), who carried out field experiments for maize for similar conditions in Spain  
 491 (Figure 10). For every given N input, their yields 25% higher than from our study, which may relate to the fact that  
 492 Berenguer et al. (2009) used a high-yield maize variety.

493



494  
495 **Figure 10.** The maize yield simulated in our study in relation to N application rate (left) and N harvested with  
496 maize (right) in comparison to the maize yields from field experiments by Berenguer et al. (2009) when corrected  
497 for zero N build-up in the root zone.  
498

499 An inter-model comparison for the case of no N stress and no water stress (taking optimal N application rate and  
500 full irrigation) for exactly the same growing conditions in Spain shows similar crop yields and net irrigation supply.  
501 The current study, using the APEX model, simulates a net irrigation supply of 638 mm and a maize yield of 11.1 t  
502 ha<sup>-1</sup>, while in an earlier study, employing the AquaCrop model (Steduto et al., 2011), we simulate an irrigation  
503 supply of 630 mm and a maize yield of 11.9 t ha<sup>-1</sup> (Chukalla et al., 2015). APEX is reported to adequately simulate  
504 evapotranspiration for different management practices with the Penman Monteith equation for semi-arid  
505 conditions in the Mediterranean, including Spain (Cavero et al., 2012). The study by Milly and Dunne (2016),  
506 however, reported that Penman Monteith overestimates evapotranspiration for non-water stress conditions,  
507 which suggests that ground-truthing with field experiments is necessary.  
508

509 While acknowledging the need for further validation of our simulation results through field experiments, we need  
510 to be aware of the limitations attached to field measurements as well. The nitrogen that can be measured in  
511 groundwater and streams can originate from different sources and represents the N coming from an experimental  
512 field only partially, so that attribution of what can be measured in groundwater and streams to certain  
513 management practices can be very difficult. Besides, field experimental results from a few years have to be  
514 interpreted cautiously, because some management practices, such as no-tillage, become effective only after  
515 some several years (Grandy et al., 2006; Derpsch et al., 2010). A practical difficulty is that field experiments  
516 generally need to focus on varying just a few management practices as it is costly to experiment with a large  
517 number of combinations of practices.  
518

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

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

527  
528 While the focus of the current study has been leaching and runoff of nitrogen, the effect of water pollution  
529 through phosphorous can be as important. The results from the current study cannot necessarily be transferred  
530 to the phosphorus-related grey WF of crop production, which requires additional study.

531

## 532 5. Conclusion

533

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

548

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

556

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561

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## 720 Appendix

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722 **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, °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 <sup>2</sup>	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 <sub>0</sub> , 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

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

Management packages			Nitrogen application rate						
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

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Table A.3. N leaching-runoff potential scores for environmental factors and agricultural practices, following the tier-1 approach (Franke et al., 2013).

Factors			Weight		Score (s)	Remark
			$\alpha$	$\beta$		
Environmental factors	Atmospheric	N-deposition	10	10	0	RFN=0.34 g m <sup>-2</sup> y <sup>-1</sup> 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 <sup>-1</sup> )		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.4.

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731Table A.4. N leaching-runoff potential scores based on fertilizer application rate and plant uptake, and calculated  $\alpha$  and  $\beta$  values following the tier-1 approach.

Fertilizer application kg ha <sup>-1</sup>	Categorized	Score for application rate	Score for plant uptake	Calculated $\alpha$ and $\beta$	
				$\alpha$	$\beta$
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

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