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4	Consistivity of simulated over wield and nitrate leaching of the wheet noise
Э	Sensitivity of simulated crop yield and nitrate leaching of the wheat-marze
6	cropping system in the North China Plain to model parameters
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22	Abstract

23 Process-based crop simulation models are often over-parameterised and are therefore difficult to 24 calibrate properly. Following this rationale, the Morris screening sensitivity method was carried out 25 on the DAISY model to identify the most influential input parameters operating on selected model 26 outputs, i.e. crop yield, grain nitrogen (N), evapotranspiration and N leaching. The results obtained 27 refer to the winter wheat-summer maize cropping system in the North China Plain. In this study, four different N fertiliser treatments over six years were considered based on a randomised field 28 29 experiment at Luancheng Experimental Station to elucidate the impact of weather and nitrogen inputs 30 on model sensitivity. A total of 128 parameters were considered for the sensitivity analysis. The ratios

31 [output changes/parameter increments] demonstrated high standard deviations for the most relevant 32 parameters, indicating high parameter non-linearity/interactions. In general, about 34 parameters 33 influenced the outputs of the DAISY model for both crops. The most influential parameters depended 34 on the output considered with sensitivity patterns consistent with the expected dominant processes. 35 Interestingly, some parameters related to the previous crop were found to affect output variables of 36 the following crop, illustrating the importance of considering crop sequences for model calibration. 37 The developed RDAISY toolbox used in this study can serve as a basis for following sensitivity 38 analysis of the DAISY model, thus enabling the selection of the most influential parameter to be 39 considered with model calibration.

40

Keywords: Morris Sensitivity analysis, Crop modelling, RDaisy toolbox, Crop yield, Nitrogen
leaching, Wheat - Maize cropping system

43 Introduction

44 Process-based models have been extensively used to assess how the interaction of genotype \times 45 environment × management may affect crop productivity and dynamics of hydrology and nitrogen 46 (N) in cropping systems (Chapman, 2008). Simulation models are also considered essential tools for 47 scenario analyses and decision support for policy making (Ewert et al., 2015). Process-based models, 48 traditionally contingent on a mathematical formulation of physical processes, typically contain a 49 broad set of parameters and are therefore often considered over-parameterised (Reichert & Omlin, 50 1997). Many model parameters are often uncertain because, among other things, of insufficient data 51 for their estimation. Generally, finding an accurate estimate for all the parameters for which a model 52 best fits the experimental data is a complicated and computationally expensive process for complex 53 simulation models (Whittaker et al., 2010). Therefore, rigorous analysis of parameter sensitivity and 54 reduction of the parameter space are essential to facilitate the calibration process.

Sensitivity analysis (SA) examines how model parameters and/or model inputs affect model outputs (Song et al., 2015; Pianosi et al., 2016). Through SA, the various parameters can be ranked based on their relative importance. The parameters having a substantial impact on the model outputs are considered for model calibration and those that are less-essential in influencing the model response can be fixed to their nominal values (Sarrazin et al., 2016) reducing hence the model dimensionality. Identifying those parameters and processes which are most influential on model outputs can guide the efforts towards improving the accuracies of the most influential parameters and help to better understand the model structure and behaviour (Saltelli et al., 2004; Sarrazin et al., 2016), and reduce model complexity (Crout et al., 2009). This is especially important for complex process-based models which are often considered as over-parameterised leading to problems of non-uniqueness in parameter sets (also called equifinality).

66 There is a wide variety of available approaches to sensitivity analysis (Hamby, 1994; Campolongo et 67 al., 2007; Saltelli et al., 2010). These techniques vary from the most straightforward approach of One 68 parameter At a Time (OAT) perturbation to more commonly used global approaches. While OAT 69 quantifies model output variation in relation to changes of one parameter at a time, global sensitivity 70 analyses evaluate model output sensitivity to simultaneous changes in several parameters and can 71 thus provide more robust sensitivity measures accounting for non-linearity and interactions among 72 model parameters. Despite OAT methods being straightforward to apply, they are usually considered 73 unreliable for high-dimensional and non-linear models. On the other hand, global methods which are 74 suitable for models of various complexity are often considered computationally intensive (Borgonovo 75 & Plischke, 2016). The Morris screening method is considered as a compromise between OAT and 76 global methods, and it is well-designed to identify influential parameters of large models since it is 77 computationally inexpensive (Campolongo et al., 2007). Moreover, it has been shown to identify the 78 same influential parameters as when using global SA methods (Confalonieri et al., 2010a; Qin et al., 79 2016). The Morris method has been widely used in analysing sensitivities in a wide range of 80 applications, including chemical (Sin & Gernaey, 2009), hydrological (Francos et al., 2003; Gan et 81 al., 2014), biological (Zi, 2011) and environmental (Cartailler et al., 2014) models.

82 Parameter sensitivities might be influenced by the crop type, the agricultural management (e.g. N 83 fertilisation) and biophysical environments (e.g. soil and weather) (Confalonieri et al., 2010b; Richter 84 et al., 2010; Zhao et al., 2014). Also, the influence of agricultural practices and weather may vary 85 among crops. For example, the importance of the parameters used in the modelling of processes 86 relevant to water stress could be altered by the timing of the crop growing season, irrigation practices, 87 soil properties and weather conditions. Further, the sensitivity of parameters used in the modelling of 88 N losses might be irrelevant when evaluated in conditions of limited N supply. Thus, ignoring the 89 influence of the specific conditions on parameter sensitivity may produce misleading results.

Despite increasing awareness of the importance of SA in model implementation and particularly in
 identifying influential parameters to consider during model calibration (Moriasi et al., 2016; Sarrazin

92 et al., 2016; Xu et al., 2016; Hjelkrem et al., 2017), screening SA methods have not yet, to the best 93 of our knowledge, been applied to the DAISY model; a widely used model for simulating water, 94 carbon and N transport and transformation processes in soils and plants (Hansen et al., 2012). 95 Although sensitivities of parts of the model have been studied using simpler local SA techniques with 96 a limited number of parameters (e.g., Salazar et al., (2013), Kröbel et al., (2010) and Manevski et al., (2016)). Therefore, this study aims to analyse the sensitivity of key outputs of a widely used process-97 98 based simulation model (DAISY), applied to the winter wheat-summer maize cropping system in 99 North China Plain (NCP), to crop and soil relating parameters and the extent to which parameter 100 sensitivities are affected by crop sequence, field management and weather conditions.

101 Materials and methods

102 The sensitivity of the four essential model outputs grain yield (Mg ha⁻¹), grain N content at harvest (kg N ha⁻¹), cumulated evapotranspiration (mm) and N leaching (kg N ha⁻¹) to crop and soil relating 103 104 parameters of the DAISY model were considered. The analysis was performed using long-term 105 experimental data of a winter wheat-summer maize double cropping system from the Luancheng 106 Experimental Station in the North China Plain. The Morris method (Morris, 1991) was selected in 107 this study as it shares many of the positive qualities of the variance-based techniques whilst having 108 the advantage of being able to screen out less influential parameters with a relatively few runs of the 109 multi-parameter model like DAISY (Campolongo et al., 2007). Because output sensitivity to crop 110 and soil input parameters may vary across seasons and crop management, the sensitivity was 111 computed for different cropping seasons with diverse weather conditions (e.g., wet, average, dry 112 seasons) and under different N fertiliser treatments (e.g. below average, average, high, and very high 113 N rates).

114 **Experimental data**

The data used for model sensitivity analysis were collected from an ongoing experiment using the conventional double cropping system, with winter wheat (*Triticum aestivum* L., early October to mid-June) and summer maize (*Zea mays* L., late June to late September) in the NCP. The field experiment was conducted at Luancheng Agro-Ecosystem Experimental Station (37°50'N, 114°40'E, elevation of 50 m) of the Chinese Academy of Sciences, located in the piedmont plain of the Taihang Mountains in Hebei Province in the NCP. A completely randomized block design with four N fertiliser rates

(200, 400, 600, and 800 kg urea-N ha⁻¹ year⁻¹) was used. These rates reflect possible fertiliser inputs 121 122 (below average, average, high, and very high) currently used in the NCP. The summary of the crop 123 management details such as tillage, wheat and maize varieties, time for crop sowing and harvest, and 124 fertilisation and irrigation amounts and application dates used to set up the DAISY model are given 125 by Hu et al., (2006) and Li et al., (2007). Data from nine consecutive years (1997 to 2006) were 126 included in our study. The first 3 years (1997-2000) were used as a warm-up period to obtain model 127 states that are independent of the chosen initial values and were excluded in the following analysis. 128 The warm-up period was judged to be sufficient for the current analysis.

Daily weather inputs required by the model were measured at a nearby weather station placed at a distance of 300 m from the field experiment. During the maize growing season, the mean seasonal precipitation recorded during the study was 310 mm, and the mean air temperature was 23°C. However, during the wheat growing season, the mean seasonal precipitation was 100 mm, and the mean air temperature was 5.9°C (Table 1).

134 <INSERT TABLE 1 HERE>

135 Model description

The DAISY model is a dynamic agro-ecosystem model combining a hydrological model, a mineral 136 137 N model, a soil organic matter (SOM) model and a crop model. It has been successfully evaluated in different environments (e.g. Denmark (Bruun et al., 2003; Salazar et al., 2013), Poland (Heidmann et 138 139 al., 2008) and China (Kröbel et al., 2010; Manevski et al., 2016)) and at different scales (Djurhuus 140 et al., 1999; Hansen et al., 2001; Jensen et al., 2001). The DAISY model has also been used in 141 comparative studies with other models used worldwide (Palosuo et al., 2011; Rötter et al., 2012; 142 Groenendijk et al., 2014). The model components have been intensively calibrated and verified 143 against comprehensive field measurements of crop leaf area index, yield, crop evapotranspiration, 144 soil water content, N₂O emissions and N leaching as well as nitrate N concentrations in the soil 145 solution.

The model structure is comprehensively described by Hansen & Abrahamsen, (2009; 2012), so only a brief outline is given here. The hydrological model simulates the key processes of water dynamics in the surface and subsurface of soils: including evapotranspiration, canopy interception, soil water transport (using Richard's equation) and soil temperature. The N model simulates transformation and 150 transport (using the convection-dispersion equation) of soil mineral N. The SOM model simulates 151 immobilisation and mineralisation of N, coupled to carbon cycle (Van der Keur et al., 2008). The crop model simulates plant growth and development, including the accumulation of dry matter and 152 153 N in different plant parts, the development of leaf-area index (LAI) and the distribution of root 154 density. It includes a detailed phenology module that considers three growth phases (i.e. sowing-155 emergence, emergence-flowering and flowering-maturity phase). Crop phenology is simulated based 156 on the calculation of the rate of development from functions of temperature, photoperiod and 157 vernalisation effects. LAI is computed as a function of leaf biomass and specific leaf area, which 158 varies according to the development stage. Aboveground biomass is partitioned to plant organs using 159 a set of stepwise linear functions driven by crop developmental stage. The soil is parameterized by a 160 one-dimensional vertical structure and the soil profile is divided into layers on the basis of physical 161 and chemical soil properties. DAISY includes as well a management module, which enables 162 simulation in the agro-ecosystems subject to various system management operations which include 163 soil tillage, crop sowing, fertilisation, irrigation and crop harvest. The model runs on a daily time step 164 at field scale and is driven by meteorological and crop biological data.

165 Model parameterisation

166 In this study, crop phenology was modelled based on $\operatorname{crop} \times \operatorname{temperature} \times \operatorname{photoperiod}$ interaction. 167 In the model, the rate of development towards a specific stage (i.e. flowering and physiological maturity) for winter wheat and summer maize was characterized by three components: the maximum 168 169 rate of crop development; any delay due to a non-optimal temperature; and any delay due to a 170 photoperiod response. The temperature effect was modelled as follows: below a base temperature 171 (Tbase), no development occurs; above Tbase, the rate of development increases up to the optimum 172 temperature (*Topt*); the rate declines immediately above *Topt*; and above a maximum temperature 173 (Tmax), development is assumed to cease. This suite of temperatures represents the cardinal 174 temperatures for development which are separately defined for the vegetative and reproductive crop 175 growth stages (Fig.1a). Furthermore, leaf photosynthesis was modelled based on Goudriaan & Van 176 Laar, (1978). Similarly, the temperature effect on leaf photosynthesis was modelled based on the 177 concept of cardinal temperature (Tbase, Topt and Tmax). However, in this case, the optimum is spread 178 over a range of temperatures where the leaf photosynthesis is constant (a plateau response) and 179 therefore the optimum is defined as having two values lower, *Topt1*, and upper, *Topt2* (Fig. 1b).

180 <INSERT FIGURE 1 HERE>

To model soil water transport, the soil water retention curve was described using the Campbell equation (Campbell, 1974). The soil was modelled as a series of three horizontal layers through which water and dissolved materials move. The first layer extends from the soil surface to a depth of 35 cm. The second and third layers extend respectively from a depth of 35 cm to a depth of 90 cm and from a depth of 90 cm to a depth of 200 cm. The data provided by Yang et al., (2006) on soil water content at saturation, field capacity and wilting point for each layer were used as default values to estimate the Campbell equation parameters (Table 2).

188 <INSERT TABLE 2 HERE>

189 Sensitivity analysis

190 The structure of the Daisy model is complex, including many simulated processes and potentially 191 many interactions; thus no a priori assumption can be made about the linearity or additivity of the 192 model response to parameter changes. Therefore, commonly applied one-parameter-at-a-time SA is 193 considered inappropriate (Saltelli & Annoni, 2010). In the present study, the sensitivity method 194 proposed by Morris, (1991) was adopted. The Morris method is considered a screening method that 195 provides a good compromise between efficiency and accuracy and it is particularly well-suited for 196 computationally costly models and/or when a high number of input parameters are considered (Xu & 197 Mynett, 2006; Campolongo et al., 2007). It has the advantage of being computationally less 198 demanding compared to the variance-based SA. By using a relatively small number of model 199 evaluations, a subset of influential and non-influential input parameters in a model could be identified.

The Morris method is based on the calculation of the so-called Elementary Effects (EE) of each input parameter on model outputs. The EE method can be conceptualised as a randomised OAT design, in which only one input parameter is modified between two successive runs of the model. This design can be regarded as a global design covering the entire space over which the parameters may vary (Wang et al., 2006). For a given parameter set $X = \{x_1, \dots, x_n\}$, the elementary effect, $EE_{Y(x_i)}$, of the parameter, x_i , on the output, y, is defined as follows:

206
$$EE_{Y(x_i)} = \frac{Y(x_1, \dots, x_{i-1}, x_i + \Delta_i, x_{i+1}, \dots, x_n) - Y(x_1, \dots, x_n)}{\Delta_i}$$
 (1)

where Y(x) is the output variable, x_i is ith model input parameter, n is number of parameters, and Δ_i is the predefined sampling increment of the model parameter x_i . However, in contrast to local 209 methods, the perturbation Δ as defined by Morris, (1991) is a predetermined multiple of $\frac{1}{p-1}$ in which 210 p corresponds to the number of intervals/levels that a parameter range is divided by. Saltelli et al., 211 (2004) suggested the use of $\Delta = \frac{p}{2(p-1)}$ with the number of levels p ranging between 4 and 10. In this 212 work, the level p was fixed to 10 according to Zhan et al., (2013).

213 The whole procedure is repeated r times (r is the number of trajectories), providing r elementary 214 effects for each parameter where r typically varies between 10 and 50 (Campolongo et al., 2007). The 215 total number of model evaluations is then given by r(n+1). For this study, r = 50 was used and 216 considered adequate given the complexity of the DAISY model. Moreover, to prevent poor coverage 217 of the parameter space, the space-filling-design, introduced by Campolongo et al., (2007) was used 218 to assure a better spread of the points over the parameter space. This was achieved by first generating 219 1000 different trajectories and then selecting the r = 50 trajectories with the largest distance between 220 couples of trajectories over the parameter space. More details of the method are given in Campolongo 221 et al., (2007).

Because the units of the EEs are the units of the model output over the units of the parameter increment, they cannot be readily compared to each other. We, therefore, used a scaled dimensionless elementary effect as was defined by Sin & Gernaey, (2009) and which was also used inter alia by Ruano et al., (2012):

226
$$SEE_{Y(x_i)} = EE_{Y(x_i)} \frac{\sigma_{x_i}}{\sigma_Y}$$
 (2)

227 where σ_Y and σ_{x_i} are the standard deviations of output Y and inputs x_i, respectively.

The mean μ and standard deviation σ from the obtained SEEs are used to assess the importance of an input parameter. A parameter with high overall importance on the output will have a high μ while a parameter with a nonlinear effect or interacting with other parameters will have a high σ . To avoid the cancelling of positive and negative effects on the mean, Campolongo et al., (2007) suggested the use of the mean of the absolute values of the elementary effects (μ^*) instead of the mean:

233
$$\mu_i^* = \frac{\sum_{i=1}^r |SEE_i|}{r}$$
(3)

To decide whether a given parameter is influential or non-influential, the Morris sensitivity distance, defined as the Euclidian distance $\epsilon_i = \sqrt{\mu_i^{*2} + \sigma_i^2}$ of (μ_i^*, σ_i) from the origin (0,0), was used. A high value of ϵ_i (> 0.1) indicates a relevant effect of the related ith parameter on the model output hence, considered as influential. In order to facilitate the comparison of the SA outputs, the same cut-off 238 value was used. The parameters tested were further ranked according to ϵ values in order of

importance. The threshold value of 0.1 was also employed for the scaled μ^* by Cosenza et al., (2013).

240 The aforementioned sensitivity index (ϵ) was also used in other modelling applications (Xu & Mynett,

241 2006; Ciric et al., 2012; Pappas et al., 2013; Ojeda et al., 2014).

242 Parameters considered for sensitivity analysis

243 DAISY contains a large number of inputs and model parameters. Ideally, all parameters should be 244 screened to determine their relative importance. However, this would result in a large number of 245 simulations making such a study impractical. Based on experience, only a few parameters account for 246 most of the variability of model outputs. Therefore, the sensitivity analysis was restricted to 39 crop 247 parameters which for two crops sum to 78 parameters (including parameters referring to, among other things, phenology, assimilation and respiration characteristics, and partitioning of assimilates to plant 248 249 organs). Furthermore, the analysis was also restricted to 28 soil parameters that for the three soil 250 layers sum to 46 (including among other things soil hydraulic parameters, SOM and soil microbial 251 biomass turnover rates). The parameters were believed to be potentially relevant parameters 252 controlling most of the processes represented by DAISY, and they have been reported in different 253 studies aiming at the calibration of DAISY for different output variables and different locations with 254 different climates, soils, crops and field management scenarios. The initial values of the selected crop 255 parameters were based partly on the values recommended for DAISY in the model crop library and 256 partly on literature screening and results from experimental studies at the Luancheng station. The 257 depth-dependent hydraulic parameters were provided by (Yang et al., 2006). The nominal values of the cardinal temperatures (Tbase, Topt and Tmax) for vegetative and reproductive stages were 258 259 obtained for winter wheat and summer maize from Porter & Gawith, (1999) and Sánchez et al., 260 (2014), respectively. The default maximum rate of development DSRate1 and DSRate2 were adjusted 261 to be within the range of observed flowering and maturity dates, respectively, as recorded in the NCP.

Since there is not enough information about the prior probability distributions for each parameter, we assumed an independent uniform distribution for each parameter. The bounds were set at 20% of either side of a parameter nominal value as was also used by Xu & Mynett, (2006), Sourisseau et al., (2008), Esmaeili et al., (2014) and more recently by Casadebaig et al., (2016). The groups of parameters and the nominal values of all parameters are given in Table A1 (Annex A). The model outputs investigated in this study are grain yield, grain N content, cumulated crop evapotranspiration 268 (ETa) and cumulated N leaching below the root zone during the cropping seasons of both crops.

269 Modelling procedure and statistical analysis

270 A total of $50^{*}(128+1) = 6450$ parameter sets were generated using the Morris method. The model is, 271 therefore, run for each parameter sets for the six cropping seasons simultaneously as winter wheat 272 and summer maize are grown in rotation (double cropping) in the NCP. This way the possible 273 contribution of the parameters of one crop on the model output of the following crop could be 274 investigated. This step is then repeated for each of the N fertiliser treatments. Finally, the model 275 selected outputs where extracted for each combination of $crop \times cropping season \times N$ fertiliser 276 treatment and used to calculate the different Morris sensitivity measures. The outcomes of the 277 sensitivity analyses were then compared within each crop, to evaluate if and to which extent the 278 relative importance of crop and soil parameters varies (i) across the different seasons and (ii) among 279 the four fertiliser N treatments, and to evaluate the stability of the parameter sensitivity. This resulted 280 in 24 sensitivity analyses for each crop.

The effect of the different cropping seasons with different weather conditions and N fertilisation rates on the number of influential parameters were tested using generalized linear models (GLM) for each crop and output variable. In order to model these effects, all GLMs were carried out using Poisson distribution with log link as we have count data (Zeileis et al., 2007). All GLM models were computed using 'glm' function of R. Over-dispersion was investigated using 'dispersiontest' function of the AER package (Kleiber & Zeileis, 2008) and was not found to be significant.

To measure the similarity between the parameter ranks resulting from different input combinations (crop × fertiliser treatment × cropping season) and for each output variable, we used the top-down coefficient of concordance (TDCC). This method was introduced by Iman & Conover, (1987) to test the agreement between multiple rankings. The method emphasises the agreement between rankings assigned to influential parameters and reduces the weight for disagreement between rankings assigned to non-influential parameters (Helton et al., 2005; Confalonieri et al., 2010a). The Savage scores and TDCC are calculated using Eq. 6 and 7, respectively.

294
$$ss(\epsilon_{ij}) = \sum_{k=R(\epsilon_{ij})}^{n} \frac{1}{k}$$
(6)
295
$$TDCC = \frac{\sum_{i=1}^{n} \left[\sum_{j=1}^{m} ss(\epsilon_{ij}) \right]^{2} - m^{2} \cdot n}{m^{2} (n - \sum_{i=1}^{n} 1/i)}$$
(7)

296 where m designates the number of rankings to compare (in this study, m represents either the number 297 of seasons or the number of treatments N); ϵ_{ij} is the sensitivity index/measure for parameter p_i (i = 1,..., n) and ranking j (j = 1,..., m), and $R(\epsilon_{ij})$ is the rank of ϵ_{ij} within ranking j. A rank of 1 is 298 299 assigned to the parameter p_i with the largest value of ϵ_{ii} , a rank of 2 is assigned to the parameter with 300 the second largest value of ϵ_{ii} and so on. In case of equal values of ϵ_{ii} , averaged ranks are assigned 301 to parameters. Values of TDCC close to one indicate a high level of concordance between compared 302 rankings, with agreement declining as TDCC decreases from one. Under the null hypothesis of zero 303 concordance between parameter rankings, the p-values for each TDCC can be calculated using the T 304 statistics (approximating a χ^2 -distribution with n-1 degrees of freedom), derived from TDCC using 305 the following equation:

$$306 \quad T = m \cdot (n-1) \cdot TDCC \tag{8}$$

307 Additionally, the comparison regarding the similarity of classification into the most influential 308 parameters among contrasting weather conditions during the seasons 2003-04 and 2004-05 was 309 performed by analysing Venn diagrams. To further endorse the differences across seasons, we 310 performed a Multi-Dimensional Scaling (MDS) analysis (Hout et al., 2013), which allows 311 representing the distance among different rankings in a reduced number of dimensions. The 312 proximities among the Savage-score transformed ranks are computed using Euclidean distance for 313 each fertiliser treatment-season combination and presented in a two-dimensional plot as outlined by 314 Richter et al., (2010).

315

316 **RDAISY toolbox**

317 Several software packages enabling the automation of the SA of process-based models have been 318 developed and used to study the influence of model parameters on model outputs. In particular, the 319 'Sensitivity' package (Pujol et al., 2017) implemented in the open source software R includes 320 algorithms for global SA including the Morris, Sobol' and FAST methods, among others. However, 321 using these methods with process-based models is not always straightforward and require that the 322 model is first coupled to the R platform in order to use one of the available functions of the 323 'Sensitivity' package. Therefore, a set of functions were created and wrapped into the RDAISY 324 toolbox to be able to operate the DAISY model through the R environment (Jabloun et al., 2014). This process allows reducing programming efforts necessary for conducting sensitivity analysis, 325

326 model calibration and model output visualisation by taking advantage of R's extensive statistical, 327 mathematical, and visualisation packages. The RDAISY toolbox comprises three main functions, 328 update.InputFiles which update the DAISY input files given specified parameter values, runDaisy to 329 run the DAISY model from the R environment given the main DAISY setup file to run and 330 read.OutputFiles, which reads the generated output files with the possibility to restrict the columns 331 to read. These functions, even though written to operate DAISY from within the R environment, are 332 written in a way to be model independent. Therefore, it can be easily adapted to manipulate any model 333 that uses text files as inputs. The interactions between RDAISY toolbox and the DAISY model are 334 shown in Fig. 2.

335 <INSERT FIGURE 2 HERE>

336

337 The update.InputFiles function requires that a text template for each of the input files be created. 338 Each text template complies precisely with the format required by DAISY and contains markers 339 (unique parameter identifier/name) for all the parameters that need to be updated. These templates 340 can be created from the study case related input files by replacing each parameter value by its unique 341 text marker. Additionally, the update.InputFiles function requires that a data.table (Dowle et al., 342 2017) is created which stores the information about the parameter names to be updated, their default 343 values, the full path to the template file where the parameter is used as well as the full path to which 344 the newly updated input file will be saved to. An example of a template file for crop input file with 345 markers and their replacement by current values is shown in Fig. 3a and b respectively.

346 <INSERT FIGURE 3 HERE>

347

The *runDaisy* requires that the full path to the main setup file and daisy.exe is provided. The *read.OutputFiles* is designed in a way to allow reading several output variables from different output files at once. Therefore, a *data.table* with the full path to each of the output files to read and the names of each output variable is required. For the function to work correctly it is crucial to set *print_header and print_dimension* to false when specifying the output variables to log in DAISY (e.g. (*output ("Soil Water Content" (when daily) (print_header false) (print_dimension false))))*. The RDAISY toolbox is given in the supplementary material.

355 **Results**

356 Screening sensitive parameters

The results of the Morris analysis showed a linear relationship between μ^* and σ , suggesting that DAISY parameters with higher overall impacts had a higher nonlinear effect and/or interacted with other parameters. The coefficient of determination (R²) considering all cropping seasons, N treatments and model outputs ranged from 0.67 to 0.94 and from 0.77 to 0.96 for maize and winter wheat, respectively. A subset of the results for the treatment N400 and the cropping season 2004-05 is shown in Fig. 4.

363 <INSERT FIGURE 4 HERE>

364

The number of sensitive parameters varied across cropping seasons and output variables and remained relatively constant among N treatments. The number of influential parameters for each crop, model output and for the seasons 2003-04 and 2004-05 and the N400 treatment is shown in Fig. 5. Regardless of the cropping season, N leaching exhibited the highest number of influential parameters for both crops (more than 38 parameters) and the number of parameters of major importance is generally higher for hot and dry seasons (e.g. 2004-5, Fig. 5) as compared to average and wet seasons (e.g. 2003-04).

372 <INSERT FIGURE 5 HERE>

373

374 In fact, the GLM models showed that cropping season characterised by different weather conditions 375 have a significant influence (p-value < 0.05) on the number of sensitive parameters (results not 376 shown). This observation was true for both crops and all model outputs except for N leaching for 377 which the number of influential parameter does not seem to be affected by weather conditions during 378 the investigated years. Besides, the N fertiliser rates have only a significant effect (p-value < 0.05) on 379 the number of influential parameters of the grain N content of both crops. The differences observed 380 between seasons was due to the model response to dry and wet conditions. In fact, when the dry 381 seasons 2004-05 and 2005-06 are excluded from the data used with the GLM models, the season 382 factor no longer have a significant effect on the number of sensitive parameters for both crops and all 383 model outputs. As for the N treatments, excluding the N200 treatment resulted in no significant effect 384 of N fertiliser rates on the number of influential parameters on the grain N content output.

To compare the relative importance of the input parameters, the calculated Morris distances (ϵ) were plotted against each input parameter for each response variable. Part of the results are reported in Fig. 6, where the parameter importance (in terms of ϵ) obtained for winter wheat and maize is shown for the N400 treatment over two cropping seasons 2003-04 and 2004-05. Parameters with ϵ below 0.1 were regarded as non-influential and were omitted from the figures. The season 2003-04 was chosen as the one with optimal growing conditions, whereas the season 2004-05 was hot during summer and dry during the wheat growing season (Table 1) and was therefore considered as dry and hot.

392 <INSERT FIGURE 6 HERE>

393 The Morris sensitivity analysis for the N400 treatment during the 2003-04 season revealed that 21 394 out of 39 crop parameters (54 %) and 28 out of 46 soil parameters (60 %) showed negligible effects 395 when all response variables were considered together. Low impact on model outputs was given inter 396 alia by parameters related to N concentration in the different plant parts (CrpNRoot, CrpNLeaf, 397 CrpNStem, CrpNOrg), maintenance respiration of the different plant parts (r_Root, r_Leaf, r_Stem, r_SOrg), maximum NH₄ and NO₃ uptake per unit root length (MxNH4Up, MxNO3Up) and to a set 398 399 of parameters that govern crop phenology and crop photosynthesis (Tmax1, Tmax2, PhotTopt2, 400 *PhotTmax*). These parameters could be fixed at their nominal values without having a substantial 401 effect on model predictions. However, the sensitivity of the remaining parameters changed 402 substantially between the different response variables and their rankings differed between the two 403 crops (Fig. 6). For instance, while 13 crop parameters affected maize yield, we found 16 crop 404 parameters that affect wheat yield. When considering only those parameters having a significant 405 effect on all response variables, we found 11 influential crop parameters for wheat but only 6 for 406 maize, and 6 soil parameters were influential for wheat but none of them for maize (Fig. 7).

407 According to the Morris sensitivity distance (Fig. 6), the parameters related to crop phenology, crop 408 photosynthesis and assimilate partitioning were key parameters. In particular, maximum development 409 rate (DSRate1), the optimum temperature for growth (Topt1) and the quantum efficiency (Qeff) had 410 a high influence on all the output variables for both crops. Cumulated ETa over the cropping cycle 411 was also quite sensitive to the crop coefficient (*EpCrop*) and specific leaf area (*SpLAI*), particularly 412 for winter wheat. Interestingly, the results of the Morris analysis over the 2003-04 season suggest that 413 the parameters associated with the previous crop affected the cumulated N leaching of the following 414 crop. In the case of cumulated N leaching during the maize seasons, sensitive parameters were related 415 to crop phenology and crop photosynthesis of winter wheat grown the season before (Fig. 6).

Similarly, N leaching and to a lesser extent grain N content over the winter wheat season were affected
by parameters related to maize. However, ETa, Yield and grain N content of maize were unaffected
by parameters relating to winter wheat.

419 <INSERT FIGURE 7 HERE>

420

421 Similar results were found for the soil parameters, and their importance also varied considerably 422 depending on the crop and the output variable considered. For instance, while maize yield was not 423 sensitive to any soil parameter, cumulated N leaching over the maize cropping season was highly 424 sensitive to water retention at field capacity (FC35 and FC90) and to the saturated hydraulic 425 conductivity (Ksat35 and Ksat90) of the topsoil (0-35 cm) and subsoil (35-90 cm) soil layer. On the 426 other hand, the output variables over the winter wheat cropping season were all sensitive to water 427 retention at field capacity and saturated hydraulic conductivity. Moreover, the soil organic matter 428 content (humus35) was a key parameter for both cumulated N leaching and grain N content of winter 429 wheat.

430 During the 2004-05 season, the results of the Morris method highlighted the importance of the 431 previous crop in affecting all the output variables of the following crop (Fig. 6). Besides the 432 parameters relating to crop phenology, crop photosynthesis and assimilate partitioning, the 433 parameters relating to root growth (PenPar1, PenPar2 and MaxPen) also had a substantial impact on 434 all outputs for both crops during this dry and hot season. Furthermore, it is remarkable that parameters 435 relating to the soil (i.e. hydraulic parameters) rank higher under limited water conditions for all model 436 outputs and both crops. In contrast to the wet season, 7 and 10 parameters relating to soil were shared 437 between the different outputs for maize and wheat, respectively (Fig. 7).

438 Morris SA excluding phenology-related parameters

439 Since most of the crop parameters considered in this analysis depend on crop phenology, the strong 440 sensitivity of DAISY to the parameterisation of crop phenology may mask the importance of other 441 parameters and processes. To investigate this, we repeated the SA with the crop phenology parameters 442 being excluded. Specifically, *DSRate1*, *DSRate2* and cardinal temperatures (*Tbase*, *Topt*, *Tmax*) were 443 fixed to their pre-assessed values (Table A1, Annex A), and the Morris sensitivity indices were 444 calculated for the remaining parameters. By excluding phenology relating parameters, the importance 445 of crop photosynthesis, assimilate partitioning, and root growth was further scrutinized, and their high 446 impact on model outcomes was also confirmed (results not shown). Most of the non-influential 447 parameters remain the same whether or not we considered the parameters related to phenology. 448 However, it is noteworthy that there are differences among the influential parameters, specifically the 449 parameters related to maize crop and influencing the output variables of the next wheat crop. We 450 found that the effect of the previous crop was more accentuated (i.e. higher overall ranks) when the 451 parameters related to phenology were included especially for crop yield. Overall, the effects of the 452 parameters relating to the previous crop and the differences between the sensitive parameters for wet 453 and dry years remained consistent and were not affected by fixing the parameters relating to crop 454 phenology.

455 Influence of weather conditions and crop management

456 The Morris SA was applied for each combination of $crop \times fertiliser$ treatment $\times cropping$ season, 457 which resulted in different Morris distance sensitivity indices. Fig. 8 depicts the variability over the 458 different cropping seasons of the Morris distance for winter wheat calculated for the N400 treatment. 459 In general, the Morris distance of the less influential parameters had low variability over seasons. 460 However, substantial variations in the Morris distance of the most influential parameters (with high 461 ϵ values) driven by the variations in weather over seasons could be observed (Fig. 8), which might 462 result in different rankings over the different seasons (Fig. 9). The parameters DSRate1, DSRate2, 463 *Topt1* and *EpCrop* presented the highest variability over seasons. These findings apply to all model 464 outputs. Similar results were also found for the other treatments. However, the results (not shown) 465 also revealed that the considered N treatments had no noticeable impact on the parameter ranking for 466 the considered output variables. In fact, the TDCC values obtained for the six cropping seasons from 467 the comparisons between parameter rankings obtained across fertilizer treatments were greater than 468 0.95 for both crops and for all output variables and years.

- 469 <INSERT FIGURE 8 HERE>
- 470 <INSERT FIGURE 9 HERE>

471

The TDCC coefficients were calculated for each output variable to provide a quantitative measure of
the concordance of the parameter rankings of the different combinations crop × fertiliser treatment ×
cropping season. All parameters were then ranked in the decreasing order of the Morris distance

475 values for each output. Summarized TDCC values are given in Table 3, where the TDCC values for 476 each output variable are displayed for each combination. The corresponding p-values are not reported 477 but were all <0.05. We obtained a different behaviour for different outputs. TDCC values were higher 478 than 0.92 for the N leaching output for both crops and around 0.9 for grain N content of winter wheat 479 suggesting that the rankings of important parameters remained relatively stable over seasons. 480 However, TDCC values were less than 0.9 for the rest of the output variables for both crops, which 481 implies that the ranks were different across years as was highlighted above.

482 <INSERT TABLE 3 HERE>

483

Fig. 10 shows the MDS plots obtained for grain yield for summer maize and winter wheat. The years,which stand apart from the other years, in such a plot are considered with different parameter ranks.

486 From Fig. 10, it is clear that clusters around the season 2004-05 and 2005-06 (qualified as dry seasons) 487 and the rest of the seasons (qualified as wet seasons) were obtained for winter wheat when yield is 488 considered. Additionally, there is a cluster around season 2002-2003 for maize yield, which was also 489 a wet season. Generally, there were more explicit clusters around the different seasons for winter 490 wheat than for summer maize. The same observations were also obtained for ETa and to a lesser 491 extent for grain N output for both crops. No clear pattern was observed for N leaching for both crops, 492 which is in accordance with the TDCC values. We conclude from this that the low TDCC values and 493 the lack of similarity between the sensitive parameter ranks among years might be mostly due to the 494 differences between parameter ranks for wet and dry years.

495 <INSERT FIGURE 10 HERE>

496 **Discussion**

It is worth mentioning that the Morris method is traditionally used for parameter screening with a very low number of sampled points. Based on the findings of Ciric et al., (2012), Zhan et al., (2013) and Vanuytrecht et al., (2014) a small sample size would not be adequate to obtain a stabilised Morris sensitivity distance for a complex model such as DAISY thus the high trajectory number (r = 50) used in this study. This choice can be further justified by the nonlinear behaviour depicted by the high σ values (Fig. 4). We further acknowledge the subjectivity in the choice of the parameter ranges which might not represent the full extent of the parameter uncertainty. When it comes to parameter screening, narrowing or broadening the range of the parameter values could significantly influence the parameter sensitivity as was delineated by Shin et al., (2013) and Paleari & Confalonieri, (2016). Shin et al., (2013) also highlighted the importance of using ranges yielding plausible parameter sets, which was believed to be the case for the $\pm 20\%$ used in this study. Therefore, we believe the results of this SA were not biased by implausible model realizations. However, it should be stressed that more work is needed to assist in the determination of parameter uncertainty ranges.

It is also important to recognise that the results of this SA were conditional on the cut-off used to select the most sensitive parameters. Interestingly, using a different measure $\beta_i = \frac{\epsilon_i}{\sigma}$ (σ is the standard deviation of ϵ_i of all parameters) instead of using ϵ_i and a threshold of 0.85 to separate the most important parameters from the less-important ones as was suggested by Lu et al., (2013) we found the same set of most influential parameters for each combination crop × fertiliser treatment × season × model output. These findings put more confidence on the parameters classified as most influential for winter wheat and maize investigated in this study.

517 Model-dependent parameter sensitivity

518 Our analysis showed that for the N400 treatment, among the 124 parameters tested, only 34 and 36 519 common parameters were identified as being influential ($\epsilon > 0.1$) for the different model outputs 520 during season 2003-04 and 2004-05, respectively. This applied to both crops. A similar high number 521 of sensitive parameters was also found for other models. For instance, Hjelkrem et al., (2017) in a 522 recent study found that the BASGRA model was sensitive to a relatively large number of parameters 523 (45 parameters). Similarly, Casadebaig et al., (2016) identified 42 parameters to substantially affect 524 wheat yield in different tested environments in Australia using the APSIM-wheat model, and Specka 525 et al., (2015) identified a subset of 28 relevant model parameters from a set of 117 analysed 526 parameters for the agro-ecosystem model MONICA applied to different crops in Germany. It is noteworthy that the same sensitive parameters, albeit differently ranked, were found for both crops 527 528 when all model outputs were considered. However, when model outputs were analysed separately, 529 the sensitive parameters and their number varied substantially with N leaching having the highest 530 number of sensitive parameters for both crops. Regardless of crop and season, N leaching was always 531 controlled by parameters relating to crop and soil; however, the other model outputs had the number 532 of their influential parameters differentiated by season whether it is a wet or dry season as was 533 suggested by the results of the GLM models. The high number of parameters controlling leaching 534 reflects on the complex processes (i.e. the integrated effect of the redistribution of soil water and 535 subsequent convection-dispersion of nitrate) driving the N leaching (Manevski et al., 2016). It is interesting to notice that some parameters, specifically soil related parameters, are shown to be 536 537 significantly more sensitive when evaluated in water-limited conditions especially for yield and grain 538 N. Thus, the sensitive (and non-sensitive) parameters cannot be assumed to be consistent across 539 seasons. These findings were confirmed for the different N treatments investigated in our study which 540 corroborates the findings of van Werkhoven et al., (2008) who demonstrated that when sensitivity 541 analyses are applied for watersheds spanning a hydroclimatic gradient, the most sensitive model 542 parameters might vary significantly across watersheds.

543 Similarly, Song et al., (2013) found that as the climate scenarios changed from wet to warmer and 544 drier conditions, the overall sensitivities of some parameters increased. In a recent study, Casadebaig 545 et al., (2016) found that the impacts of the influential parameters were strongly dependent on 546 environmental and management conditions. However, Tan et al., (2016) found that the weather 547 conditions had negligible effects on the identification of influential parameters of the ORYZA model 548 and that they only had slight effects on the ranks of the parameters' sensitivity for outputs in the 549 panicle-formation phase and the grain-filling phase of rice grown in China. The effect of dry and wet 550 years observed in our study might also be confounded with the effect of irrigation management since 551 irrigation amounts varied across seasons (Table 1). It should be noted, however, that the seasons 552 2004-05 and 2005-06, which are relatively hot and dry with a high cumulative ETo of 875 and 863 553 mm, respectively, showed relatively similar tendencies of parameter sensitivities (results not shown) 554 despite the difference in irrigation amounts for the two seasons (Table 1). Thus, the combined effect 555 of seasons and irrigation management would be worthy of further study.

556 Generally, the DAISY output responses were strongly influenced by the parameters related to crop 557 phenology, corroborating the findings of Kröbel et al., (2010) and Manevski et al., (2016) who also 558 conducted a local SA on key parameters of the DAISY model for winter wheat and summer maize in 559 the NCP. We speculate that this is because many of the parameters in DAISY are formulated to 560 depend on crop phenology (Hansen et al., 2012).

The model behaviour proved to be highly consistent with the nature of the different processes that it integrates. For instance, simulations of grain yield were influenced by the parameters related to crop photosynthesis and to assimilate partitioning. Besides, simulations of crop evapotranspiration were influenced by the crop coefficient and the soil water retention at field capacity at the surface layer on

565 the one hand, and by other parameters linked with the responses of plants to light (Qeff) and temperature (Topt1) on the other hand. In fact, a lower FC value means that the soil water holding 566 capacity is very low and thus a smaller amount of water is available for evapotranspiration and vice 567 568 versa (Abebe et al., 2010). These results are in concordance with the findings of Salazar et al., (2013) 569 who showed that the soil water balance simulated by DAISY was most sensitive to the potential 570 evapotranspiration and soil hydraulic parameters included in the Campbell model. Similarly, Esmaeili 571 et al., (2014), who conducted a global sensitivity analysis on the RZWQM model, found that the field 572 capacity in the upper 30 cm of the soil horizon had the most significant contribution (>30%) to 573 evapotranspiration uncertainty. The high sensitivity to the *EpCrop* parameter in all N treatments and 574 especially during dry and hot years reflects the role of evapotranspiration as a process of direct loss 575 of water from the soil-plant system, which has a considerable impact on the water balance 576 components of the winter wheat-summer maize double cropping system. Similarly, EpCrop and top 577 and sub-soil hydraulic properties were identified as sensitive parameters in simulating N leaching for 578 both crops, because these parameters directly affect soil water movement and the root water 579 uptake. The root water uptake also depends on the rooting depth and the root density distribution, as 580 well as on the soil water status in the rooting depth which was also depicted by the SA. In fact, the 581 parameters related to the root penetration rate (*PenPar1*) and root maximum penetration depth 582 (*MaxPen*) were identified as sensitive parameters in simulating ETa, N leaching, grain yield and grain 583 N content of winter wheat under water shortage conditions.

584 The absence of influence of parameters affecting N uptake (e.g., parameters related to N concentration 585 in the different plant parts) on simulated crop yield and N content indicate that N was not limiting 586 crop growth with current management setup. These results agree with the findings of Hu et al., (2006) 587 who, using the same dataset, found no statistically significant difference in grain yield and grain N 588 content between the different N treatments, implying no N shortage for the investigated N treatments. 589 It could also explain the strong rank concordance between the different fertiliser treatments. A 590 potential explanation of the similarities between N treatments is the issue of over-fertilisation. In fact, 591 a recent investigation by Ju et al., (2009) shows that the fertilisation rate in the NCP exceeds crop 592 requirements for maximum grain yield. In reality, the results of the SA might have been different if 593 there had been a zero N treatment. In fact, Zhao et al., (2014) found that N input with two fertilisation 594 rates (0 and 100 kg N ha⁻¹) influenced the rank order of parameter sensitivities of the APSIM model. 595 It is noteworthy that N leaching depended mainly on the soil hydraulic parameters of the three soil 596 layers, which presented the highest ranks among the other sensitive parameters. We also found that

597 humus content and C/N ratio of the surface soil layer (0-35 cm) as well as the leaf photosynthetic 598 capacity (*Fm*) and photosynthetic quantum efficiency (*QEff*), were among the influential parameters. 599 This corroborates the findings of Manevski et al., (2016) who found, based on a sensitivity analysis 600 applied to 10 parameters of the DAISY model setup for the NCP, that a 10% change in humus content 601 and C/N ratio affected simulated nitrate leaching. They also found that nitrate leaching was strongly 602 affected by parameters governing crop vegetative development and growth (*DSRate1* and *Qeff*).

603 Based on the Morris results, parameters associated with the previous crop showed major effect on 604 cumulated N leaching for the following crop and this was true for winter wheat and summer maize 605 regardless of the weather conditions. Besides, parameters relating to the previous crop also showed 606 major effect on crop yield, grain N content and cumulative ETa of the following crop only under dry 607 conditions (e.g. 2004-05 season). We speculate that the effect of the previous crop is driven by the 608 soil status (i.e. soil water content, organic matter and soil nutrients) left after crop harvest and before 609 sowing of the following crop, This has generally been referred to as the carry-over effects (Kollas et 610 al., 2015) such as N mineralising from the harvest residues of the previous year or altered soil water 611 content due to crop water uptake by the previous crop which was mainly the case in our study. For 612 instance, Li et al. (2007) showed that soil moisture before sowing of summer maize in the NCP is a 613 crucial factor that determines seedling growth, yield, and water use.

614 **Practical implications for model calibration**

615 Parameterization and identification of reliable estimates of the different parameters are a crucial issue 616 in modelling. Sensitivity analysis identifies the parameters that deserve more attention (Ma et al., 617 2012; Hjelkrem et al., 2017). The high σ values associated with the most relevant parameters (Fig. 4) 618 indicated a high degree of parameter non-linearity/interactions. Moreover, our findings showed that 619 there are multiple influential parameters for a single output variable that was considered sensitive for 620 multiple other processes (Fig. 4). This might substantially increase the frustration and subjectivity 621 that often characterize manual calibrations with increasing risk of calibrating parameters with 622 compensating effects. We therefore argue that the multi-objective calibration estimating all 623 parameters related to all output variables at once might be the best approach in this case.

624 Our analysis showed that about 34 parameters greatly influenced the outputs of the DAISY model for 625 both crops in the NCP. It is a valuable indication for the DAISY model users who may opt for 626 approximating the other less-influential parameters to their nominal values while focusing efforts on calibrating the parameters that have the most substantial impact on winter wheat and summer maize grown in the NCP. Because of high N fertiliser rates in the NCP, the N treatments did not affect parameter rankings. Therefore the calibration of the DAISY model in Luancheng could be limited under these conditions to only one treatment. Consequently, the remaining treatments could be used to validate the calibrated model. This approach was adopted by Hu et al., (2006) who used crop and soil data of the same field experiment with N fertiliser at 200 kg N ha⁻¹ yr⁻¹ (N200) for the calibration of the RZWQM model, which was subsequently evaluated using the other N treatments.

634 Moreover, our results suggest that the parameter rankings may differ between cropping seasons 635 depending on whether the cropping season is dry or wet. Specifically, the parameters relating to the 636 soil are more sensitive to seasons than other parameters, and significant uncertainty might be 637 introduced if the calibration is based only on wet years or dry years and the parameters are transferred 638 thereafter to conditions different from the calibration period. These findings support the idea that both 639 wet and dry periods should be included in the calibration and validation periods which was also 640 supported by Gan et al., (1997) and Arnold et al., (2012). Similarly, Li et al., (2012) stressed that a 641 sufficiently long period of records for model calibration should be used to ensure proper 642 representation of climate variability and to achieve stable model parameters. Furthermore, Bastola et 643 al., (2011) and Li et al., (2012) recommended that if model parameters are calibrated against a long 644 time series of historical data containing both wet and dry periods then these parameters can be 645 assumed to be valid also under future climates, with a higher degree of confidence. Moriasi et al., 646 (2016) also stressed that it is very important to ensure that the calibration period captures dry, average 647 and wet years to ensure that parameter values obtained are representative of the study area climate. 648 Our SA results further imply the importance of including different irrigation and/or nitrogen 649 treatments in the calibration process to have more representative parameter sets.

Another insight from our analysis is that parameters related to the previous crop could affect some of the model outputs of the following crop, suggesting the need to consider the continuous crop rotation when calibrating the most relevant parameters of both winter wheat and summer maize, especially when calibrating ETa and/or N leaching. This is in line with the Teixeira et al., (2015) and Kollas et al., (2015) who recently demonstrated the advantage of simulating continuous crop rotations compared to single crops and years in New Zealand, particularly under limited growing conditions as the carry-over effects could affect the growth of the next crop to some degree.

657 In the end, it is worth mentioning that using a higher threshold will result in a lower number of

658 sensitive parameters. This signifies that it would be necessary to examine to which extent the 659 performance of the DAISY model will be affected with respect to reduction in the number of 660 influential parameters.

661 Conclusions

662 The dependence of process-based models on input parameters makes it particularly important to 663 understand their effects on model response outputs. The Morris screening analysis used in this study 664 helped identify the parameters with the greatest impact on the simulated grain yield, grain N content, cumulated ETa and cumulated N leaching below the root zone of winter wheat and summer maize. 665 Our application of the Morris method to DAISY successfully tracked changes in sensitivities of the 666 667 most influential parameters with model outputs. The sensitivities of most parameters changed 668 substantially with cropping season, which represented different weather conditions. We also explored 669 the influence of N fertiliser rates on parameter sensitivities.

670 Out of 128 parameters, the Morris method identified 34 parameters to be most influential for the simulation of investigated model output. These parameters mainly cover processes associated to crop 671 672 phenology, crop photosynthesis, assimilate partitioning, and root growth. The parameters associated 673 to soil hydraulics had major effect on winter wheat outputs and exhibits considerable influence on 674 the cumulative N leaching simulations and the water balance through their effects on the cumulative 675 ETa, as well as on the simulation of crop yield. Their effect on maize yield and grain N content, 676 however, was only apparent under hot and dry conditions suggesting that greater attention should be 677 paid to soil hydraulic parameters when the model is evaluated under dry weather and/or deficit water 678 conditions. The remaining 94 parameters only showed minor sensitivity. The large number of 679 parameters of minor importance indicates that the DAISY model could be simplified.

The parameterisation of the previous crop was shown to substantially affect cumulative N leaching of the following crop as well as crop yield and grain N content depending on whether the cropping season is dry or wet suggesting the importance of considering crop rotations especially when N leaching is the target output. Ranking and relevance of most influential parameters hence depended on weather conditions. Conversely, parameter rankings were shown to be consistent across N input treatments when the amounts of N exceeds crop requirements for maximum grain yield.

The SA presented here has provided a deeper insight into how those sensitivities change dependingon the considered crop, model output and weather condition combinations. The application of the

688 Morris method has considerably improved the understanding of the complex DAISY model and 689 enabled an extensive insight into the model response under limited conditions in the NCP. 690 Furthermore, the obtained results will considerably accelerate the calibration process of the DAISY 691 model when used in the NCP. Nevertheless, it should be noted that the most sensitive parameters 692 highlighted in this study might differ substantially if the model is used in different soil and weather 693 conditions. However, we believe that the developed RDAISY toolbox will serve as a basis for 694 following sensitivity analysis of DAISY. The primary functions developed for RDAISY are not 695 limited to the DAISY model, besides they could be readily applied to process-based models that 696 consider text files as inputs. These functions can also serve as a basis to implement automatic 697 calibration for the DAISY model by taking advantage of R's extensive optimisation packages.

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1018 **Annex A**

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Parameter Name Nominal Value Units Description No. **Crop parameters*** DSRate1 0.026 (0.031) Development rate in the vegetative 1 stage °C 2 8 (4) Development base temperature Tbase1 during vegetative stage 3 Topt1 30.5 (21) °C Development optimum temperature during vegetative stage 4 Tmax1 °C Development maximum 37.3 (31) temperature during vegetative stage 5 DSRate2 Development rate in the 0.03 (0.046) reproductive stage °C 6 Tbase2 Development base temperature 8 (9.2) during reproductive stage 7 °C Development optimum temperature Topt2 26.4 (20.7) during reproductive stage °C 8 Tmax2 36 (35.4) Development maximum temperature during reproductive stage 9 Fm 6(5) $g CO_2 m^{-2}/h$ Maximum assimilation rate 10 Oeff 0.04 (0.05) $g CO_2 h^{-1}/W$ Quantum efficiency at low light 11 PhotTopt1 25 (10) °C Photosynthesis optimum temperature °C Photosynthesis optimum 12 PhotTopt2 35 (25) temperature °C 13 PhotTmax Photosynthesis maximum 45 (45) temperature DSLAI05 DS at CAI=0.5; initial phase 14 0.13 (0.15) $(m^2/m^2)/(g$ 0.03 (0.022) Specific leaf weight 15 **SpLAI** DM/m^2) 16 LeafAIMod Specific leaf weight modifier 1(1)PAR extinction coefficient 17 PARext 0.6 (0.6) Interception capacity 18 IntcpCap 0.5(0.5)mm Crop coefficient 19 EpCrop 1.15 (1.15) 20 **EpFacDS** Crop coefficient modifier 1(1)21 PenPar1 0.25 (0.25) cm/°C/d Penetration rate coefficient 22 PenPar2 4 (4) °C Penetration rate threshold 23 MaxPen 120 (150) Maximum penetration depth cm $2.5 \ 10^{-7} \ (2.5 \ 10^{-7})$ 24 Maximum NH4 uptake per unit MxNH4Up g/cm/h root length

1020 Table A.1. List of input parameters considered in the se	ensitivity analysis.
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1021 *The first entry is the nominal value for maize. Nominal values for winter wheat are given between
1022 parentheses.

No.	Parameter Name	Nominal Value [*]	Units	Description
25	MxNO3Up	$2.5 \ 10^{-7} \ (2.5 \ 10^{-7})$	g/cm/h	Maximum NO3 uptake per unit
•				root length
26	Partit	1(1)	-	Assimilate partitioning
27	r_Root	0.015 (0.015)	-	Maintenance respiration
20	T	0.01 < (0.01 <)	1 -1	coefficient, root
28	r_Leaf	0.016 (0.016)	day ¹	Maintenance respiration
20	r Stom	0.01(0.01)	day-1	Maintenance respiration
29	I_Stem	0.01 (0.01)	uay	coefficient stem
30	r SOrg	0.01 (0.01)	dav ⁻¹	Maintenance respiration
50	1_5015	0.01 (0.01)	duy	coefficient, storage organ
31	ShldResC	0.35 (0.4)	_	Capacity of shielded reserves
		()		(fraction of stem dry matter)
32	ReMobilDS	1 (1.5)	-	Remobilization of stem reserves,
				Initial DS
33	ReMobilRt	0.1 (0.03)	day ⁻¹	Remobilization, release rate
34	ExfoliationFac	0.9 (0.7)	-	Exfoliation factor
35	LfDR	1 (1)	-	Death rate of Leafs
36	CrpNRoot	1 (1)	-	N-concentration in roots
37	CrpNLeaf	1 (1)	-	N-concentration in leaves
38	CrpNStem	1 (1)	-	N-concentration in stem
39	CrpNOrg	1 (1)	-	N-concentration in storage organ
Soil pa	rameters**			
40	BD	1.44;1.49; 1.55	g/cm ³	Soil bulk density
41	clay	0.07; 0.12; 0.35	%	Clay fraction
42	silt	0.86; 0.84; 0.55	%	Silt fraction
43	humus	0.5; 0.2; 0.1	%	Humus content of the soil
44	CN	11; 11; 11	g C/g N	Soil C/N ratio
45	SAT	43.3; 43.1; 45.1	%	Soil water content at saturation
46	FC	35.6; 33.8; 37.1	%	Soil water content at field capacity
47	WP	9.6; 13.9; 14.4	%	Soil water content at wilting point
48	Ksat	3.9; 1.8; 0.08	cm/h	Soil water conductivity at
				saturation
49	SOMs_turnRate	0.00000179	h^{-1}	Turnover rate of the slow SOM
				pool
50	SOMf_turnRate	0.00000583	h^{-1}	Turnover rate of the fast SOM pool
51	SOMs_CN	6.7		C/N ratio of slow SOM pool
52	SMBs_turnRate	0.00000771	h^{-1}	Turnover rate of the slow SMB pool

1024 Table A.1. Continued.

1025 *The first entry is the nominal value for maize. Nominal values for winter wheat are given between1026 parentheses.

1027 ** the three values given are the values corresponding to the three soil layers, 0-35cm, 35-90cm and

1028 90-200cm, respectively.

No.	Parameter Name	Nominal Value [*]	Units	Description
53	SMBs_maint	0.000075	h ⁻¹	Maintenance respiration of the slow SMB pool
54	SMBf_CN	6.7	-	C/N ratio of the slow SMB pool
55	SMBf_turnRate	0.000416667	h^{-1}	Turnover rate of the fast SMB pool
56	SMBf_maint	0.000416667	h ⁻¹	Maintenance respiration of the fast SMB pool
57	OMinit	5000	kg C/ha/year	Initial organic matter content
58	KNH4	0.5	day ⁻¹	Maximal immobilization rate for ammonium
59	KNO3	0.5	day ⁻¹	Maximal immobilization rate for nitrate
60	RMax	0.5	g DM/m²/h	Maximal speed of AOM incorporation
61	Resp	0.5	-	Fraction of Carbon lost in respiration
62	F_turnRate	0.002 (0.002)	h ⁻¹	Turnover rate of the fast AOM pool
63	S_CN	90 (90)	-	C/N of the slow AOM pool
64	S_turnRate	0.0002 (0.0002)	h ⁻¹	Turnover rate of the slow AOM pool

1030 Table A.1. Continued.

	U											
Winter wheat							Summer maize					
Season	Tmean*	ЕТо	Р	Ι	ETo-P		Tmean	ЕТо	Р	Ι	ETo-P	
2000-01	6.2	395	86	200	309		24.3	311.1	215.6	150	95.5	
2001-02	7.2	363	107	373	256		23.9	312.3	263.4	325	48.9	
2002-03	5.0	297	156	233	141		23.5	340.2	292.6	187	47.6	
2003-04	6.0	396	121	140	275		22.2	350.4	434.4	0	-84.0	
2004-05	5.1	448	99	70	349		24.9	426.8	312.5	140	114.3	
2005-06	6.4	490	34	280	456		24.2	372.9	347.2	140	25.7	

Table 1. Weather and irrigation data for winter wheat and summer maize growing seasons at the NCP during the study period.

*Tmean: Mean temperature (°C); ETo: Reference evapotranspiration (mm); P: Precipitation (mm); I: Irrigation (mm)

Table 2. Hydrological properties of the soil profile used in the DAISY model for Luancheng Experimental Station (Yang et al., (2006))

		Soil layer (cm)	
	0-35	35-90	90-200
Organic carbon content (%)	0.5	0.2	0.1
Bulk density (g cm ⁻³)	1.44	1.49	1.55
Soil water at saturation (cm ³ cm ⁻³)	0.433	0.431	0.451
Field capacity (cm3 cm ⁻³)	0.356	0.338	0.371
Permanent wilting point (cm ³ cm ⁻³)	0.096	0.139	0.144
Clay (<0.002 mm) content (%)	7.0	12.0	35.0
Silt (>0.002 and <0.05 mm) content (%)	86.0	84.0	55.0

Table 3. Top-down concordance coefficients (TDCC) obtained for the four fertiliser treatments from the comparisons between parameter rankings obtained across cropping seasons.

Summer Maize							Winter Wheat				
Treatment Yield Grain N ETa N Leaching		Yield	Grain N	ЕТа	N Leaching						
N200	0.88	0.92	0.90	0.92	_	0.89	0.92	0.83	0.93		
N400	0.87	0.88	0.89	0.93		0.89	0.90	0.82	0.93		
N600	0.87	0.87	0.89	0.92		0.89	0.90	0.82	0.92		
N800	0.87	0.86	0.89	0.92		0.89	0.90	0.82	0.92		

Fig 1. Cardinal temperatures for the effect of temperature on (a) crop development and (b) crop photosynthesis.

Fig. 2. Flow chart demonstrating the interactions between RDAISY toolbox and the DAISY model.

Fig. 3. An example of a template file for crop input file with markers (a), and their replacement by default values (b). The example is shown for maize.

Fig. 4. Average Morris mean effects (m*) and spread (s) for different conditions. The labels of the first 10 most sensitive parameters are shown and their abbreviations are given in Table A1 (Annex A).

Fig. 5. Number of most influential parameters for winter wheat and summer maize.

Fig. 6. Morris sensitivity analysis results for all DAISY output responses for the N400 treatment during the wet and dry seasons 2003-04 and 2004-05, respectively. Morris distance (ϵ) indicates the importance of each parameter. Parameter abbreviations on the y-axis are given in Table A1 (Annex A).

Fig. 7. The Venn diagram for crop and soil parameters indicating the number of shared important parameters between all DAISY output responses for summer maize and winter wheat. The results are shown for the N400 treatment during the season 2003-04.

Fig. 8. Box-plots of Morris distance showing the sensitivity of all key output variables to crop parameters, calculated over all six cropping seasons. The results are shown for winter wheat under the N400 treatment.

Fig. 9. The 10 highest ranked parameters of all key output variables, calculated for each cropping season. The ranks are shown for winter wheat under the treatment N400. The parameters were ranked from 1 to 10 based on the ascending order of the Morris sensitivity distance. (W) and (M) denote crop parameters for winter wheat and preceding maize crop, respectively. The numbers represent the ranks for each parameter.

Fig. 10. Proximity of Morris sensitivity distance represented in a common space using multidimensional scaling, displaying the effect of different fertilizer treatments and years on sensitivity analyses results of summer maize and winter wheat yield.









a) Crop template input file with parameter text markers

b) Crop input file with parameter text markers replaced by their default values

```
(defcrop "CN_Maize" "Pioneer Maize"
    (Devel original
        (DSRate1 0.026)
        (TempEff1 (8 0.01) (30.5 1.00) (37.3 0))
        (DSRate2 0.03)
        (TempEff2 (8 0.01) (26.4 1.00) (36 0))
)
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Fig. 3



Fig. 4







Fig. 6















