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A sound understanding of a cropping system model with the global sensitivity analysis

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ABSTRACT

The capability of cropping system models of depicting the crop and soil-related processes implies a high number of parameters. The aim of this work was to detect the key parameters, and the associated processes, of the ARMOSA cropping system model, considering two target outputs, crop yield and nitrogen leaching. A global sensitivity analysis (SA) was carried out in two steps: (1) the Morris method considering the whole set of parameters; (2) Sobol analysis was applied to the Morris outcome. The simulation was run on winter wheat in four soil types in Marchfeld (Austria, 2010–2018). Parameters affecting crop yield was the critical nitrogen concentration, the potential CO_2 assimilation rate, and the drought sensitivity parameter. Nitrogen leaching was mainly affected by the decomposition of litter and the early aboveground biomass growth. The parameters ranking did not appreciably change across soil types. This study offers a quick and replicable methodology for model calibration.

1. Introduction

Adequate management and preservation of natural resources is a current challenge in agriculture, also due to the impact of climate change. The need to maintain good yield productions complicates this challenge since agriculture is regarded as the main driver of environmental degradation in Europe (Chukalla et al., 2018; Young et al., 2021; Bancheri et al., 2022). Indeed, agricultural intensification is often regarded as a key driver of global warming (Wezel et al., 2015), along with biodiversity and ecosystem services loss (Díaz et al., 2019). To tackle this issue, the scientific community has been studying and developing strategies to support multiple ecosystem services, among which the yield production, soil fertility and water quality improvement (Schulte et al., 2014; Gagic et al., 2017; Meena et al., 2020; Montanarella and Panagos, 2021). With this regard, site-specific strategies have been applied in experimental field trials to test the effect of single practices, or a combination of them, on a restricted set of variables, in short, and long-term perspectives.

In this context, mathematical models that depict cropping systems are powerful instruments to evaluate the long-time effect of agronomic management strategies on different crops, soil types, and pedoclimatic conditions, without performing costly and time-consuming field tests. Therefore, cropping system models allow for overcoming the limited temporal and spatial conditions of the experimental trials (Deytieux et al., 2016). Given the great potential of the mathematical models, depicting the effect of the pedoclimatic conditions and of the agricultural practices on target variables is strictly required for a reliable representation of the cropping system (Keating and Thorburn, 2018). While most of the cropping systems models adequately simulate crop growth, fertilization, and irrigation (e.g., STICS (Brisson et al., 2009), APSIM (Holzworth et al., 2014) and EPIC (Izaurralde et al., 2006)), the effect of tillage on soil state variables is rarely addressed and, when present, it is not linked to carbon and nitrogen cycling. Such an aspect is pivotal when the aim of the modeling analysis is the quantification of the effect of contrasting farming systems (e.g., conventional vs conservation agriculture) on soil and crop-related variables (Valkama et al., 2020). To do that, it is strictly required to mathematically describe the effects of soil tillage (e.g., ploughing and sod seeding) in detail, especially when it interacts with the management of the crop residues.

ARMOSA (Analysis of cRopping systems for Management Optimization and Sustainable Agriculture) is a process-based model that has

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been developed to quantify the effects of crop management practices on soil nitrogen and carbon cycles, on nitrogen leaching, and on soil carbon sequestration (Perego et al., 2013). ARMOSA has the peculiarity to dynamically quantify the effect of tillage and soil organic carbon evolution, on the soil water retention curve and the bulk density, for a consistent representation of the field practices; this aspect enables the model application in decision support systems. The model simulates crop growth and development by including soil water dynamics, carbon and nitrogen cycling and evapotranspiration. These complex and interconnected processes, which take place in the soil-crop–atmosphere continuum, are described at such a detailed level of representation that ARMOSA relies on a large number of parameters (approximately 100).

The calibration of the ARMOSA model was performed in many applications by considering contrasting pedoclimatic conditions and cropping systems with specific purposes, i.e., the quantification of nitrogen leaching (Groenendijk et al., 2014; Perego et al., 2014), net ecosystem exchange (Sandor et al., 2017), soil organic carbon evolution (Valkama et al., 2020), and crop yield (Pirttioja et al., 2015; Fronzek et al., 2018; Puig-Sirera et al., 2022; Kimball et al., 2023). To set the values of the model parameters for a given situation with a selected purpose, information and data are usually retrieved from specific experiments which are time and money-consuming. Moreover, an important aspect is that the number of parameters considered in a robust calibration must be low to ensure valid values also for further model applications (Confalonieri et al., 2009). In fact, optimizing a high number of parameters might well fit the data of the calibration dataset, but often fail to represent other datasets (Seidel et al., 2018), typically the one used in the validation step. It is therefore useful to identify strategies to help users to apply the model in different situations.

In this perspective, an effective strategy is based on the evaluation of the influence of each input parameter, and possibly of combinations of them, on the target state variables of interest. In fact, this indicates which are the most important input parameters that therefore require an accurate estimate, and which are almost not influential ones that can be thus neglected in the calibration phase (Razavi et al., 2021). Moreover, it provides useful information about the formalism used to model the cropping system: i.e., it highlights which parameter values change according to crop or soil type, and which are instead generally valid being characteristic of physical, chemical or biological processes. Such a knowledge of the model is therefore crucial to decide either which time and money-consuming data collections are needed, or how the calibration phase can be optimized according to the purpose of the study.

With this regard, global sensitivity analysis methods (Iooss and Lemaître, 2014; Saltelli et al., 2004; Saltelli, 2008) are developed to estimate the influence of input parameters on the state variable of interest, and thus identify the most influencing ones, by considering all the admissible values of the input parameters and combinations of them (Richter et al., 2010; Saltelli et al., 2019). In other words, global sensitivity analysis methods allow the understanding of the model behavior (Confalonieri et al., 2012) spotting the key parameters for which admissible range results in the highest variability of the output (Monod et al., 2006; Diel and Franko, 2020). In this context, this work aimed to gain insight into the ARMOSA model, to understand the parameter effects and the possible interactions between parameters. Specifically, a global sensitivity analysis of the model was carried out to identify the key parameters (and the relative processes) affecting the variability of the mean annual yield and the average annual nitrogen leaching at 1 m depth, being good indicators of productivity and environmental impact, respectively. The analysis was performed on winter wheat (*Triticum aestivum* L.), in four soil types in an intensive agriculture area (Marchfeld, eastern Austria), from 2010 to 2018. Dealing with a large number of input parameters, the sensitivity analysis was conducted by following a two-step approach. The screening method of Morris (with the improvement proposed in Campolongo et al. (2007)) was first applied to obtain a ranking of the majority of parameters without extensive computations (Paleari et al., 2021). Then, as already done in DeJonge et al. (2012), Confalonieri et al. (2013), Bregaglio et al. (2020) and Xiang et al. (2022), the more accurate and CPU-expensive Sobol method (Sobol, 2001; Homma and Saltelli, 1996) was applied to the top parameters resulting from the first screening. In addition, the top-down correlation coefficient between the parameter rankings returned by the Morris method was used (i) to verify that the two target outputs are mainly regulated by different parameters/processes, and (ii) to evaluate the contribution of the pedological conditions on each output target.

2. Material and methods

In this section, the ARMOSA model and the case study of our interest are described, then the statistical methods used to perform our analysis is stated.

2.1. The ARMOSA model

The ARMOSA model (Perego et al., 2013; Valkama et al., 2020) is a process-based model that depicts the cropping system with a modular approach. This enables the progressive inclusion of new modules (e.g., intercropping, mulch decomposition on the soil surface, agroforestry) to enrich the model. The description of the complex system implies the simulation of many processes whose algorithms include over 100 parameters. The three main modules daily simulate the water dynamics, the crop growth and development, and the carbon and nitrogen cycling. The water dynamic is simulated with the bucket approach with travel time (Savabi and Williams, 1995). In this respect, the soil characteristics required for each pedological horizon are sand, silt and clay percentages; bulk density; soil organic carbon and nitrogen contents in stable, litter, and manure fractions; and van Genuchten equation parameters (which can be either set a priori or internally derived from HYPRES Pedotransfer Function). In addition, the soil horizons are further split into 5 cm layers for the daily estimation of the soil-related variables. Crop growth and development are implemented according to the WOFOST approach (Van Diepen et al., 1989) but including two improvements presented in Valkama et al. (2020): i.e., (i) the canopy is divided into 5 layers with a different light interception, and (ii) the phenology is described with the BBCH scale (Biologische Bundesanstalt, Bundessortenamt and Chemische Industrie). This allows a detailed simulation of the development (i.e., crop phenology) and the thermal time required to reach the stages. The reference evapotranspiration (ET0) can be estimated using the Penman–Monteith, Priestley–Taylor, or Hargreaves equation. Crop evapotranspiration (ETc) is estimated using the FAO 56 approach (Allen et al., 1998). Actual evapotranspiration (ETa) is calculated as the product of ET0, crop coefficient at a given theological stage and the water stress factor (Sinclair et al., 1987), which also directly influences crop-related processes such as carbohydrate production and photosynthate partitioning. Carbon and nitrogen cycling is simulated following the approach of the SOILN model (Johnsson et al., 1987) with the difference that the organic and inorganic input of nitrogen are assumed independent by considering distinct decomposition rates and fates. This applies also to the application of organic matter inputs (e.g., slurry, dung, compost, green manure, crop residue), which are described by the carbon and nitrogen contents, decomposition rates and burial depths. Regarding the drivers affecting the soil processes, tillage operations affect mineralization (Rádics et al., 2014), hydrological parameters and bulk density and are simulated as a function of tillage depth, timing, degree of soil layers mixing and perturbation. This was implemented following the WEPP model (Flanagan et al., 2007). The mixing of two or more consecutive soil layers (e.g., the first two in the topsoil, involved in the tillage operation) determines pool mixing and the recalculation of pools (e.g. mass or volumetric variables, such as C-litter and soil water content). Bulk density is daily computed based on tillage and the soil organic carbon content.

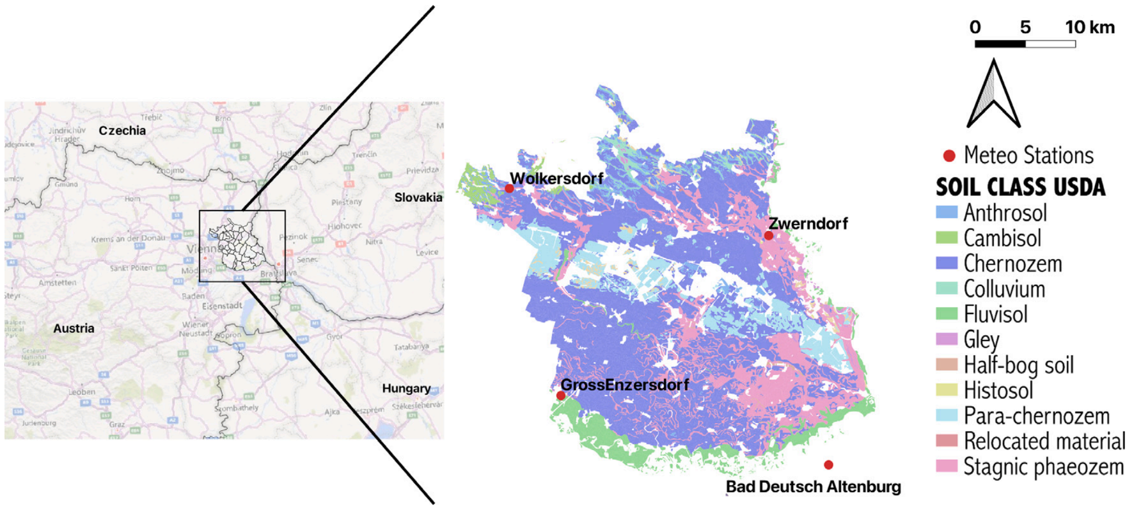

Fig. 1. Soil units and the associated representative soil types (triangles) in the Marchfeld area.

Table 1
Main characteristics, USDA soil classification, classification according to the World Reference Base for Soil Resources (WRB, https://www.isric.org/explore/wrb, last accessed on 28 November 2023) and properties of the four soil types considered in the sensitivity analysis.

USDA classification	WRB classification	Horizon	Depth (cm)	Clay (%)	Silt (%)	Sand (%)	Bulk density (gcm^{-3})	O. M. (%)
loam	Stagnic Phaeozem	Ap	0–35	17	45	38	1.44	2.4
		A	35–55	15	42	43	1.55	0.7
		A/Cg	55–75	17	35	48	1.59	0.2
		Cg	75–200	11	39	50	1.62	0.1
clay-loam	Stagnic Phaeozem Clayey	Ap	0–25	33	49	18	1.22	5.8
		A	25–55	37	46	17	1.28	3.6
		C1k	55–90	23	47	30	1.52	0.4
		C2g	90–150	1	14	85	1.70	0.2
sandy-loam	Chernozem	Ap	0–20	13	28	59	1.47	2.0
		A	20–60	13	30	57	1.48	2.0
		C	60–200	12	29	59	1.64	0.8
silt-loam	Anthrosol	Ap	0–30	20	67	13	1.45	2.2
		A	30–200	20	61	19	1.46	1.8

Input parameters and initialization. Besides daily weather data and soil parameters (texture, bulk density, SOC), with the option to insert the observed values of the water retention curve parameters, the model setting requires information related to (i) the cropping system, i.e., crop sequences, sowing and harvesting dates, residues management; (ii) the irrigation, i.e., water amount, timing, possibly automatic irrigation as a function of water depletion threshold; (iii) the nitrogen fertilization, i.e., mineral or organic, amount, timing, application depth, carbon over nitrogen ratio, ammonia nitrogen over total nitrogen; and (iv) the tillage operations, i.e., depth, timing, degree of soil layers mixing and perturbation.

Output state variables. The main model outputs are above-ground biomass, grain yield, gross primary production, nitrogen crop recovery, soil water content, water percolation, nitrogen leaching, ammonia volatilization, carbon dioxide as the result of soil respiration, nitrous oxide emissions, and soil organic carbon in the three pools (i.e., stable, litter, and manure). Outputs are simulated on a daily basis. Moreover, soil-related outputs are computed by the model for all the soil 5 cm layers.

2.2. Case study

The global sensitivity analysis was carried out to identify the most important parameters (and thus the relative processes) affecting the variability of the mean annual yield of winter wheat, i.e., *Triticum aestivum* L., and of the average annual nitrogen leaching at 1 m depth, in the region of Marchfeld in Austria, i.e., an area of about 1000 km^2, located at the North-Eastern border of Vienna (Lat. 48.20 °N, Long. 16.72 °E), see Fig. 1. This area is one of the primary sources of agricultural products in Austria, and winter wheat is one of the main cultivated crops in Europe.

The considered region is characterized by a flat topography, an altitude within 160−180 m a.s.l. In particular, the dominant soil types in Marchfeld are Chernozem and Para-Chernozem, Stagnic Phaeozem, Fluvisol and Anthrosol, characterized by humus-rich surface horizons and sandy deep horizons, followed by fluvial gravel from the former river bed of the Danube. In this respect, our analysis was performed on four distinct soils largely representative of the 205 soil mapping units recognized in the area, as shown in Fig. 1. The main characteristics and properties of these four selected soils are reported in Table 1. In particular, the main differences between the two selected Stagnic Phaeozem soils are due to the clay content and, for clarity, their classification according to USDA is added. Therefore, from now on, the four considered soils would be named loam, clay-loam, sandy-loam and silt-loam soils, as reported in Table 1.

Concerning the meteorological data, the Marchfeld region is characterized by a temperate continental climate with cold winters and dry summers, with a mean annual precipitation of around 550 mm. The average annual temperature is 10 °C and the mean annual reference evapotranspiration is around 800 mm. Data from four representative weather stations (Zwerndorf, Gross-Enzersdorf, Wolkersdorf, and Bad Deutsch Altenburg, whose position is shown in Fig. 1) highlight a low spatial variability of the climatic and weather conditions. A standard deviation of 31.17 mm year^{-1} in the mean annual precipitation of 570 mm year^{-1}; of 0.30 °C in the mean maximum temperature of 15.20 °C; of 0.73 °C in the mean minimum temperature of 6.45 °C; and of 21.98 mm year^{-1} in the mean annual reference evapotranspiration of 890.00 mm year^{-1} were calculated between the four stations, as reported in the Supplementary Material file named Syntesis.xlsx (available with the ARMOSA software in the repository https://unimibox.unimi.it/index.php/s/pnJ9rRxWfwLT9a3, last accessed on 5 December 2023). Therefore, homogeneous in-space meteorological data was assumed, considering the Wolkersdorf station, which showed to be the most representative in terms of annual cumulative and mean temperatures. In particular, the meteorological data over a period of nine years (i.e., from 2010 to 2018) were used.

Referring to the model description in Section 2.1, in all the forthcoming numerical simulations, the reference evapotranspiration was estimated through the Hargreaves equation by considering the minimum, maximum temperature and the extraterrestrial radiation, while water dynamic was reproduced with the bucket approach with travel time. Finally, the crop management is set as follows:

- sowing time in early October and harvesting time in early July;
- inorganic fertilization of 180 $\mathrm{kgNha^{-1}}$, which was partially applied as urea at sowing and then applied twice during stem elongation;
- ploughing at 30 cm soil depth after the harvesting;
- crop residues were retained in the field after harvesting and incorporated into soil with ploughing.

2.3. Statistical methods

Among the many parameters of the model, our global sensitivity analysis focused on the 70 parameters related to the output variables of our interest, i.e., the mean annual yield and the average annual nitrogen leaching at 1 m depth. In particular, they consist in:

- 18 parameters related to the carbon–nitrogen cycle, accounting for mineralization, immobilization, nitrification, denitrification, volatilization, water and temperature effect on microbial activity, and atmospheric deposition;
- 52 parameters related to the photosynthetic activity, crop maintenance, leaf area growth and duration, vernalization, photoperiod, dry matter partitioning, nitrogen dilution, root growth, and sensitivity to drought.

Specifically, in Table A.1, the parameters are grouped according to the process they are mainly involved in. For each parameter, a short description as well as the range of values considered in the analysis is provided. These ranges of values have been either retrieved from the literature or calibrated through previous applications of the ARMOSA model.

In order to identify the most important processes affecting the variability of the mean annual yield ($\mathrm{Mg\ ha^{-1}}$) or the average annual nitrogen leaching at 1 m depth ($\mathrm{kg\,NO_3\text{-}N\ ha^{-1}}$), a two-step global sensitivity analysis is performed as it follows. Firstly, the screening method of Morris (1991), with the improvement proposed in Campolongo et al. (2007), was adopted to rank the 70 model parameters listed in Table A.1 from the more to the less affecting the variability of the output variables. In particular, for each output variable, the Morris method is applied four times, i.e., once for each soil type defined in Table 1. The top-down correlation coefficient is then used to state if the resulting parameter rankings depend on the considered output variable and/or on the soil properties. Lastly, the more accurate (but also computationally expensive) method of Sobol (Sobol, 2001; Homma and Saltelli, 1996) was applied to the parameters that mostly affect the variability of each output variable. For reader's convenience, details about the application of the methods of Morris and Sobol, and the computation of the top-down correlation coefficient was summarized in Appendix B. The Morris and Sobol analysis was performed by using the SALIB Python library (Herman and Usher, 2017; Iwanaga et al., 2022).

Table 2
Top-down correlation coefficients between the parameter rankings obtained by applying the Morris method to evaluate the effect of model parameters on mean annual yield by considering different soil types, see Fig. 4, to highlight the contribution of soil characteristics.

	loam	clay-loam	sandy-loam	silt-loam
loam	1.0	0.79	0.99	0.78
clay-loam	0.79	1.0	0.77	0.99
sandy-loam	0.99	0.77	1.0	0.78
silt-loam	0.78	0.99	0.78	1.0

3. Results

3.1. Morris' sensitivity analysis

For each soil type, the screening method of Morris modified by Campolongo et al. (2007), was applied to qualitatively rank the 70 parameters in Table A.1 according to the importance of their mean elementary effect μ^* (see Appendix B) on the variability of either the mean annual yield of winter wheat or the average annual nitrogen leaching at 1 m depth.

Before analyzing the Morris sensitivity measures, Figs. 2 and 3 show the distributions of the mean annual yield and of the average annual nitrogen leaching at 1 m depth, respectively, obtained with the 1420 combinations of parameters used for the Morris analysis. Interestingly, all the considered combinations of parameters result in admissible values of both the output variables of our interest. In addition, differences in soil properties mainly affect the distribution of the average annual nitrogen leaching at 1 m depth (see Fig. 3) rather than mean annual yield (see Fig. 2).

In order to investigate the elementary effects of the parameters in Table A.1, for each target output and for each soil type, the Morris' sensitivity measures related to the input parameters were displayed in the (μ^*, σ) plane, see Figs. 4 and 5. According to the considerations reported in Campolongo et al. (2007), the 70 input factors were then ranked according to the sensitivity measure μ^*. The complete parameter rankings obtained for each soil type were reported in Tables S1 and S2 in the Supplementary Material.

Regarding the mean annual yield, Fig. 4 shows that the variability of the grain yield is mainly affected by aCrit, followed by PCO2 and WSPar, for all soil types. A slightly less relevant effect was detected for DeathLeavesStart, kc50, LAITHMin, MaintenanceStorage, CO2compensation25 and maxRootsDepth.

On the other hand, Fig. 5 shows that the variability of the annual leaching was most influenced by CmicrobEfficiencyL and LAI0, followed by TGLAI, kStable, kCstableFractionLM, MicrobialWCbase, maxRootsDepth, NstemHarvest, TBaseLAI, NleavesHarvest, PCO2, aCrit, and SLA. It is further worth noticing that the elementary effects of the parameters LAI0, TGLAI, and TBaseLAI are also characterized by very high variance σ (so that $\sigma > \mu^*$), suggesting that these inputs have large non-linear and/or interaction effects.

The top-down correlation coefficient (Iman and Conover, 1987) was applied to the results of the Morris analysis to quantify the agreement between the parameters ranking obtained for the two target variables (i.e., crop yield and nitrate leaching) for each soil type. The analysis resulted in a weak correlation index, ranging from 0.29 to 0.4 (data not shown). Conversely, high values of correlation coefficients were obtained when comparing the rankings obtained with different soil types for crop yield (Table 2) and nitrate leaching (Table 3).

3.2. Sobol' sensitivity analysis

In order to apply the Sobol method for each of the output variables of our interest (i.e., mean annual yield of winter wheat and annual nitrogen leaching at 1 m depth), a subgroup of the most influential

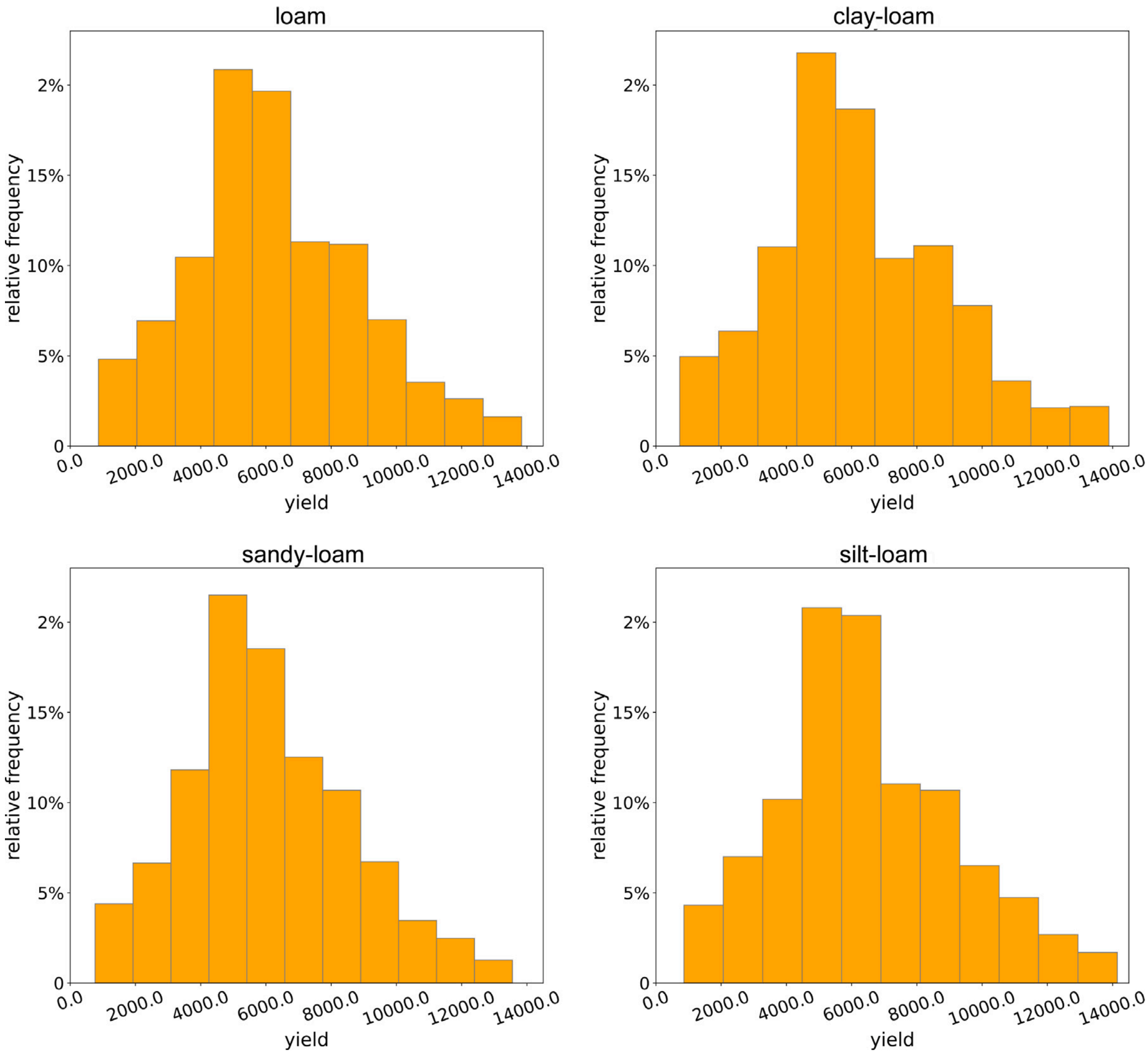

Fig. 2. Distribution of the values of annual yield obtained with the combinations of parameters used for the Morris analysis.

Table 3
Top-down correlation coefficients between the parameter rankings obtained by applying the Morris method to evaluate the effect of model parameters on the annual nitrogen leaching at 1 m depth by considering different soil types, see Fig. 5, to highlight the contribution of soil characteristics.

	loam	clay-loam	sandy-loam	silt-loam
loam	1.0	0.55	0.99	0.55
clay-loam	0.55	1.0	0.56	0.96
sandy-loam	0.99	0.56	1.0	0.56
silt-loam	0.55	0.96	0.56	1.0

parameters detected by the Morris method is first selected. Specifically, as recalled in Appendix B.1, the most important parameters are those displayed in the right region of the (μ^*, σ)-plane in Figs. 4 and 5, respectively, (see those represented with colored markers) that thereby appear in the top positions of the parameter rankings in Table S1 or Table S2 in the Supplementary Material. This provided a group of 9 parameters affecting the variability of the mean annual yield, and a group of 13 parameters for the variability of the average annual leaching at 1 m depth. The selected parameters are listed in Table 4. These subgroups of parameters are thus investigated by applying the Sobol method to estimate how they affect the variance of the respective output variable. The resulting Sobol' indices (i.e., main and total effects) are plotted in Figs. 6 and 7.

Fig. 6 points out that all the parameters listed in the left column of Table 4 are influential parameters that affect at least 1% of the variability of the mean annual yield of winter wheat (having both main and total effects larger than 0.01, see Section 2). In addition, it emerges that the variability of the mean annual yield is mainly due to the parameter aCrit, followed by WSPar and PCO2, as they affect at least 10% of the output variance (having both main and total effect larger than 0.1) regardless the soil type. Other parameters that have an important effect on the mean annual yield variance are maxRootsDepth, except in the case of the clay-loam soil, and kc50, only on sandy-loam soil. It is further remarkable that in the soil type having a high concentration of clay in the layers explored by the roots (i.e., clay-loam), the contribution of aCrit is lower than in the other cases, while that of PCO2 is higher than in other soil types. This behavior can be likely due to the no-limiting water and nitrogen availability in a clay soil such as the clay-loam one (see soil characteristics in Table 1) in which the effect of the genetic crop potential increases (Peng et al., 2020). Lastly, for all soil types, interactions involving aCrit and WSPar have an important effect on the mean annual yield variance (as $0.01 < S_i^T - S_i < 0.1$). Referring to Fig. 4, these parameters in fact fall in the top-right region of the (μ^*, σ) plane for all soil types.

The Sobol' sensitivity measures plotted in Fig. 7 indicate that all the parameters listed in the right column of Table 4 have an important effect on the variance of the annual nitrogen leaching at 1 m depth, having both main and total effects larger than 0.01 for all soil types.

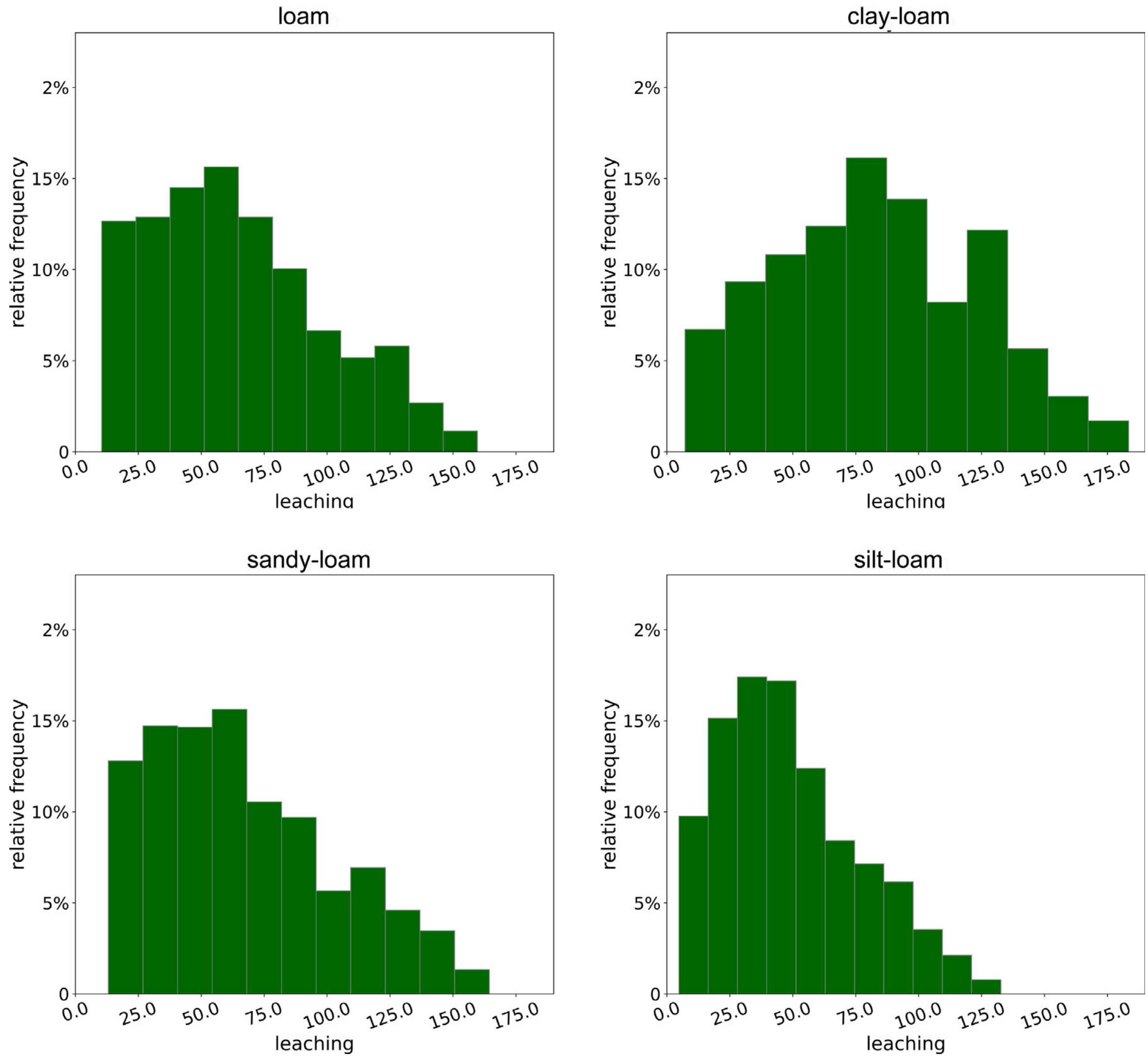

Fig. 3. Distribution the values of average annual leaching at 1 m depth obtained with the combinations of parameters used for the Morris analysis.

Table 4
Lists of input parameters considered in the sensitivity analysis performed by applying the Sobol' method. According to the Morris method, they are the parameters that mainly affect the variability of the mean annual yield (left column) and of the average annual nitrogen leaching at 1 m depth (right column).

Mean annual yield of winter wheat	Average annual nitrogen leaching at 1 m depth
aCrit	CmicrobEfficiencyL
PCO2	LAI0
WSPar	TGLAI
DeathLeavesStart	kStable
kc50	kStableFractionLM
LAITHMin	MicrobialWCbase
MaintenanceStorage	maxRootsDepth
CO2compensation25	NstemHarvest
maxRootsDepth	TbaseLAI
	NleavesHarvest
	PCO2
	aCrit
	SLA

The key input parameters affecting more than 10% of the annual nitrogen leaching variance are CmicrobEfficiencyL and TGLAI for all soil types. In addition, other parameters that have an important effect on the variance of the nitrogen leaching are LAI0 and maxRootsDepth in the case of the silt-loam soil, and kStable in the case of the clay-loam soil. Moreover, consistently with the results in Fig. 5, interactions

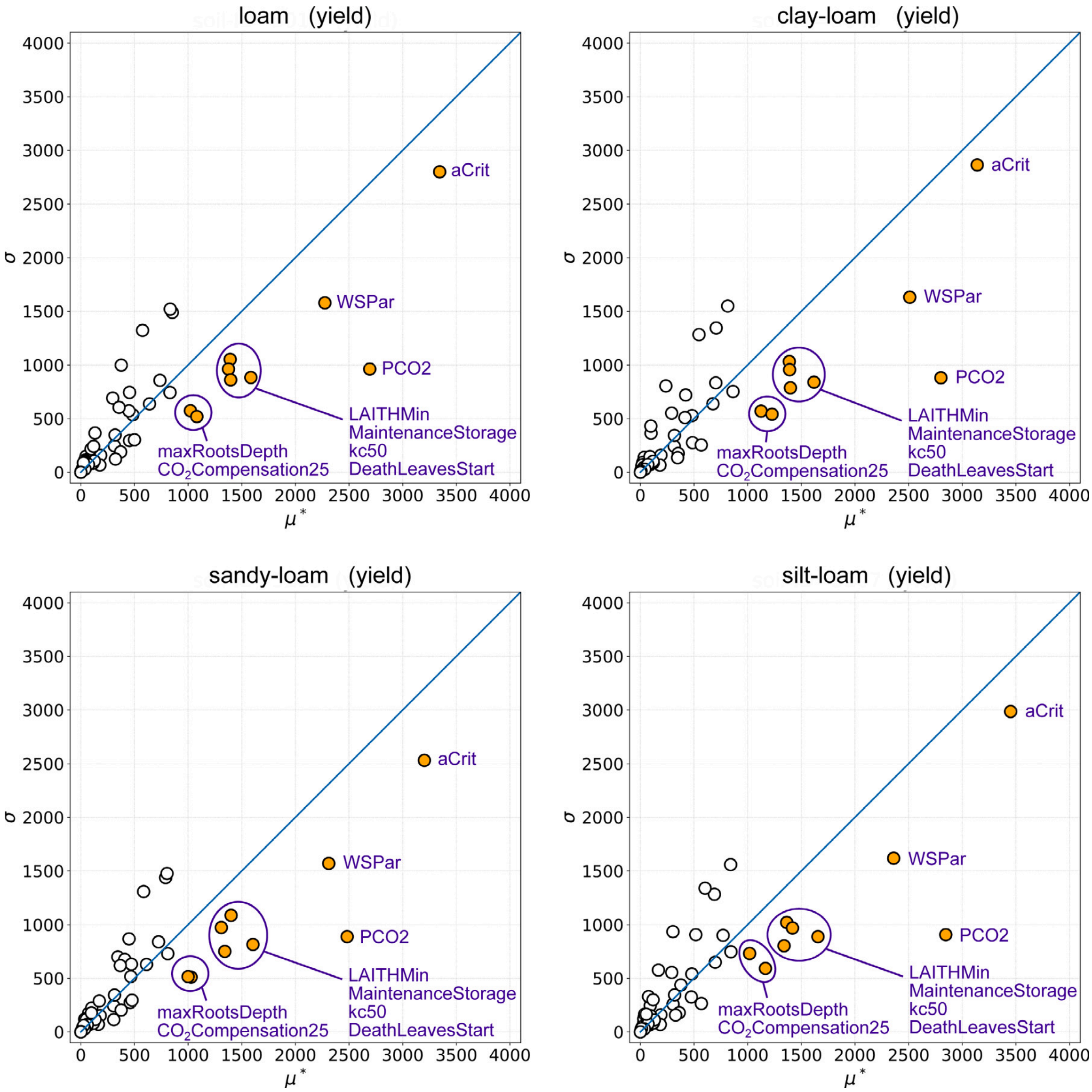

Fig. 4. Plot of the Morris' sensitivity measures indicating how the input parameters affect the variability of the annual yield, in the (μ^*, σ)-plane. In each panel, the line denotes the threshold $\sigma = \mu^*$ and colored circles denote the sensitivity measures of most important parameters. The complete rankings are reported in Table S1 in the Supplementary Material. As a remark: (i) inputs with low μ^* and σ have negligible effects; (ii) inputs with high μ^* and low σ have large linear effects with negligible interaction effects; and (iii) inputs with high μ^* and high σ have large non-linear and/or interaction effects (see Appendix B for further details).

involving LAI0, TGLAI, and TBaseLAI have a not negligible effect on the annual nitrogen leaching variance (as $0.01 < S_i^T - S_i < 0.1$) in the four soils.

4. Discussion

4.1. Discrepancy between the parameter rankings

The top-down correlation coefficient quantified the discrepancy between the parameter rankings returned by the Morris method for crop yield and nitrate leaching. These low values indicate that elementary effects strongly changed for the two target outputs. This is consistent with the fact that the annual yield and the leaching reflect different process domains, which involve different groups of model parameters. Moreover, this result reflects the complexity of the model, in which the processes are described with detailed mechanisms. In particular, the parameter rankings related to the yield, which is a crop-related variable, indicate that the process mostly relies on genetic-based processes rather than on water and nitrogen dynamics. Therefore, the low correlation between the ranking of parameters governing the two output variables confirms that the choice of running the sensitivity analysis to estimate the variability of either the crop yield or the nitrogen leaching allows for exploring different aspects of the ARMOSA model. When studying the correlation between the elementary effects of the four soils, high values were returned, with a larger extent for the crop yield. In the case of the mean annual leaching, the highest agreement was obtained when comparing the Morris outcomes obtained with soils having a similar clay concentration in the top layers (i.e., loam and sandy-loam soils). Looking at the correlation results reported in Tables 2 and 3, it results that the hydro-pedological properties of the soil types have little impact on the sensitivity rank of influential variables on the crop yield. This result was obtained in sub-optimal conditions with no limiting N fertilizer rate in a limiting climate, which is characterized by limited annual rainfall (i.e., 500 mm) with dry summer. Results of low plasticity in yield were also reported by Richter et al. (2010) on durum wheat in two Mediterranean sites having water-limiting climates and contrasting soils with the resulting differences in water and nitrogen availability. The scarce effect on parameters ranking the different soil

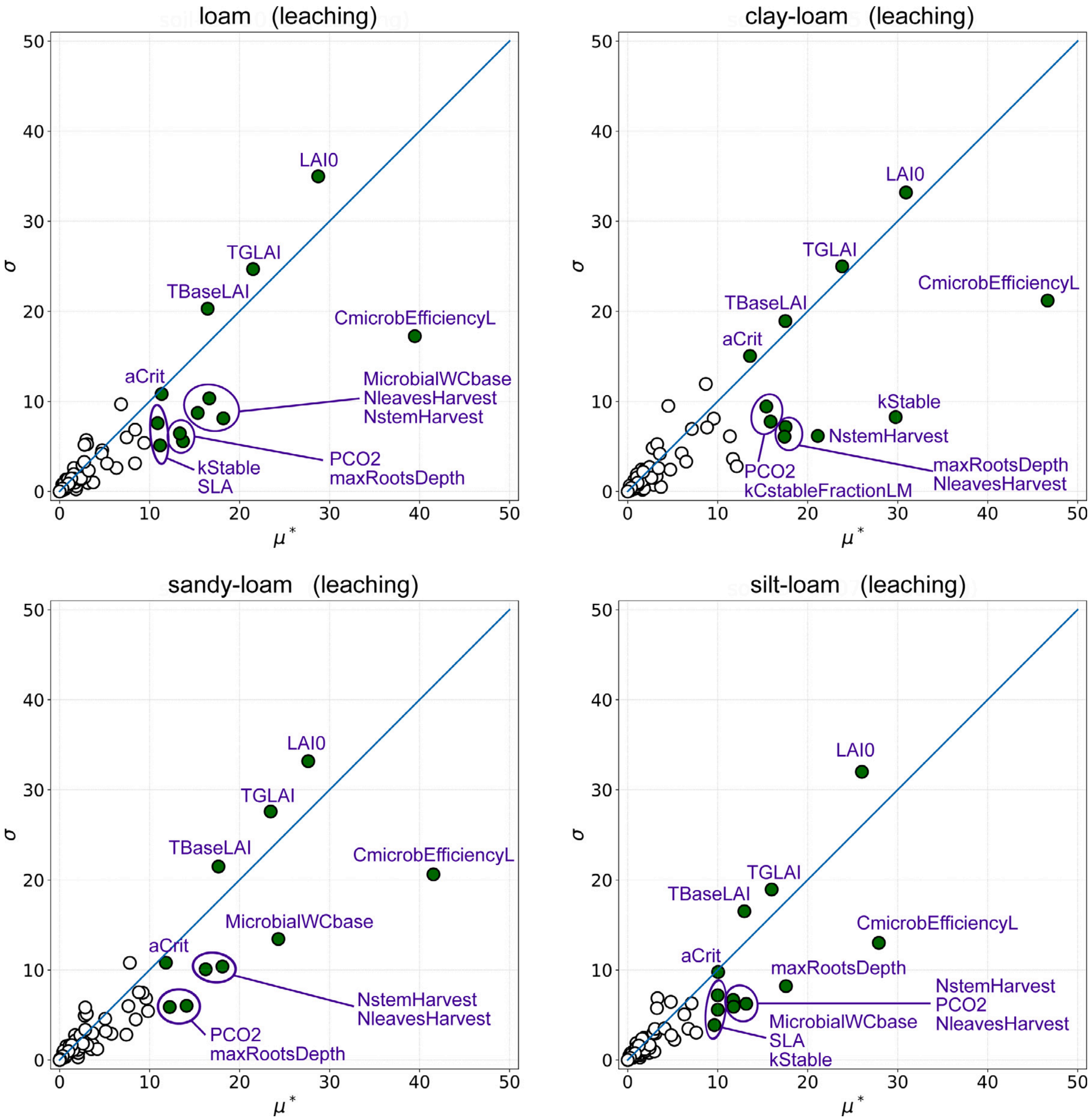

Fig. 5. Plot of the Morris' sensitivity measures indicating how the input parameters affect the variability of the average annual leaching at 1 m depth, in the (μ^*, σ)-plane. In each panel, the line denotes the threshold $\sigma = \mu^*$ and colored circles denote the sensitivity measures of most important parameters. The complete rankings are reported in Table S2 in the Supplementary Material. As a remark: (i) inputs with low μ^* and σ have negligible effects; (ii) inputs with high μ^* and low σ have large linear effects with negligible interaction effects; and (iii) inputs with high μ^* and high σ have large non-linear and/or interaction effects (see Appendix B for further details).

conditions suggests that the ARMOSA model is characterized by low plasticity, which is the model's tendency to change behavior when applied to different conditions (Confalonieri et al., 2012). Regarding the nitrate leaching, a lower correlation resulted when comparing the results of the coarse soils (loam and sandy-loam) with the fine soils (clay-loam and silt-loam). However, these correlations were significant and this was confirmed by a generally similar pattern (Fig. 7). Only two discrepancies resulted due to the effect of the organic matter. In particular, for clay-loam soil kStable was highly significant due to the very high organic matter content, and in silt-loam soil maxRootsDepth resulted in high sensitivity because of the high organic matter at a deeper soil depth. A general low sensitivity of the model to hydro-pedological conditions is likely due to the method by which the parameters of the water retention curve were estimated. In our case study, as in many other cropping system models, the parameters of the van Genuchten function were derived from applying a Pedo-Transfer Function, due to the difficulty of having measured data of hydraulic properties, especially for large-scale studies. This estimation method, as well-known, tends to smooth out the differences between soils (Basile et al., 2019).

4.2. *The relevant parameters and processes of yield and leaching simulation*

Crop yield. The two combined sensitivity analysis methods highlighted that the variability of the annual yield is mainly affected by the parameters that regulate five processes: (i) the nitrogen dilution, i.e., aCrit; (ii) the potential dry matter assimilation, i.e., PCO2; (iii) the susceptibility to drought, i.e., WSPar; (iv) the crop coefficient for the maximum crop ET estimation during the stem elongation stage, i.e., kc50; and (v) the potential root depth, i.e., maxRootsDepth. The similar pattern of the results observed between the four soils having contrasting properties indicates that all these five processes have a key role in yield simulation. It means that an adequate selection of the parameters related to these processes allows for depicting the growth of the crops in different pedoclimatic conditions. In particular, among the studied parameters, aCrit and WSPar have the largest difference between the

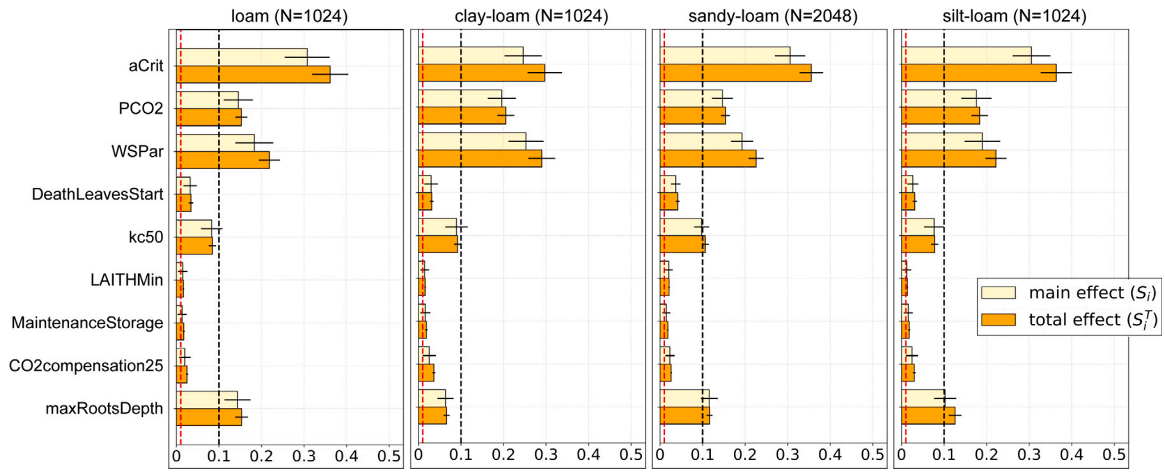

Fig. 6. Sobol' main and the total effects on the variance of the mean annual yield of the input parameters in the left column in Table 4. As a remark, influential parameters are characterized by S_i or S_i^T higher than 0.01 (see the red dashed line); while key parameters have S_i or S_i^T higher than 0.1 (see the black dashed line).

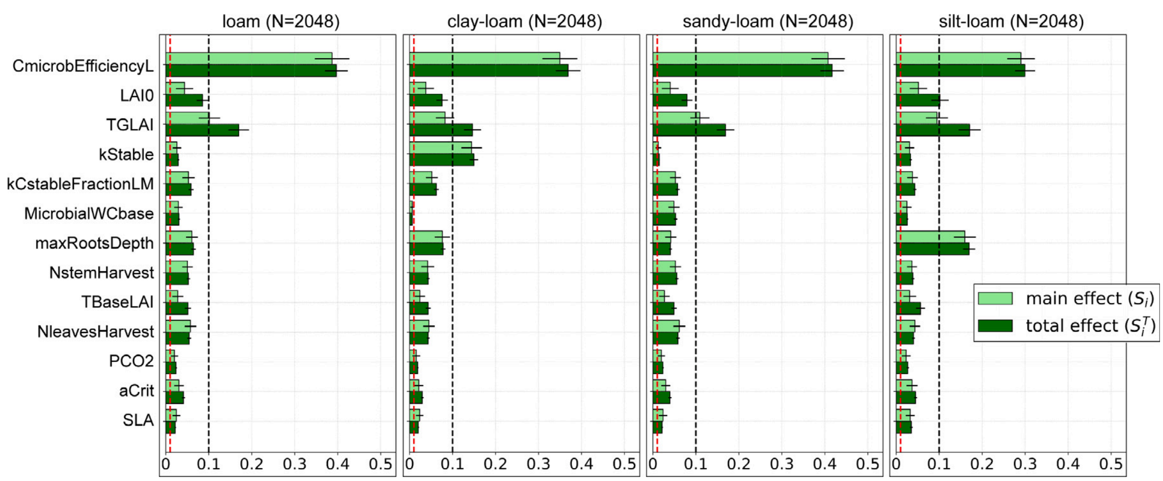

Fig. 7. Sobol' main and the total effects on the variance of the annual leaching of the input parameters in the left column in Table 4. As a remark, influential parameters are characterized by S_i or S_i^T higher than 0.01 (see the red dashed line); while key parameters have S_i or S_i^T higher than 0.1 (see the black dashed line).

main effect and the total effect, regardless of the soil type. It is then likely that the effect of these parameters significantly depends on the value assumed by the other ones. In particular, aCrit is the leading parameter in the critical nitrogen dilution curve (see Table A.1). Each point of the curve corresponds to the nitrogen concentration at which the dry matter accumulation does not increase, despite rises in nitrogen availability and root nitrogen uptake (Justes et al., 1994). It thus guides the fertilization plan, as matching the fertilizer rate with the nitrogen concentration allows for the maximization of nitrogen use efficiency. Moreover, the present ranking analysis found the parameter of the sensitivity to drought as an important function in different soils, also in combination with other crop parameters. In addition, the key role of the sensitivity to drought is pivotal in possible simulations under future climate scenarios, being characterized by more severe drought (Fronzek et al., 2018). In this study, maxRootsDepth had a higher response in soils with higher sand content, in which water availability can be limiting. The crop yield estimation strongly depends on the water availability and water consumption and this agrees with the high sensitivity of maxRootsDepth and kc50, respectively. In modeling studies, these two parameters were addressed while designing *in silico* ideotypes of maize to reduce water loss in drought-prone environments (Lynch, 2013; Perego et al., 2014).

Annual nitrogen leaching. The present analysis highlighted that the variability of the annual nitrogen leaching at 1 m depth is mainly affected by two main processes: (i) the decomposition of the litter and the immobilization of the organic matter coming from the crop residues decomposition into the stable fraction, i.e., CmicrobEfficiencyL; and (ii) the leaf area index growth in the early stages of the crop development, i.e., LAI0 and TGLAI. The first result fully agrees with previous studies which identified the key role of crop residue retention in the soil as a driver of the mineral nitrogen availability and, in turn, of nitrogen leaching. In particular, a review highlighted the effectiveness of estimating nitrogen in soil accounting for different forms of plant residue carbon and nitrogen, and for soil characteristics, rather than dealing with indexes using the carbon-to-nitrogen ratio of crop residues (Chen et al., 2014). Other authors found that crop residue retention allows for a decrease in nitrogen leaching (Wang et al., 2018). A recent work by Tadiello et al. (2023) highlighted the strong interaction between carbon and nitrogen cycling while simulating the crop residue decomposition on the soil surface. In this respect, improvements of the ARMOSA model should consider such an aspect for a closer representation of the complexity of the agro-ecosystem especially when the simulation aims at estimating the effect of the conservation agriculture practices on nitrogen leaching and other environmental variables. The importance of the process related to the growth of the aboveground biomass at the early stages and the related nitrogen demand, which was indicated by the significant effect of the parameters related to the LAI growth, emphasizes that the crop uptake has a higher impact on nitrogen leaching than the soil organic matter mineralization. The earlier the growth of the LAI, which is mainly driven by air and soil temperature, the lower the risk of leaching during the autumn rainfall (Lemon, 2007). With the same regard, in a recent experimental and modeling study (Vogeler et al., 2022), the authors found decreasing nitrogen leaching with early sowing when nitrogen leaching derives from nitrogen mineral fertilizer and the nitrogen that is mineralized from the soil organic matter pool. When the content of organic matter is large (i.e., clay-loam), kStable is a key parameter due to the high nitrogen rate that can be mineralized and made available for both crop uptake and leaching. The calibration of this parameter can benefit from the availability of soil organic matter over time, especially in the topsoil layer (Valkama et al., 2020). Moreover, maxRootsDepth had a large response in silt-loam soil in which the high organic matter in the deeper layer caused a varying nitrate leaching depending on the maximum roots depth because the crop N uptake reduces the N loss downwards.

4.3. The reliable use of the two-step sensitivity analysis in crop modeling

The application of the Morris method to screen the more relevant parameters affecting the outcome of crop models, followed by the estimation of the Sobol indices of the most important parameters is a consolidated practice already used in different works as, for instance, in DeJonge et al. (2012), Confalonieri et al. (2013), Bregaglio et al. (2020), Xiang et al. (2022), Specka et al. (2015), Silvestro et al. (2017). For the sake of clarity, among these works, only in DeJonge et al. (2012), Confalonieri et al. (2013), Bregaglio et al. (2020) and Xiang et al. (2022) the Morris screening method was coupled with the variance-decomposition based Sobol method. Conversely, in Specka et al. (2015) and Silvestro et al. (2017), the Sobol indices of the most important parameters detected by the Morris method were then analyzed by using the Extended Fourier Amplitude Sensitivity Test (eFAST) method, i.e. a robust and computationally efficient method to estimate the Sobol indices (Cukier et al., 1973; Saltelli, 1999). In this respect, in our case, the extremely high computational performance of the ARMOSA code allowed to directly compute the total and main effects with the Sobol method based on the Saltelli sampling, which allows, differently from the eFAST method, a progressive increase of the sample size to reach the convergence.

Going into details, in DeJonge et al. (2012) the two-step sensitivity analysis combining the Morris screening and Sobol methods was performed on CERES-Maize crop model with the aim to evaluate the effect of input parameters regulating water balance and crop growth on different outputs and scenarios, as in our work. Specifically, they consider: anthesis date, maturity date, leaf number per stem, maximum leaf area index, yield, and cumulative ET, under both full and limited irrigation treatments. Instead, Confalonieri et al. (2013) reports the first multi-year spatially distributed sensitivity analysis executed on two complex agroecological models, i.e. CropSyst and WOFOST. Focusing on the production of wheat production in Morocco, the Morris and Sobol methods highlighted that, differently from other crop models, photosynthesis parameters are more relevant than those related to leaf area expansion, under the explored conditions. In Bregaglio et al. (2020) the two-step sensitivity analysis based on the subsequent application of the Morris and Sobol methods, was carried out on a process-based hazelnut simulation model by considering four orchards located in Italy, Chile, and Georgia. The peculiarity of this work is the formalization of a methodological workflow that integrate different sensitivity analysis techniques to support an automatic calibration of the model able to enhance prediction accuracy. In this respect, having a three-year experimental dataset, the sensitivity was performed on the relative root mean square error between the predicted and the estimated quantities, to evaluate the influence of parameter changes on model predictions of fruit yield, leaf area index, and soil water content. It would be surely interesting to adopt this approach in future works to calibrate ARMOSA on proper dataset. Conversely, in Xiang et al. (2022) the Morris screening followed by the Sobol variance-based method were conversely used to determine the governing environmental and management factors that control the groundwater storage and crop yield predicted by the linked DSSAT-MODFLOW modeling system, in an intensively irrigated groundwater region basin. Specifically, they focus on Finney County, southwest of Kansas (USA), in the Ogallala Aquifer, where the main crops are corn, winter wheat, soybeans, sorghum, and triticale. Results indicate that climatic parameters importantly affects crop yields (e.g., 40% for winter wheat), with differences among crops; while hydrogeologic parameters have relatively limited influence on crop yield, as in our case.

Concerning the works where the Sobol's indices were computed with the eFAST method, in Specka et al. (2015), a sensitivity analysis was carried out on the agro-ecosystem model MONICA for six different crops (i.e., winter wheat, spring barley, silage maize, sugar beet, clovergrass ley and winter rape) to identify model parameters that mainly regulate the above-ground biomass. The analysis highlighted that parameters related to photosynthesis and plant development had a dominant effect for all crops, despite the set of important parameters differed for each crop. Lastly, in Silvestro et al. (2017), the Morris and eFAST methods were used to compare the crop models Aquacrop and SAFYE, both describing yield response to water, with the aim to quantify their complexity and plasticity. Specifically, the global sensitivity analysis was carried out on the response of winter wheat yield with a wide range of water limited conditions. Moreover, as in the present work, the top-down correlation coefficient was used to compare the rankings. It was found that SAFYE has a lower complexity and plasticity than Aquacrop.

5. Conclusion

The applied two-step approach identifies only few key parameters of the model due to the constitutive properties of the selected sensitivity analysis methods. While the Morris method handles large amounts of parameters, by providing qualitative information about how much they affect a state variable, the Sobol method is suited to give reliable qualitative estimates of the contribution of a moderate number of parameters on the output variability. It means that this two-step approach is effective in the understanding of the model uncertainty.

The application of a two-step sensitivity analysis pointed out that the variability of the annual yield is mainly affected by five parameters, i.e., aCrit, PCO2, WSPar, kc50, and maxRootsDepth, which are respectively related to the critical nitrogen concentration, the potential carbon assimilation, the drought sensitivity, the maximum crop ET during the stem elongation stage, and the potential root growth. For crop yield, the top down correlation showed a very low level of plasticity.

The variability of the annual nitrogen leaching is mainly impacted by three parameters, i.e., CmicrobEfficiencyL, LAI0 and TGLAI, which regulate the litter decomposition and the crop growth in the early stages. The effect of kStable and maxRootsDepth was detected in soils with high organic matter content. Moreover, the top-down correlation coefficient highlighted that the variability of the two target outputs is regulated by different processes, with a limited effect of soil type on nitrogen leaching. The sensitivity analysis highlighted the complexity of the model and the interaction of crop, nitrogen and carbon processes. The limited plasticity of the model ensures possible applications in varying soil conditions.

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CRediT authorship contribution statement

Annachiara Colombi: Data curation, Investigation, Methodology, Software, Visualization, Writing – original draft, Writing – review & editing, Formal analysis. **Marialaura Bancheri:** Data curation, Visualization, Writing – review & editing. **Marco Acutis:** Methodology, Supervision. **Angelo Basile:** Methodology, Supervision, Funding acquisition. **Marco Botta:** Data curation, Software. **Alessia Perego:** Investigation, Supervision, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Angelo Basile reports financial support was provided by European Commission.

Software and data availability

Software name: ARMOSA (**A**nalysis of c**R**opping systems for **M**anagement **O**ptimization and **S**ustainable **A**griculture), SA-ARMOSA.

Developer: Marco Botta (ARMOSA), Annachiara Colombi (SA-ARMOSA).

First year available: 2021.

Hardware requirements: PC/Mac/Linux.

Software requirements: JRE 1.8 or higher, Python 3.8, SALib Python Library 1.4.5.

Program language: Java 1.8, Python 3.8.

Software and data availability (under request): https://unimibox.unimi.it/index.php/s/pnJ9rRxWfwLT9a3

Cost: free.

Appendix A. Statistical methods for the sensitivity analysis

See Table A.1

Appendix B. Statistical methods for the sensitivity analysis

B.1. Morris method

The Morris method (Morris, 1991), also called Elementary Effects (EE) method, is a screening method based on the one-at-a-time (OAT) design, i.e., it is specifically designed to evaluate the effect of changes in one input parameter at a time on a given target output. The Morris method, as revised in Campolongo et al. (2007), returns three sensitivity measures for each input parameter. Specifically, μ and μ^* describe the overall importance of the parameter on the variability of the model output; while σ indicates the presence of non-linear effects and/or parameter interactions. This method results particularly well-suited to handle models with a large amount of parameters (as in our case) and/or that require expensive numerical simulations. In fact, it returns good qualitative information about the model from a quite low number of realizations.

In more detail, the Morris method is based on the assumption that the model parameters under investigation are independent and uniformly distributed so that the space of the input parameter of our interest is a k-dimensional hypercube, with $k = 70$, defined by the ranges of values reported in Table A.1. For each output variable and for each soil type, the ranking of the input parameters results from the following procedure. The k-dimensional hypercube of the input parameters is discretized into a k-dimensional p-level grid, and $r(k+1)$ points of this p-level grid are selected (see Morris (1991), Campolongo et al. (2007), Iooss and Lemaître (2014) for further details). In summary, following the optimized strategy proposed in Campolongo et al. (2007), the $r(k+1)$ points are obtained by first generating a large amount M of trajectories in the k-dimensional p-level grid. Each trajectory is obtained starting from a randomly given point in the grid, and then performing k steps, one for each dimension, and whose lengths are random multiples of the grid size. The above $r(k+1)$ points are those constituting the r trajectories that maximize the coverage of the space of parameters. In this work, this sampling of the space of parameters is performed by setting $k = 70$, $M = 500$, $p = 16$ and $r = 20$. Each of the forthcoming experiments thus consists in $r(k+1) = 1420$ different setting of the input parameters (each corresponding to one of the selected points in the k-dimensional hypercube) and the same number of realizations of the ARMOSA model: i.e., for each one of the selected $r(k+1)$ points, the mean annual yield of winter wheat and the average annual nitrogen leaching at 1 m depth were calculated. Then, for each output variable, the Morris' sensitivity measures (μ, μ^* and σ) are statistics of the distributions of the Elementary Effects EE_i of the parameter i (with $i = 1, \dots, k$) defined as

$$\mathrm{EE}_i(\mathbf{x}) = \frac{Y(\mathbf{x} + \Delta\mathbf{e}_i) - Y(\mathbf{x})}{\Delta}, \tag{B.1}$$

where $\mathbf{x}$ and $\mathbf{x} + \Delta\mathbf{e}_i$ are two of the $r(k+1)$ selected points in the space of the input parameters; $\mathbf{e}_i$ is a k-dimensional vector with the ith component equal to 1 and all the others equal to 0; Δ is the distance between $\mathbf{x}$ and $\mathbf{x} + \Delta\mathbf{e}_i$; $Y(\mathbf{x})$ denotes the value of the output variable of interest obtained when the parameter setting $\mathbf{x}$ is assumed. In particular, for any input parameter j, μ is the mean, μ^* is the mean of the absolute values, and σ is the standard deviation of the distribution of the Elementary Effects EE_i. According to Morris (1991) and Campolongo et al. (2007), these measures allow the classification of the input parameters into three groups: (i) inputs having negligible effects (with low μ^* and σ); (ii) inputs having large linear effects without interaction effects (with high μ^* and low σ); and (iii) inputs having large non-linear and/or interaction effects (with high μ^* and high σ). For each output variable and soil type, the input parameters are then ranked according to the value of μ^*.

B.2. Top-down correlation coefficient

The top-down correlation coefficient proposed by Iman and Conover (1987) is a concordance measure to compare different rankings. Specifically, this measure is highly sensitive to agreements in the top positions and neglects disagreements at the bottom of the rankings. In this work, it was used to highlight if the rankings resulting from the Morris method are strongly related to either the soil properties or the considered output variable. In detail, let r_i^p be the rank assigned to the ith parameter, with $i = 1, \dots, k$, as achieved in a given test said p. The top-down correlation coefficient C^{pq} between the rankings obtained in two different tests, said p and q respectively, is computed as the ordinary Pearson correlation coefficient on the Savage scores (Savage, 1956). If there are no ties among the variables being ranked, the Savage scores of the ith parameter, related to the rankings obtained from test p, is given by

$$S_i^p = \sum_{j=r_i^p}^{k} \frac{1}{j}, \tag{B.2}$$

and the top-down correlation coefficient writes

$$C^{pq} = \frac{\left(\sum_{i=1}^{k} S_i^p S_i^q - k\right)}{k - S_1}, \tag{B.3}$$

where S_i^p and S_i^q are the Savage scores of the ith parameter, related to the rankings obtained from tests p and q, respectively; while $S_1 := \sum_{j=1}^{k} 1/j$.

Table A.1
Model parameters considered in our sensitivity analysis. SWC means Soil Water Content. SWCSat is SWC at Saturation. "Fraction" denotes constants in the range $[0, 1]$. d denotes day. The reported values have been retrieved from literature or identified with the ARMOSA application (the latter are denoted by "$*$").

Process	Parameter	Description	Values&Units	References
Immobilization of C and N from litter and manure	kCstableFractionLM	Humification fraction of litter and manure	0.2–0.6 [–]	Perego et al. (2013)*, Valkama et al. (2020)*
Mineralization	kStable	Mineralization rate of humus (stable pool)	0.00005–0.0001 $[\mathrm{d}^{-1}]$	Perego et al. (2013)*, Valkama et al. (2020)*
Denitrification	kHalfSatDenitr	Half-saturation constant for denitrification	5–20 $[\mathrm{mg\,L^{-1}}]$	Perego et al. (2013)*
	kDenitrPotential	Potential denitrification rate	0.1–0.4 $[\mathrm{kg\,ha^{-1}\,d^{-1}}]$	
	ThetaDenitrLimited	SWC threshold below which no denitrification occurs	0.15–0.25 $[\mathrm{m^3\,m^{-3}}]$	
Water effect on microbial activity	MicrobialWaterCoeff	Microbial response to water availability	0.1–2 [–]	Johnsson et al. (1987), Perego et al. (2013)*
	MicrobialSaturation	Microbial activity at saturation	0.4–0.8 [–]	
	MicrobialWCbase	Fraction of SWCSat below which there is no microbial activity	0.1–0.5 [–]	
Temperature effect on microbial activity	MicrobialTemp	Temperature at which microbial efficiency is maximum	18–22 [°C]	Johnsson et al. (1987)
Nitrification	kNitrification	Nitrification rate	0.3–0.8 $[\mathrm{d}^{-1}]$	Johnsson et al. (1987)
	NitrateAmmRatio	NO3 over NH4 ratio at equilibrium	5–10 [–]	
Volatilization	kVolatilization	Volatilization rate	0.1–0.3 $[\mathrm{d}^{-1}]$	Johnsson et al. (1987)
N athmospheric deposition	AtmDryNH4	Atmosferic dry deposition	0.005–0.015 $[\mathrm{kg\,ha^{-1}\,d^{-1}}]$	Perego et al. (2013)*
	AtmWetNH4	Atmosferic wet deposition (amount of NH4 in 1 mm of rain)	0.005–0.015 $[\mathrm{kg\,mm^{-1}}]$	
	AtmDryNO3	Atmosferic dry deposition	0.005–0.015 $[\mathrm{kg\,ha^{-1}\,d^{-1}}]$	
	AtmWetNO3	Atmosferic wet deposition (amount of NO3 in 1 mm of rain)	0.005–0.015 $[\mathrm{kg\,mm^{-1}}]$	
Mineralization of organic matter due to tillage	fOx	Mineralization adjustment coefficient during the tillage consolidation process	1–2 [–]	Valkama et al. (2020)*
Photosynthetic activity	EarTmin	BBCH stage after which the ear photosynthetic activity starts	55-65 [–]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
	EarTmax	BBCH stage after which the ear photosinthetic activity stops	80-90 [–]	
	EarRelativeSurface	Ear area/weight ratio	0.0005–0.0007 $[\mathrm{m^2\,g^{-1}}]$	
	EAIfactor	Percentage of EAI that contributes to photosynthesis	0.4–1 [–]	
	MaxCO2net	Max photosynthetic rate capacity	1200–2200 $[\mathrm{\mu g\,m^{-2}\,s^{-1}}]$	
	CO2compensation25	CO_2 compensation point at 25 °C	0–50 $[\mathrm{mg\,kg^{-1}}]$	
	DarkRespiration20	Dark respiration at 20 °C	10–50 $[\mathrm{\mu g\,m^{-2}\,s^{-1}}]$	
	PCO2	CO_2 potential assimilation rate at light saturation	0.001–0.003 $[\mathrm{g\,m^{-2}\,s^{-1}}]$	
	EffPot	Initial light conversion factor	15–17 $[\mathrm{\mu g\,J^{-1}}]$	
	TbaseCO2	Temperature below which CO_2 is not absorbed	0–10 [°C]	
Root growth	RootsElongationC	Roots elongation rate	0.009–0.015 $[\mathrm{mm\,d^{-1}}]$	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
	maxRootsDepth	Maximum roots depth	0.5–1 [mm]	
Dry matter partitioning	FromStemToStorage	Fraction stem weight possibly translocated to storage organ	0.05–0.25 [–]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
	BeginTranslocation	Start BBCH stage of translocation	60–70 [–]	
	FDMshoot9	Fraction of total dry matter allocated to shoot at BBCH stage 9	0.3–0.5 [–]	
	FDMshoot21	Fraction of total dry matter allocated to shoot at BBCH stage 21	0.3–0.5 [–]	
	FDMshoot30	Fraction of total dry matter allocated to shoot at BBCH stage 30	0.4–0.6 [–]	
	FDMshoot45	Fraction of total dry matter allocated to shoot at BBCH stage 45	0.6–0.8 [–]	
	FDMshoot60	Fraction of total dry matter allocated to shoot at BBCH stage 60	0.7–0.9 [–]	
	FDMshoot97	Fraction of total dry matter allocated to shoot at BBCH stage 97	0.9–1 [–]	

(*continued on next page*)

Table A.1 (*continued*).

Process	Parameter	Description	Values&Units	References
Leaf area growth	LAI0	Initial leaf area index	0.01–0.1 [$m^2\,m^{-2}$]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
	LAIexp	Threshold above which LAI increases exponentially	0.7–0.9 [$m^2\,m^{-2}$]	
	SCP	Scattering coefficient of leaves for PAR	0.03–0.2 [–]	
	SLA	Specific leaf area	0.015–0.025 [$m^2\,g^{-1}$]	
	TGLAI	Relative LAI growth rate in response to temperature	0.005–0.025 [$°C\,d^{-1}$]	
	TBaseLAI	Base temperature for juvenile leaf area growth	0–5 [°C]	
Leaf area duration	LAITHMin	Value of LAI when relative death rate due to self-shading starts	3–5 [$m^2\,m^{-2}$]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
	LAITHMax	Max value of relative death rate due to self-shading	0.035–1 [–]	
	ParAgeDLAI	Tuning coefficient for relative leaves death rate due to ageing	0.3–2 [–]	
	DeathLeavesStart	Start BBCH stage for leaves ageing death	75–90 [–]	
Canopy type	KDF	Extinction coefficient for diffuse PAR flux	0.3–0.7 [$m^2\,ha^{-1}$]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
Crop physiological maintenance	MaintenanceLeaves	Maintenance respiration of leaves	0.01–0.035 [$g\,g^{-1}\,d^{-1}$]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
	MaintenanceRoots	Maintenance respiration of roots	0.01–0.015 [$g\,g^{-1}\,d^{-1}$]	
	MaintenanceStem	Maintenance respiration of stem	0.01–0.015 [$g\,g^{-1}\,d^{-1}$]	
	MaintenanceStorage	Maintenance respiration of storage	0.01–0.035 [$g\,g^{-1}\,d^{-1}$]	
Vernalization	EAIstart	Minimum optimum temperature for vernalization	2–5 [°C]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
	EAIstop	Maximum optimum temperature for vernalization	8–10 [°C]	
	VernBBCHStart	BBCH stage after which the vernalization process can start	1–10 [–]	
	VernBBCHEnd	BBCH stage after which the vernalization process stops	25–31 [–]	
Crop ET	kc50	Crop coefficient at BBCH stage 50	0.9–1.2 [–]	Allen et al. (1998)
N uptake	NUPmax	Maximum nitrogen uptake coefficient	3–6 [$kg\,kg^{-1}$]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
Crop residues mineralization	kleaves	Leaves mineralization rate	0.01–0.02 [d^{-1}]	Sandor et al. (2017)*, Valkama et al. (2020)*
	kstem	Stem mineralization rate	0.01–0.02 [d^{-1}]	
	kstorage	Storage mineralization rate	0.01–0.02 [d^{-1}]	
	kroots	Roots mineralization rate	0.0001–0.001 [d^{-1}]	
	NleavesHarvest	Nitrogen concentration fraction in leaves at harvest	0.5–1 [–]	
	NstorageHarvest	Nitrogen concentration fraction in storage at harvest	0.5–1 [–]	
	CNroot	carbon–nitrogen ratio in roots at harvest	60–90 [–]	
	NstemHarvest	Nitrogen concentration fraction in stem at harvest	0.5–1 [–]	
Photoperiod	PhotoPeriodCritical	Photoperiod critical hours	9–12 [h]	Ritchie (1985), Van Diepen et al. (1989), Richter et al. (2010), Perego et al. (2013)*
N dilution curve	aCrit	Critical value of nitrogen for dilution curve	0.013–0.04 [–]	Justes et al. (1994)
Immobilization and mineralization due to microbial activity	CmicrobEfficiencyL	Microbial efficiency in C-litter utilization	0.2–0.7 [–]	Perego et al. (2013)*, Valkama et al. (2020)*
Sensitivity to drought	WSPar	Water stress factor tuning coefficient	6–14 [–]	Richter et al. (2010)

B.3. Sobol method

The Sobol method is a form of global sensitivity analysis based on the decomposition of the variance of a model output into sums of conditional variances. Being computationally expensive, the method of Sobol has been not applied by considering all the input parameters in Table A.1, but rather, taking advantage of the screening method of Morris, by dealing only with a selection of the most influential parameters detected by the Morris method. Specifically, for each output variable of our interest, we consider the subgroup of input parameters that appear in the top positions of the Morris' rankings for at least a soil type.

Going into details, let Y be the output variable of our interest, and k_Y the number of most influential parameters detected with the Morris method. Denoting by X_i the i-th input parameter, and assuming again the independence between the input parameters, the output variance decomposition writes

$$\mathrm{Var}(Y) = \sum_{i=1}^{k_Y} D_i(Y) + \sum_{i<j}^{k_Y} D_{ij}(Y) + \cdots + D_{12\ldots k_Y}(Y), \tag{B.4}$$

where $D_i(Y) := \mathrm{Var}[\mathbb{E}(Y|X_i)]$, $D_{ij}(Y) := \mathrm{Var}[\mathbb{E}(Y|X_i, X_j)] - D_i(Y) - D_j(Y)$ and so on for higher order interactions (refer, among others, to Saltelli and Sobol (1995), Sobol (2001), Iooss and Lemaître (2014) for further details). The method then returns the so-called *Sobol' indices* or *variance-based sensitivity indices*

$$S_i(Y) = \frac{D_i(Y)}{\mathrm{Var}(Y)}, \quad S_{ij}(Y) = \frac{D_{ij}(Y)}{\mathrm{Var}(Y)}, \quad S_{ijh}(Y) = \frac{D_{ijh}(Y)}{\mathrm{Var}(Y)}, \quad \ldots \tag{B.5}$$

and so on, which quantify the fraction of the output variance that is due to either an individual factor i only (i.e., S_i, thereby said *first-order indices* or *main effects*) or to a combination of factors. Additionally, as the number of indices grows exponentially with the number of input parameters under investigation, Homma and Saltelli introduced the so-called *total indices* or *total effects* to assess the impact of parameter i including all possible interactions with the other factors (Homma and Saltelli, 1996). These indices write as it follows

$$S_i^T = S_i + \sum_{i<j} S_{ij} + \sum_{j\neq i, h\neq i, j<h} S_{ijh} + \cdots = \sum_{g\in\#i} S_g, \tag{B.6}$$

where $\#i$ denotes all the subsets of $\{1, \ldots, k_Y\}$ including i. Moreover, the total effects allow the estimate of the so-called *interaction indices* (defined as the difference $S_i^T - S_i$) which represent the fraction of the output variance due to parameters interactions. In practice, especially when the number of parameters is large, it is sufficient to compute the main effects and the total effects to have good information about the model. The Sobol indices can be then interpreted as proposed by Liu et al. (2020): (i) only parameters affecting more than 1% of the output variance, having $S_i > 0.01$ or $S_i^T > 0.01$, are *influential* factors, i.e., they have a not negligible effect; (ii) parameters influencing more than 1% of $\mathrm{Var}(Y)$, having $S_i > 0.1$ or $S_i^T > 0.1$, are *key/important* input factors.

In the present work, for each experiment (i.e., for each pair of target output and soil type), the main and the total effects was computed by applying the quasi-Monte Carlo sampling-based method described in Saltelli (2002) with a sample size of $N(k_Y + 2)$ model input sets, where k_Y is the number of input parameters considered to quantify the variability of the output Y, while N has to be taken large enough to assure the convergence of both the Sobol indices (Saltelli, 1999). As specified in Section 3, taking into account the results that emerged by the Morris method and the top-down correlation coefficients, the Sobol method was applied by considering $k_Y = 9$ parameters to estimate the variability of the mean annual yield, and $k_Y = 13$ parameters in the case of the average annual nitrogen leaching at 1 m depth. These parameters are listed in Table 4. The value of N used for each experiment is specified in Section 3.2.

Appendix C. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.envsoft.2023.105932.

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