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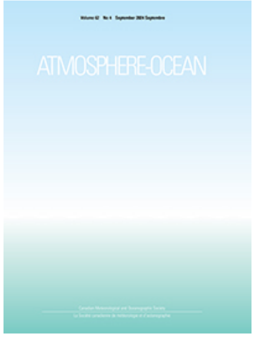

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ABSTRACT *Land surface models (LSMs) have become indispensable for understanding the role of the terrestrial biosphere in the global climate system. However, the ability of LSMs to reproduce observed carbon, water, and energy fluxes varies considerably among models. Some of these deficiencies can be attributed to parameter uncertainties. Global sensitivity analysis (GSA) quantifies model output uncertainties caused by the uncertainty in model inputs. Our study conducts, for the very first time, a GSA for the Canadian Land Surface Scheme Including Biogeochemical Cycles (CLASSIC) model. Focusing on a site in the humid tropics, we evaluate the model's sensitivity for a wide range of ecosystem variables (17 in total). Considering a total of 90 parameters, we identify the top five most influential parameters using the qualitative Morris method per output variable. These influential parameters are then analysed using the quantitative Sobol' method. The analysis shows that the maximum carboxylation rate parameter has the greatest influence on almost all output variables considered. The impact of the maximum carboxylation rate is partially regulated by the canopy extinction coefficient's uncertainty. The results of this research will guide future efforts to optimize the model's performance more efficiently, focussing on a small subset of the 90 parameters.*

RÉSUMÉ *[Traduit par la rédaction] Les modèles de surface terrestre (MST) sont devenus indispensables pour comprendre le rôle de la biosphère terrestre dans le système climatique mondial. Cependant, la capacité des MST à stocker les flux de carbone, d'eau et d'énergie observés varie considérablement d'un modèle à l'autre. Certaines de ces lacunes peuvent être attribuées à l'incertitude des paramètres. L'analyse de sensibilité globale (ASG) quantifie les incertitudes de sortie du modèle causées par l'incertitude des entrées du modèle. Notre étude effectue, pour la première fois, une analyse de sensibilité globale pour le schéma canadien de la surface terrestre incluant le modèle des cycles biogéochimiques (CLASSIC). En nous concentrant sur un site des tropiques humides, nous évaluons la sensibilité du modèle pour un large éventail de variables écosystémiques (17 au total). Sur un total de 90 paramètres, nous identifions les cinq paramètres les plus influents au moyen de la méthode qualitative de Morris par variable de sortie. Ces paramètres influents sont ensuite analysés à l'aide de la méthode quantitative de Sobol. L'analyse révèle que le paramètre du taux de carboxylation maximal a la plus grande influence sur presque toutes les variables de sortie considérées. L'impact du taux maximal de carboxylation est partiellement régulé par l'incertitude du coefficient d'extinction de la canopée. Les résultats de cette recherche guideront les efforts futurs pour optimizer le rendement du modèle plus efficacement, en se concentrant sur un petit sous-ensemble des 90 paramètres.*

KEYWORDS global sensitivity analysis; land surface model; Morris method; Sobol' method

1 Introduction

Land Surface Models (LSM) are components of climate models that simulate the exchange of mass, energy, and momentum between the land surface and the atmosphere. The complexity of LSMs has increased over time as more processes have been added (Fisher & Koven, 2020; Pitman, 2003). Sellers et al. (1997) proposed a classification for LSMs based on their degree of complexity. They characterize the first generation of LSMs as those using a simple surface energy balance equation and processes related to a combined surface-vegetation layer (Manabe, 1969). The second generation of LSMs took the first generation a step further by

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dividing the surface-vegetation layer into a separate soil and vegetation layer. This approach recognizes that the canopy cover shields a fraction of the ground from incoming solar radiation. Additionally, moisture diffusion into multiple soil layers and the impact of snow cover on the soil are also considered (Deardorff, 1978). The third generation of LSMs includes a representation of carbon fluxes through stomatal conductance, photosynthesis, and respiration (Farquhar et al., 1980). The next generation of LSMs included carbon pools, allowing climate models to simulate an interactive global carbon cycle. Further processes include competition among Plant Functional Types (PFTs), wildfires, land cover changes (Lawrence et al., 2019). The role of nutrients in photosynthesis has been incorporated through the addition of nitrogen (Lawrence et al., 2019) and phosphorous cycles (Goll et al., 2017; Reed et al., 2015; Yang et al., 2014). The increasing complexity of LSMs creates the demand for advanced methods of model evaluation, including a systematic approach to assessing model sensitivity.

LSMs require a wide range of inputs, such as meteorological data, atmospheric CO_2 concentration, land cover change, initial conditions, and model parameter values. However, many of the model parameter values are not well constrained due to a lack of observations, and uncertain inputs lead to uncertain outputs. Sensitivity analysis allows for the quantification of parameter value uncertainties' impact on model output variables (Saltelli et al., 2004; Wagener & Pianosi, 2019). Two types of sensitivity analysis are commonly used: local sensitivity analysis, and global sensitivity analysis (GSA). Local sensitivity analysis evaluates the effect on the model output of small changes in input parameter values around a base point (e.g. local derivatives), and is typically performed one parameter at a time. In contrast, GSA computes the importance of parameters based on changes in model output(s) over the full uncertainty range of parameter values for multiple input parameters simultaneously (Saltelli et al., 2008). When parameters are allowed to vary, each parameter or combination of parameters accounts for a fraction of the total model output variance.

Sensitivity analysis is an important step for model development and optimization, which can be done by constraining very few parameters with optimal values using observations (Bagnara et al., 2019; J. Li et al., 2016; Y. Li et al., 2022; Ma et al., 2020; Zhu & Zhuang, 2014). LSM groups have used GSA methods to identify parameters that are influential on output variables by studying a single eddy covariance site (Ma et al., 2020; Tang & Zhuang, 2009; Verbeeck et al., 2006), multiple sites (Alton et al., 2006; Arsenault et al., 2018; Hou et al., 2015; Y. Li et al., 2022; Pappas et al., 2013; Rosolem et al., 2012; Zhu & Zhuang, 2014) or by using global model data (J. Li et al., 2016; Lu et al., 2013). The results of these studies consistently show that most of the model output uncertainty associated with parameters is governed by very few parameters. The most influential parameters for the model output variables net ecosystem exchange, gross primary productivity (GPP), sensible heat flux, and latent heat flux are frequently identified as maximum carboxylation rate (*vmax*), quantum efficiency, specific leaf area, parameters related to stomatal conductance, and roughness length (Alton et al., 2006; Arsenault et al., 2018; J. Li et al., 2016; Y. Li et al., 2022; Lu et al., 2013; Ma et al., 2020; Rosolem et al., 2012; Zhu & Zhuang, 2014). Other studies have identified influential parameters such as the Clapp and Hornberger *b* parameter, soil respiration parameters, the canopy extinction coefficient (k_n), and the scaling parameter from leaf to canopy (J. Li et al., 2013; Pappas et al., 2013; Verbeeck et al., 2006). The differences can be due to the choice of models, sites, sensitivity approaches, and/or parameter uncertainty ranges.

The Canadian Land Surface Scheme Including Biogeochemical Cycles (CLASSIC; Melton et al., 2020) model is the land surface component of the Canadian Earth System Model (CanESM; Swart et al., 2019) and has undergone decades of development. There has been no prior formal sensitivity analysis conducted on the CLASSIC model. Conducting such an analysis is important for understanding the importance of various parameters and how different processes are affected based on parameter uncertainty interactions. Additionally, it provides valuable insights to support ongoing model development efforts and tuning.

In the present study, we use GSA methods to identify the most influential parameters for a broad range of model outputs, including variables that form part of the carbon, water, heat, and radiation fluxes simulated by the CLASSIC model at a single FLUXNET2015 site in the humid tropics. We consider 90 independent parameters in a screening test to identify a subset of parameters that are then used in a quantification test, wherein the effects of variations in input parameters on various model outputs such as gross primary productivity, autotrophic and heterotrophic respiration and transpiration rates, latent and sensible heat fluxes are studied. We also study the interactions of uncertainty ranges of the two most influential parameters on all model output variables.

The following Section 2 describes the model, site characteristics, parameter uncertainty ranges, GSA methods and sampling method used. Section 3 presents the results from the GSA methods, and the importance and interactions of the two most influential parameters' uncertainty ranges on all processes. A discussion on limitations, future research, and conclusions are presented in Section 4.

2 Methods

a *The CLASSIC Model*

The CLASSIC model can be used both in a coupled mode inside CanESM, and offline as a standalone model. The model is composed of two main components, namely the Canadian Land Surface Scheme (CLASS; Verseghy, 2017) and the Canadian Terrestrial Ecosystem Model (CTEM; Melton & Arora, 2016). The CLASS component simulates physical processes such as radiation, heat, and water fluxes of the land surface vegetation, soil, and snow. CTEM is the dynamic vegetation model in the CLASSIC model that simulates biogeochemical processes such as photosynthesis, phenology, allocation of carbon to the live and dead carbon pools, canopy conductance, and tissue turnover (Arora & Boer, 2005); maintenance, growth and heterotrophic respiration (Melton et al., 2015) and dynamic root distribution (Arora & Boer, 2003). For the present study, for the current model configuration, some processes, such as competition, land use change, fire, moss, and the diffusion of carbon in the soil, are turned off, as these processes are either not relevant for the site considered or are under active development in the model. The CLASSIC model has 134 input parameters, of which only parameters that are site-relevant (91) are considered in this study. The processes represented by these parameters are generally non-linear and are obtained empirically.

For our analysis, the model has been spun up to a state of equilibrium with the observed meteorological data that is obtained from the site. The spin-up is performed separately for each combination of input parameter values. The spin-up starts from a bare ground state, where the leaf, stem, root, litter biomass and soil carbon pools are each set to values of zero. The model is determined to be in an equilibrium state if the annual soil carbon changes are less than 0.1% and/or the absolute net biome productivity value for the last two sets of spin-up years is less than $2 \times 10^{-12}\,\mathrm{kgC\,m^{-2}\,year^{-1}}$. To reach equilibrium, we spin the model up for 500 years by looping over the available 11-year meteorological dataset, for the FLUXNET2015 site location (described in detail in Subsection b). Once the equilibrium state is attained, the model is run for an additional 11 years using the observed meteorological forcing. The 11-year annual average value of each output variable is chosen for analysis by the GSA methods.

The photosynthesis module of the CLASSIC model simulates the net canopy-level photosynthetic rate that includes GPP (Eqs. (S1)–(S8); Melton & Arora, 2016) and autotrophic respiration fluxes, which are computed from the living components: the vegetation carbon pools (cVeg, cRoot, cStem). Heterotrophic respiration is the respiration from microbes that decompose litter (dead leaves, stems and roots) and soil organic carbon (cSoil). The carbon pool in the land is referred to as cLand. The model also simulates variables such as the leaf area index and vegetation height. The net canopy-level photosynthetic rate, along with the atmospheric CO_2 concentration and vapour pressure is used to compute the canopy conductance, which is used by the physical component of the CLASSIC model to obtain the surface energy budget variables, such as latent heat flux and sensible heat flux; and water cycle variables, such as the total run-off (including drainage through the base of the soil model) per unit area leaving the land portion of the grid cell, and transpiration. The net longwave and net shortwave radiation fluxes and the surface albedo are also simulated by the physical component of the CLASSIC model.

The response of modelled processes to changes in parameter uncertainties can be studied by identifying the influential parameters. In this study, the following variables have been analysed using GSA methods: individual carbon cycle components (GPP, autotrophic respiration, heterotrophic respiration, leaf area index, vegetation height, cLand, cLitter, cRoot, cStem, cSoil, cVeg); turbulent heat fluxes (latent and sensible heat fluxes); radiation fluxes (net longwave and shortwave); and water cycle components (transpiration and total run-off). The subsections that follow provide further detail on the site selection process, parameter uncertainty ranges, and sensitivity analysis methods used. A more comprehensive discussion of the model equations used to compute GPP is provided in Supplementary Information.

b *Site Selection*

The FLUXNET2015 database provides measurements from 204 eddy covariance sites around the world (Pastorello et al., 2017). The CLASSIC model has been evaluated for the performance at 31 sites (Melton et al., 2020), of which 17 have various degrees of gap-filling (Pastorello et al., 2020). Multiple selection criteria have been considered before choosing a site for our analysis. These include the gap-filling score, age of the forest, time from previous catastrophic disturbance, available number of years of measured meteorological data, and homogeneity of the landscape and vegetation.

The site chosen for this study is a tropical wet primary forest (evergreen broadleaf forest) located in French Guiana, South America (5°16′54″N, 52°54′44″W; Pastorello et al., 2017). The site is surrounded by over 400 ha of undisturbed forest, in the northernmost region on the Guiana Plateau with small hills ranging from 10 to 40 m a.s.l. This forest site is home to old-growth trees, with the oldest trees over 300 years of age. The average canopy height is 35 m, with an overgrowth of 5 m. The flux tower is 55 m tall, and the sensors are placed 3 m above the top of the tower. The positioning of the sensors are such that there is little disturbance to the upper canopy, with the presence of over 1 km of forest cover in the direction of the prevailing winds (Bonal et al., 2008). The tower was erected in 2003 and continuous meteorological data such as atmospheric pressure, precipitation, specific humidity, atmospheric temperature and horizontal winds; and fluxes such as net radiation, GPP, ecosystem respiration (RECO), and net ecosystem exchange are available for 11 years from 2004 to 2014 (Pastorello et al., 2017). The gap-filling score for this site is high, where the data for 121 out of 132 months are available (Pastorello et al., 2020).

FLUXNET2015 sites measure various fluxes between the land and the atmosphere, typically employed for model optimization. The reader should note that our study does not involve any optimization. Instead, we use the observed meteorological data from the FLUXNET2015 site as the forcing for our model, which is forced from a bareground state. Spinning up and running the separately for each set of parameter uncertainty values is crucial for computing differences in outputs during GSA sensitivity measure calculations.

c *Parameter Uncertainty Ranges*

Parameter ranges represent a critical choice for any sensitivity analysis, and these ranges will inevitably affect the sensitivity results (Wallach & Genard, 1998). Of the 134 input parameters, only 91 were used for the GSA (Table S1), of which 88 are independent by definition. As mentioned earlier, some parameters were not considered as they correspond to processes that are turned off in the present model configuration, or are not relevant to our site, or have virtually no uncertainty. The parameter uncertainty ranges were determined in the following ways: *vmax*, a well-documented parameter, has been assigned a specific range based on observations of the evergreen broadleaf plant function type (from the TRY plant traits database; Kattge et al., 2020); 35 parameters (38.5%) have been assigned plausible ranges based on our modelling experience and expert advice, and 30 parameters (32.3%) have been assigned values based on a literature survey, of which the ranges for the lower and upper temperature thresholds for photosynthesis (*tlow* and *tup*) have been modified to include the default values used in the CLASSIC model. All other parameters for which documented uncertainty ranges are not available (28.5%) were assigned ±10% ranges, except for the lower temperature threshold used to estimate cold stress-related leaf loss rate (*lwrtrsh*). The parameter *lwrtrsh* was assigned a ±2 K range (Table S1).

All parameters considered in GSA methods must be independent, and thus the three dependent parameters, namely, the base allocation parameters for leaf (*epsilonl, epsilons, epsilonr* in Table S1) have to be converted to independent variants. The dependent parameters are transformed using the spherical coordinate system to achieve the required parameter independence (Eqs. (S10)–(S12)). With just two spherical parameters, the three dependent parameters can be converted to independent parameters. This transformation further reduces the total number of independent parameters used in the screening test to 90. For interested readers, more details about the spherical coordinate conversion used in this article are available in the Supplemental document.

d *Global Sensitivity Analysis*

GSA can be described as the class of statistical methods where the relationship between variations in the input parameters and variations in single or multiple output variables can be quantified across the specified uncertainty range of multiple input parameters (Saltelli et al., 2004). GSA methods can be used to identify parameters that individually do or do not influence the model outputs, as well as identify the interactions among parameters.

1 SCREENING: MORRIS ELEMENTARY EFFECTS METHOD

Pareto's principle is an empirical observation stating that in general the variability of model output is largely determined by the uncertainty of only a few parameters (Box & Meyer, 1986). If variations of a parameter over its range of uncertainty induce larger output variations than comparable variations of other parameters, the input parameter is influential (Wagener & Pianosi, 2019). The method of distinguishing significant parameters from those with the least impact is referred to as screening or qualitative GSA. The Morris elementary effects method, proposed by Morris (1991) and later modified by Campolongo and Braddock (1999), is a screening test based on the one-at-a-time design. This method perturbs only one parameter between consecutive steps in a realization/simulation, generating a random walk through the parameter space (Eqs. (S14)–(S15)). Multiple realizations of such random walks are performed to sample the parameter space for all parameters. The ratio of difference of any two consecutive random walks to the step size is an elementary effects value. Statistical measures, such as the absolute mean and standard deviation of the elementary effects value from multiple evaluations, are the sensitivity measures used to determine the influence of the parameters on the model output(s). The elementary effects method is simple, and effective at identifying the set of important parameters among all parameters considered and distinguishing between those with negligible effects (small absolute mean and standard deviation values), linear and additive effects (large absolute mean and small standard deviation values), and non-linear effects (large absolute mean and standard deviation values) on the model output variable(s). While the method can allow parameters to be ranked according to the type of effect, it cannot quantitatively assess the individual importance or parameter interactions.

The statistical measures mean (μ), absolute mean ($\mu*$), and standard deviation (σ) are given by Saltelli et al. (2008):

$$\mu_i = \frac{1}{r}\sum_{j=1}^{r}(EE_i^j), \tag{1}$$

$$\mu_i^* = \frac{1}{r}\sum_{j=1}^{r}|EE_i^j|, \tag{2}$$

$$\sigma_i^2 v = \frac{1}{r-1}\sum_{j=1}^{r}(EE_i^j - \mu_i)^2, \tag{3}$$

where r is the total number of realizations, and EE_i^j is the elementary effects value for the ith parameter and jth realization. We have used the Euclidean distance (κ) from the origin and points (μ_i^*,σ_i) as the sensitivity measure to identify the influential parameters (Eq. (S19)). The influential parameters will have a larger value of κ, which is indicative of greater sensitivity of the output variable to the parameter(s). Details about the hypercube, step-size, and random-walk trajectory used by the Morris method, are provided in the Supplemental document for interested readers.

To compute one elementary effects value for a single parameter, two points in the unit hypercube are necessary. For n parameters, which yields n elementary effects values, $(n+1)$ model evaluations are required. In addition, r realizations/trajectories result in a total of $r \times (n+1)$ evaluations (Saltelli, 2002; Saltelli et al., 2004). In this study, 90 independent parameters and 80 realizations were used for the elementary effects method, requiring 7280 runs. The top five influential parameters for each of the output variables were obtained from the elementary effects method, which were further analysed to quantify their individual contributions and interactions using the Sobol' variance-based GSA method. The screening test robustly identifies the most influential parameters, but the ranking of less influential parameters experiences substantial sampling variability. There is no perfect way to select the subset of parameters for the Sobol' method, as the same selection procedure applied to two sets of realizations in the screening test would produce the same most influential parameters but would differ in some of the less influential parameters. When repeating the screening test with a different set of realizations, we find that those parameters which are not robustly identified as influential have negligible contribution to the variance-based sensitivity analysis to which we now turn.

2 VARIANCE-BASED SENSITIVITY TEST: SOBOL' METHOD

A GSA method used to quantify the uncertainty of output variables due to the uncertainty in input parameters is the Sobol' method, based on a variance decomposition. The influence of individual parameters on the output can be determined by calculating the variance of conditional expectation ($V[E(\cdot \mid \cdot)]$). To study variations in the output with the uncertainty in a single input parameter ($Y \mid x_i$), the output can be split into subsets based on quantile ranges of the ith parameter's uncertainty range. For each quantile slice, an average can be computed, representing the conditional expectation ($E_{x_{\sim i}}(Y \mid x_i)$) of the output when the ith parameter is held constant, while the expectation is estimated by sampling over all other ($\sim i$) parameters. The variance of the conditional expectation, $V_{x_i}[E_{x_{\sim i}}(Y \mid x_i)]$, quantifies the influence of a single parameter on the output variable when all other parameters change. We use the first-order and total-order sensitivity indices (SI) in this study to quantify influential input parameters and their interactive effects. The first-order SI for the ith parameter (SI_{1_i}) is given as Saltelli et al. (2008):

$$SI_{1_i} = \frac{V_{x_i}[E_{x_{\sim i}}(Y \mid x_i)]}{V(Y)}, \tag{4}$$

where $V(Y)$ represents the output variance. The total-order SI for the ith parameter (S_{tot_i}) is given as Saltelli et al. (2008):

$$SI_{tot_i} = 1 - \frac{V_{x_i}[E_{x_i}(Y \mid x_{\sim i})]}{V(Y)}, \tag{5}$$

where $V_{x_i}[E_{x_i}(Y \mid x_{\sim i})]$ represents the variance of the conditional expectation of the output when all parameters other than the ith are varied, while the expectation is estimated by sampling over the (ith) parameter. S_{T_i} close to zero implies that the influence of a parameter is negligible, and an error bar crossing zero implies that even if the mean is away from zero the influence of the parameter is not robust. Fixing the parameter within its uncertainty range will not affect the output variable if $SI_{tot_i} \simeq 0$. We have included the derivation of equations to obtain the sensitivity indices using the Sobol' method, and a tutorial example in the Supplemental document. Interested readers are requested to view the document.

To compute the first-order and total sensitivity indices using the Sobol' variance-based method, a total of $N \times (k+2)$ model evaluations are required, where N is the number of perturbation points for each parameter (Saltelli et al., 2008). The computational cost to run each perturbation is the main drawback of variance methods. As the dimensionality (k) increases, more points have to be sampled to evaluate the whole variability space. The parameter values are drawn randomly from their range, so a large number of realizations is necessary to adequately cover the parameter space. In this study, 14 parameters and 512 perturbation points were used for the Sobol' analysis, resulting in a total of 8192 model evaluations.

Various sampling techniques can be used to perform variance-based GSA, but in this study, quasi-random numbers were used. Quasi-random or Quasi-Monte Carlo (QMC) methods were employed to improve sampling of the whole variability space of each parameter (Morokoff & Caflisch, 1994; Niederreiter, 1978, 1992; Sobol', 1998). QMC methods consider the position of previously generated samples to create a spread of samples that are neither random nor completely predictable. These methods utilize an algorithm that generates distributions of points with a low measure of deviation from uniformity, known as low-discrepancy sequences. These methods have low disorderliness and gaps, resulting in efficient utilization of the sampling space. We have used the Sobol' low-discrepancy sequences, which produces successive points in a deterministic pattern, while performing the Sobol' analysis. This sampling technique is known for producing a highly uniform distribution as the sample size increases, making it an efficient method for sampling the input space in variance-based sensitivity analysis (Bratley et al., 1992; Sobol', 1967, 1976). This technique has been shown to be faster than pseudorandom Monte Carlo methods because of its improved sampling of parameter uncertainty ranges (Chan et al., 2000; Kucherenko & Sytsko, 2005; Sobol', 1967; Sobol' & Kucherenko, 2005).

It is important to consider the sampling uncertainty of the outputs when considering model output statistics based on a finite number of runs. In this study, the sampling uncertainties of the sensitivity indices that are computed by the bootstrap confidence intervals span from the 2.5th to 97.5th percentiles. It is possible to have slightly negative values of the Sobol' indices and the confidence intervals due to properties of the estimator used for the sample estimates (Eq. (S20); Saltelli et al., 2008). If the SI values are close to zero, or if zero falls well within the confidence interval of the parameters of interest, it suggests that the parameter might be non-influential, particularly if the interval has a small spread in range.

3 Results

a *Morris Elementary Effects Method*

All model variables evaluated in this study are sensitive to fewer than 15% (10–11) of the total number of parameters (90; Fig. 1). The relative sensitivity to each parameter varies among output variables. At least five parameters that are part of the photosynthesis module, especially *vmax*, are highly influential across all output variables (Fig. 1). At least two parameters that are part of the phenology parameterization are influential across all output variables. Most of the least influential parameters form part of parameterizations related to physical processes and heterotrophic respiration.

The elementary effects method used in this study assesses the relative influence of each parameter on the individual model output variables, rather than quantifying the individual contribution of each parameter to changes in the model outputs. To further investigate the influential parameters, the Morris method was utilized to identify a subset of 14 parameters for more detailed analysis using the Sobol' variance-based decomposition (Table 1). While the allocation fractions are not found to be influential, they are included in the Sobol' analysis along with *rtsrmin* as otherwise the model was found to crash.

b *Variance-based Sobol' Analysis*

1 FIRST AND TOTAL ORDER SOBOL' INDICES

The output values from all the runs were analysed using the Sobol' method for each of the model output variables considered. We first consider the main order effects, where the SI values denote the conditional variance of the model output(s) for a single conditioning variable. The results indicate that the variance of all model output variables is primarily dominated by only one parameter, *vmax*, which accounts for approximately 50–80% of the output variance for all model variables (Fig. 2a). For most model outputs, the importance of *vmax* is comparable, as the ranges of confidence intervals of the sensitivity indices overlap. However, for net shortwave radiation (denoted as RSS in Figs. 1 and 2), the importance of near-infra-red albedo (*albnir*) and *vmax* are comparable (Fig. 2a). The parameter k_n is the second most influential parameter for most output variables except for net shortwave radiation, vegetation height (denoted as vegHeight) and cStem. All other parameters considered have negligible influence on a majority of model outputs, as their SI values are very small. The confidence intervals of the first order SI of all other parameters except for *vmax*, for all variables (except net shortwave radiation), cross zero, indicating that the first order SI values for these parameters cannot robustly be distinguished from zero (Fig. 2a).

Total order indices include the interactive effects of all the parameters considered (Fig. 2b). The total order of each output variable includes the first-order effect and is theoretically greater in value for the same set of input parameters analysed. The ranking of parameters follows similar patterns of importance as of the first order, wherein the photosynthetic parameter *vmax* has the highest total SI values for all model outputs. This parameter also exhibits the largest interactive features for all output variables (except for total run-off, denoted as MRRO, and sensible heat flux, denoted as HFSS), due to the fact that the strength of the interactions is based on the difference between the total and first-order indices. As most of the output variables behave similarly to each other, we focus on GPP as broadly representative of the GSA. The total variance in GPP explained by *vmax* is about 88% (confidence intervals 68 to 100%; Fig. 2b), of which the individual effect is about 75% (confidence intervals 52 to 90%; Fig. 2a), such that the interactions account to about 13%. Most of the parameters that did not exhibit any first-order influence on the model outputs have some positive interactive effects that are not generally robust (Fig. 2b), which is

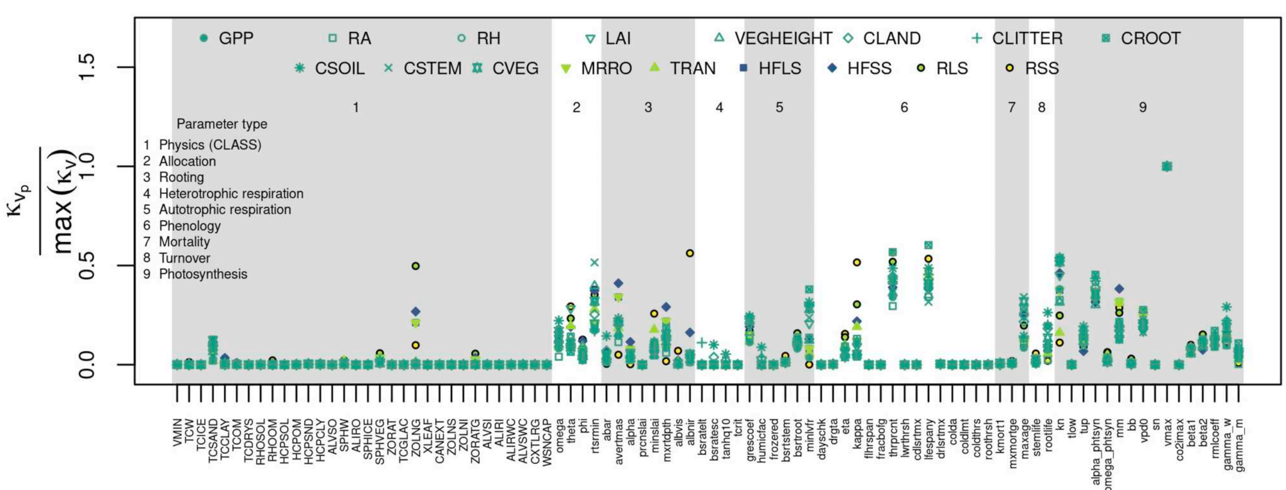

Fig. 1 Normalized distances (κ) of each parameter (p) computed from the sensitive indices (μ^*, σ) of the Morris elementary effects method for the output variables (represented as coloured symbols, v). The κ values were normalized with the maximum distance across parameters for a given output variable, as the output variables have different units.

TABLE 1. List of parameters selected for Sobol analysis, their minimum and maximum uncertainty ranges, default values, units, and description used in Sobol'.

Parameter	Min.	Max.	Default	Unit	Description
vmax	10.0e −06	80.0e −06	35.0e −06	$molCO_2m^{-2}s^{-1}$	Max. carboxylation rate
lfespany	0.6466	2.5979	1.50	years	Leaf life span
alpha_phtysn	0.05	0.120	0.08	$\mu molCO_2$ $(\mu mol\ photon)^{-1}$	Quantum efficiency
k_n	0.4	0.7	0.50	–	Canopy light extinction coefficient
rtsrmin	0.1	1	0.16	–	Minimum rootshoot ratio for support and stability
thrprcnt	30	60	40	%	Percentage of max. leaf area index that can be supported, used as a threshold for determining leaf phenology status
avertmas	0.1	8.7	2.45	$kgC\ m^{-2}$	Average root biomass
ZOLNG	−6.908	−0.5108	−4.605	–	Natural log of roughness length of soil
albnir	20.7	25.3	23	–	Near IR albedo
maxage	100	2100	600	years	Maximum plant age. used to calculate intrinsic mortality rate
mm	9	15	12	–	Used in photosynthesis-stomatal conductance coupling
kappa	1.44	1.76	1.6	–	Exponential parameter of allometric relations, required to support green leaf biomass
epsilonl	0.15	0.5	0.35	–	Base allocation fraction for leaf (epsilon L)
epsilons	0.01	0.1	0.05	–	Base allocation fraction for stem (epsilon S)
epsilonr	0.4	0.8	0.60	–	Base allocation fraction for roots (epsilon R)

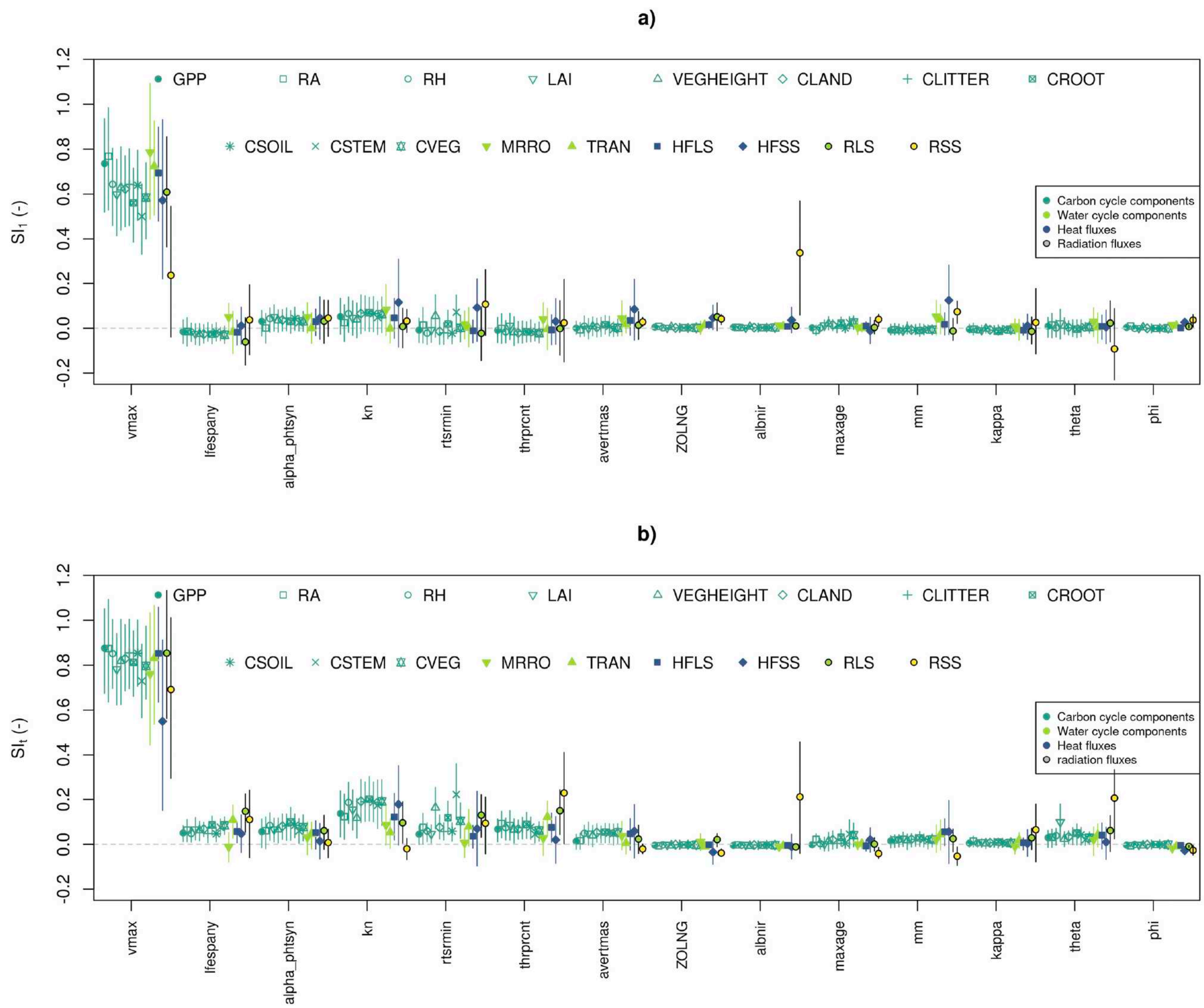

Fig. 2 First order (a) and total order (b) sensitivity indices, and their confidence intervals for all outputs for the 14 parameters.

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indicative of the interactions of each parameter considered with other parameters. For almost all model outputs the interactive effects add on to the first order indices, while for a few model outputs (e.g. sensible heat flux, total run-off and net shortwave radiation) the total order is less than the first order, which cannot be true theoretically, and must be the result of sampling variability in the estimators used for the indices.

2 INTERACTIONS OF INFLUENTIAL PARAMETERS

Figure 3 shows the distributions of GPP variability conditioned on the top four influential parameters from the first-order SI. Values were plotted on conditional hexagonal histogram distributions along with their variations in conditional means. The histograms illustrate the conditional dependence of the output on individual parameters. As described in the previous section, the influence of the parameter is measured by the variance of the conditional mean. If the conditional mean depends strongly on the parameter, the model output is sensitive to the uncertainty of the parameter value, and if the conditional mean's dependence on the parameter is low, the sensitivity of the model output is low to the uncertainty of the parameter value.

The first four influential parameters for GPP (from highest to lowest first-order SI values) are *vmax*, canopy light

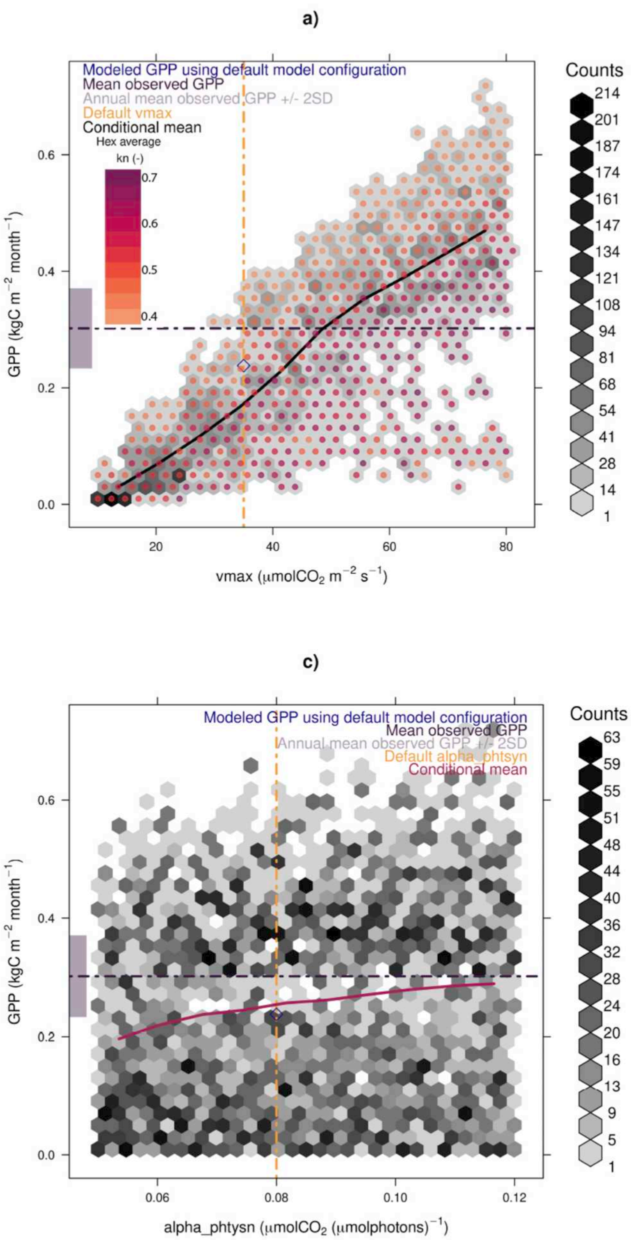

Fig. 3 Conditional hexagonal plot of the distribution spread, modelled value using default configuration, annual mean observed value with ± 2 standard deviation, conditional mean of GPP and modelled GPP using default configurations for (a) *vmax*, with average k_n for runs in each hexagonal grid as coloured dots, (b) k_n, (c) *alpha_phtsyn* and (d) *lfespany*.

extinction coefficient along the depth (k_n), quantum efficiency (*alpha_phtsyn*) and leaf lifespan (*lfespany*; Fig. 2a). As is illustrated graphically by the variation of the conditional means in each plot (Fig. 3a–d), the parameter *vmax* has the greatest variation in the conditional mean, followed by k_n, *alpha_phtsyn* (Fig. 3a–c). The variation of the conditional mean of GPP to *lfespany* (Fig. 3d) is the least among the four parameters, reflecting that *lfespany* has the least influence among the four parameters. The dependencies of the conditional means of GPP on the other parameters are close to zero, as the sensitivity of the output to the inputs reduces as the ranking increases (not shown).

As mentioned in the previous section, the parameter k_n represents the rate at which the canopy reduces the availability of light. To investigate interactions between k_n and *vmax*, the average k_n values for simulations falling within each hexagonal grid have been included as coloured stipples along with the conditional distribution of GPP on *vmax* (Fig. 3a). For a given *vmax* value, the GPP values tend to reduce as the average k_n values increase. Figure 4 further illustrates the dependence of GPP on *vmax* and k_n for an instantaneous state obtained from Eqs. (S1)–(S8). To obtain this state, the output variable leaf area index is fixed, and no soil moisture stress effects are considered. The instantaneous dependence of GPP reflects the pattern seen in the conditional distribution in Fig. 3(a). The slope of GPP vs *vmax* reduces as k_n values are increased. This analysis shows that even if *vmax* values are high, GPP may be less depending on the availability of light. Since all output variables are directly or indirectly affected by the vegetative biomass present, all output variables are sensitive to *vmax* and k_n. Our analysis also highlights the importance of interactions between the influential parameters' uncertainty in driving the carbon cycle.

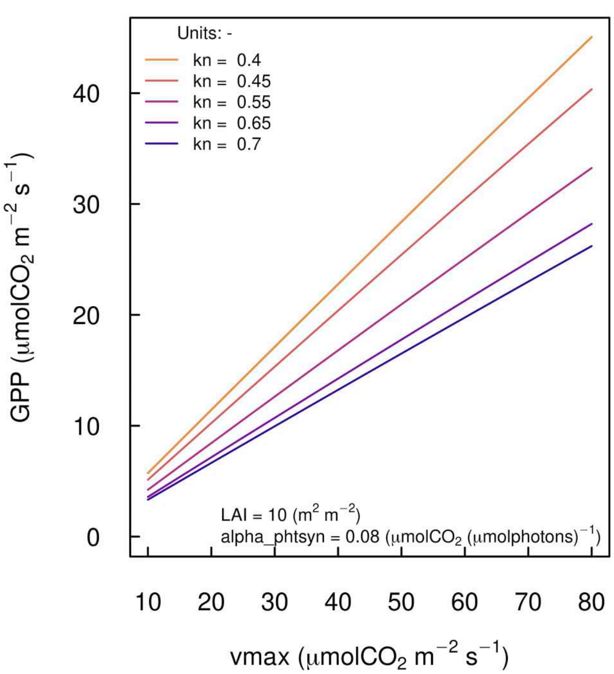

Fig. 4 Functional dependence of GPP vs *vmax* and k_n for a particular state with site-specific PPFD = 2100 mol photons m^{-2} s^{-1}, atmospheric CO_2 (2009's) = 387.64 ppm, mean atmospheric pressure = 1005.93 hPa, and defined leaf internal CO_2 concentration ($c_i = 240$ ppm) and canopy temperature ($T_c = 29°C$).

4 Discussion and conclusions

This study screened the influence of 90 independent input parameters in the CLASSIC model using the Morris elementary effects method and found a small number of influential parameters for any given model output. The most influential parameters across output variables, when combined and quantified using Sobol' analysis, a variance-based GSA method, showed that the photosynthetic parameter *vmax* by far has the greatest impact on the model output variance for all output variables, regardless of the type of variable. The overall importance of photosynthetic parameters is consistent with previous studies that analysed carbon fluxes, latent heat flux, and carbon pools (Alton et al., 2006; Arsenault et al., 2018; J. Li et al., 2013, 2016; Lu et al., 2013; Pappas et al., 2013; Rosolem et al., 2012; Verbeeck et al., 2006).

Remarkably, a wide range of output variables are sensitive to the same set of primarily photosynthetic parameters (e.g. *vmax* and k_n). An upper limit of how much CO_2 a plant can assimilate and how the slope of the reaction rate versus inter-cellular CO_2 concentration changes is given by *vmax*, while k_n determines the amount of light in the depth of the canopy and thereby the absorption of photons as a function of leaf area index. The autotrophic respiration is a function of *vmax* and the factor for scaling photosynthesis from the leaf to the canopy (fPAR in the Supplementary document), the latter depending on k_n, as in Eq. (S9). For heterotrophic respiration to occur, a sustained supply of litter and detritus is required and is provided by the biomass, which is sensitive to the parameters *vmax* and k_n. Parameters such as the litter respiration rate (*bsratelt*) and soil carbon respiration rate (*bsratesc*) may be expected to be more influential for heterotrophic respiration but, as shown by the results from Morris elementary effects, are far less influential in comparison to *vmax*. The variance in biomass, in response to photosynthetic parameter variations, affects the amount of carbon that enters the litter pool and ultimately the soil pool, and thus affecting heterotrophic respiration more compared to the variations of individual respiration parameters. We note that there are far more parameters in the model's photosynthesis parameterization compared to respiration, and more complex parameterizations may lead to more uncertainty. We also note that the site in this study is tropical, and soil-related parameters may be of more importance in colder climates where decomposition is slower.

Since the carbon and water cycle are directly linked through stomatal conductance, changes in the two photosynthetic parameters also influence the water cycle outputs, transpiration and total run-off. The photosynthetic parameters affect stomatal conductance and thereby the latent heat flux, which then affects soil moisture. The most influential photosynthetic parameters (*vmax*, k_n) affect the carbon cycle variables (GPP, autotrophic respiration, heterotrophic respiration, leaf area index, vegetation height, and the carbon pools) directly through processes described in Eqs. (S1)–(S9) and indirectly affect the heat, water, and radiation fluxes through stomatal conductance and plant growth.

The parameter *vmax* dominates the sensitivity of a wide range of output variables simulated by the CLASSIC model, but the k_n controls the slope of this dependence (e.g. GPP vs. *vmax* as depicted in the previous section). For the tropical site selected in this study, *vmax* and k_n were the only parameters that had robust interactive effects for various output variables, as observed in the Sobol' method. It is important to note that different biomes may exhibit different interactive effects among various influential parameters.

The uncertainty range for quantum efficiency (*alpha_phtsyn*, Table S1) in our study is narrower than that used by previous sensitivity analyses of LSMs. This decision was motivated after performing the GSA methods using uncertainty ranges provided by earlier studies (J. Li et al., 2013; Lu et al., 2013; Ma et al., 2020; Pappas et al., 2013), where assigning broader ranges to *alpha_phtysn* and *vmax* resulted in *alpha_phtsyn* being much more influential for all model outputs compared to *vmax*. The extreme values of these two photosynthetic parameters interacted to produce unrealistic low and high biomass states, which are not observed when plant function type-specific and/or narrower ranges are used. Uncertainty ranges must be chosen with caution, as the sensitivity of an output variable strongly depends on the uncertainty range of each parameter, highlighting the importance of carefully examining and evaluating the ranges assigned to all parameters. Plant function type-specific uncertainty ranges must be used whenever possible (e.g. from the TRY plant traits database; Kattge et al., 2020), especially if the parameter could be highly influential (e.g. *alpha_phtsyn* and *vmax*).

Insights from GSA allow for the targeted optimization of specific parameters, making the optimization process more efficient. Better optimized parameters in a model should in principle lead to improved output results. Model performance can be optimized by comparing observed output variables with model outputs, using metrics like root mean square error, squared correlation coefficient, and absolute errors. As we have shown in our study, GSA can identify the influential parameters for the CLASSIC model's output variables. This knowledge can then be used to optimize CLASSIC model's output variables. Since the CLASSIC model is the land component of CanESM, improvements in the CLASSIC model will ultimately enhance CanESM as well. Currently, parameter optimization using a machine learning algorithm is under progress by one of the co-authors.

Our study, like many other GSA studies performed on LSMs, is not without limitations. As mentioned earlier, this research was conducted for a tropical FLUXNET2015 site with 11 years of available observed meteorological forcing. The 11-year period considered for the mean state is too short to represent the historical period, and this affects the mean state of the model. While the site was well suited given a high gap-filling score, the influential parameters identified may vary if a different FLUXNET2015 site is chosen, or if a greater number of available years are considered for GSA.

To address the high dimensionality of the parameter space considered in the study, we performed the GSA in two steps. Various other GSA techniques are available, but by performing the Morris and Sobol' methods sequentially, we were able to screen out parameters that have limited influence on the output variables and quantify the absolute effects of the most influential parameters. We chose to use the first and total-order sensitivity indices to study the individual effects of parameters and their interactive effects. We assume that the difference between total index and first-order index is dominated by interactions between two parameters namely *vmax* and k_n, since only these two parameters showed robust differences between the first-order and total-order indices. In such cases, second-order effects could be studied instead of/or in addition to the total-order effects to identify parameters that have interactive effects on the output variables.

Based on the computational load, we chose to use the top five influential parameters from all output variables for the Sobol' method. This number is arbitrary, as even three or ten could be used. Modelers should keep in mind that as the dimensionality increases, so does the number of runs. They should also consider the extent to which the parameter space needs to be studied and will be studied. With 512 perturbation points, the confidence intervals computed through the Sobol' method are broad. The confidence intervals would be smaller if the number of perturbation points were increased. Just like the Morris method, the computational time and parameter search space should be kept in mind while performing the Sobol' method. We did not perform a test with various perturbation sizes due to time constraints. Additionally, this study focuses on the sensitivity of the average annual mean of output variables. The influential parameters may vary if a different statistical measure such as the trend over the period concerned is chosen instead of the mean state.

Our analysis involved performing a large number (15,472) of simulations with the CLASSIC model. An alternative to ease computational load while performing GSA is to use emulators. Emulators are statistical proxies of complex models such as LSMs or even Earth system models. These models provide a statistical relationship between model input parameters and model output, and are less complex, thereby, are far less computationally demanding. Emulators can be used for identifying optimum parameter ranges, and global sensitivity analysis (Baker et al., 2022; McNeall et al., 2020, 2023; Petropoulos et al., 2014). Using the original model is more reliable than using a proxy when identifying influential parameters.

To conclude, we have identified that for the CLASSIC model and considering an evergreen broadleaf forest site in French Guiana, the photosynthetic parameters, maximum carboxylation rate (*vmax*) and canopy extinction coefficient (k_n), are the most influential among 90 input parameters. This influence is observed across the mean state of 17 output variables representing the budgets of carbon, water, and turbulent energy fluxes. Our findings were derived from a two-step global sensitivity analysis (GSA). The parameter *vmax* dominates the sensitivity of all the output variables while k_n controls the slope of the output variables. Together these two parameters account for a majority of the interactive effects on the output variables.

This finding underscores the critical importance of *vmax* (and k_n) in LSMs, and that the most influential parameters have to be accurately parameterized to improve model performance and reliability. As mentioned earlier, the influential parameters may vary for different biomes, and for different statistical measures. Our future research will assess how the sensitivity of various output variables varies across biomes, and what effect a changing climate might have on the influential parameters. The main objective of this study was to develop a framework to identify the most influential parameters in the CLASSIC model using GSA. This study does not delve into optimizing the CLASSIC model for optimal values or ranges of these influential parameters but forms the basis for future optimization work. We leave the development of an optimization framework for future research.

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Disclosure statement

No potential conflict of interest was reported by the author(s).

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Author contribution

All three authors defined the experimental setup; RDSN designed, tested, and performed the experimental framework for the model runs; CS provided the input data for the model; RDSN performed the analysis and wrote the manuscript with inputs from CS and AHM.

Supplemental data

Supplemental data for this article can be accessed online at http://dx.doi.org/10.1080/07055900.2024.2396426.

Code and data availability

This study has been conducted using the *R* Statistical Software (v3.6.3; R Core Team, 2020). The GSA was performed using the *sensitivity R* package (v1.27.1; Iooss et al., 2022), in which the screening test was performed using the *morris*() function, and the quantitative analysis was performed using the *sobol*2002() function. Quasi-random numbers for the quantitative method were generated using the *sobol*() function within the *randtoolbox* R package (v1.31.1; Christophe & Petr, 2021).

The scripts used to perturb the name list files, to run the CLASSIC model, and to produce the Morris elementary effects, Sobol' SI, hexagonal distribution plots and instantaneous state of GPP are available at https://doi.org/10.5281/zenodo.10582208. The repository also includes the input matrices and the output files that can be used to reproduce the results shown in this study.

The source code and the model data for the CLASSIC model v1.0 used to run all model simulations for the GSA in this article can be downloaded from https://doi.org/10.5281/zenodo.3522407, the singularity container with required packages to run the model is at https://doi.org/10.5281/zenodo.3525249 and site-level meteorological input files used for the model runs are available through https://doi.org/10.5281/zenodo.3525336. The three external open-access components of the CLASSIC model mentioned here, have to be downloaded and, if needed, installed to produce data for other FLUXNET2015 sites, but are not necessary for the reproduction of GSA/ parameter uncertainty interaction results shown in our study. All datasets and software used in this article are licensed under the Creative Commons Attribution 4.0 International.

The runs presented in this study were performed on a single shared server with two CPUs of 8 cores each and one node. Since each run is independent, 14 cores were used simultaneously to run the CLASSIC model. Under these conditions, the run time for each core for one run was 45 minutes, totalling almost four weeks for all the Morris and Sobol' runs. The runs for each Morris and Sobol' analysis were set up with a model spin-up of 500 years looped over with the available meteorological data, and a transient period of 11 years.

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