MODEL RELEVANCE

Frameworks for Exploring the Complexity-Sensitivity-Uncertainty Trilemma

S. MULLER, R. MUÑOZ-CARPENA, G. KIKER
University of Florida
PO Box 110570, Gainesville, FL 32611-0570
carpena@ufl.edu

Abstract

Ever more complex models play an important role in environmental assessment and adaptation to climate change. Model complexity is fundamental to the ability of environmental models to address questions, as well being a crucial determinant of uncertainty in model results. However, while increasing model complexity is introduced to answer new questions or reduce the uncertainty of the model outputs by considering refined process, often increased model complexity can have unexpected (and often unexplored) consequences on the overall model sensitivity and uncertainty. Thus modelers face a difficult trilemma relating model complexity, sensitivity, and uncertainty that can ultimately compromise the relevance of the model for a particular problem. We propose a methodological framework based on global sensitivity and uncertainty analysis to objectively and systematically explore this trilemma. An application is presented where a spatially distributed biogeochemical model to describe phosphorous dynamics in the Everglades (USA) is built and evaluated at different complexity levels. By increasing complexity, key model outputs were found to lose direct sensitivity to specific input factors and gain sensitivity to interaction effects between inputs. The relationship between complexity and uncertainty was found to be less predictable. Output uncertainty was generally found to reduce with increased complexity for summative outputs affected by the overall model (i.e., phosphorus surface water concentration), but reverse relationships were found for other outputs. The conceptual and methodological framework proved insightful and useful for characterizing the interplay between complexity, sensitivity, and uncertainty, and is proposed as an indispensable component in the model development and evaluation process.

1. Complexity, Uncertainty, and Sensitivity: A Modeling Trilemma

> That is what we meant by science. That both question and answer are tied up with uncertainty, and that they are painful. But that there is no way around

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> them. And that you hide nothing; instead, everything is brought out into the open [16].

A recent summary of the NATO Advanced Research Workshop on Global Climate Change and Local Adaptation [28] identifies models providing an integrated environmental assessment and management as a central component of the nexus of climate change adaptation. The study also concludes that additional emphasis is urgently needed on rational approaches to guide decision making through uncertainties surrounding climate change. This is because as is the case with all models [39,21], those predicting climate change itself or models simulating the response of natural systems to this change (or to our proposed plans to address this change) produce unavoidable uncertainty around the predicted responses. However, in spite of the difficulties that the consideration of modeling uncertainty represent for the decision process, this consideration should not be avoided or the value and science behind the models will be undermined [5].

These two issues; i.e., the need for models that can answer the pertinent questions and the need for models that do so with sufficient certainty, are the key indicators of a model's *relevance*. For instance, a model may answer a question but its usefulness might be limited if the uncertainty surrounding the answer is large. Conversely, a model may be able to address many questions with acceptable accuracy, but if it cannot address the particular question of interest then it is not relevant. Model relevance is inextricably linked with model complexity. Zadeh [55] expressed this relationship in his *principle of incompatibility* for humanistic systems or similarly highly complex systems. According to this author:

> …stated informally, the essence of this principle is that as the complexity of a system increases, our ability to make precise and yet significant statements about its behavior diminishes until a threshold is reached beyond which precision and significance (or relevance) become almost mutually exclusive characteristics.

Although model complexity has advanced greatly in recent years, yet there has been little work to rigorously characterize the threshold of relevance in integrated and complex models. Formally assessing the relevance of the model in the face of increasing complexity would be valuable because there is growing unease among developers and users of complex models about the cumulative effects of various sources of uncertainty on model outputs [31,30,11,34]. In particular, this issue has prompted doubt over whether the considerable effort going into further elaborating complex models will in fact yield the expected payback [1].

More complex models include more state-variables, processes and feedbacks, and therefore have fewer simplifying assumptions. Model complexity, in turn, has direct implications for uncertainty [15], as shown in Figure 1a.

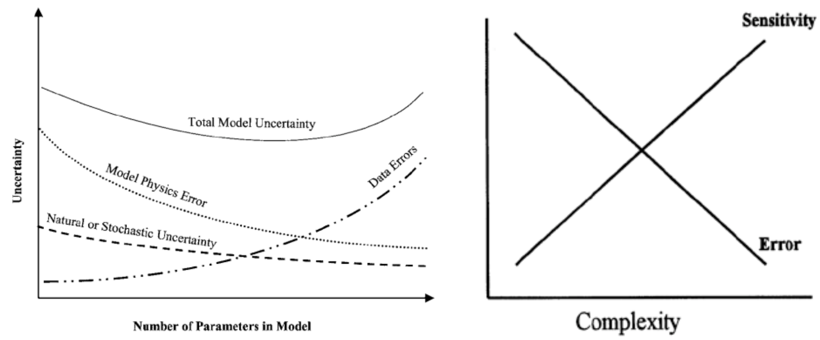

Figure 1. a) Trends in model uncertainty versus complexity [15]; b) Trends in model sensitivity and error versus complexity [49].

Increased complexity can translate into less structural uncertainty (model physics error in Figure 1a) and natural stochasticity (from spatial and temporal discretization). However, each additional process in a model requires additional model input factors, each of which is subject to uncertainty because of its intrinsic variability or data sampling errors. As complexity is increased and input factors accumulate, so too do the input uncertainties, which propagated onto the model outputs. Eventually a critical point is reached beyond which any additional complexity to reduce structural uncertainty is undermined by the accumulated input uncertainty—the threshold described by Zadeh [55].

In addition to input and structural uncertainty, overparameterization is another important source of uncertainty that is related to complexity. This issue can lead to problems of non-identifiability and non-uniqueness, which can fundamentally undermine trust in the validity of a given model [4]. Though difficult to quantify, the potential for overparameterization can be studied in terms of the sensitivity of an output to input factors [6,49]. Though a general relationship relating complexity and sensitivity has been suggested (Figure 1b) by Snowling and Kramer [49], this is another area that has not been widely studied [27].

Uncertainty analysis is the formal process of propagating input uncertainties through the model and onto the outputs. Sensitivity analysis determines what portion of the output uncertainty is attributable to the uncertainty in a given input factor, or to the interactions between input factors. Global sensitivity methods (those in which the complete parametric space of all the model input factors is sampled concurrently) should be used when evaluating complex models. However, the use of local sensitivity methods (derivative-based over a limited range and one factor at a time) remains pervasive [42]. Global sensitivity analyses offer additional benefits for managing uncertainty by helping to identify not only the important input factors for a given model output, but also their interactions. This information can be used to direct resources toward those input factors that would offer the best returns on resource investment. Conversely, unimportant input factors may indicate ways in which a model is unnecessarily complex, and therefore how it could be simplified. In addition, some cutting-edge methods of global sensitivity analysis have the benefit of employing Monte Carlo simulations, so results can be used for both uncertainty and sensitivity analysis [44]. This is an important efficiency since both global sensitivity and uncertainty analyses are generally computationally demanding, but work best when applied in tandem [44].

All modelers, but especially environmental modelers who often use complex models in increasingly integrated systems, face a difficult task. Relevant models must be available for environmental assessment of climate change, but in general we do not yet have a thorough understanding of how increasing complexity affects the behavior of models, particularly with respect to uncertainty. Rational and useful guidance is therefore needed to inform how model complexity is selected and managed. We propose that model relevance can be approached as a trilemma among model complexity, uncertainty, and sensitivity, and that this represents a useful conceptual framework within which to study the matter. Further, we propose a methodological framework of combined global sensitivity and uncertainty analysis as an efficient and effective means to explore and implement the relevance trilemma.

To demonstrate the utility of this approach, we present results obtained during the development of a complex, spatially distributed but user-definable numerical model of wetland biogeochemistry, including solute transport and reactions, developed for the Everglades wetlands of south Florida [17,18]. The flexibility provided to the user to define the description of the wetland biogeochemistry offered the opportunity to explore, using global sensitivity and uncertainty analysis in a systematic and step-wise fashion, the effect of incrementally increasing the complexity of the conceptual biogeochemical model.

2. Challenges of Integrated Modeling for Evaluation of Climate Change Impact Scenarios

Throughout the history of environmental modeling there has been a natural tendency propelling the emergence of ever more complex models. There are many reasons: our knowledge has grown and we use models to synthesize this; we have a natural inclination to push our technological and intellectual boundaries; advances in processing speeds and programming languages have fueled this urge; and both the study and the globalization of environmental concerns have exposed more complex problems that legitimately require more complex tools to tackle. Meanwhile, efforts to facilitate simplification of models have also been growing [20,24,38, 41]. However models of large and growing complexity are here to stay.

Integrated modeling exemplifies today this tendency toward greater complexity, and represents an important modeling frontier. Integrated models link independent models (environmental, social, economic, and risk management) together, such that the output of one becomes the input for another, in an effort to take the holistic approach to the next level. This methodology is already being adopted as the best practice for future modeling in support of environmental assessment and management [12]. While technologically admirable, integrated models represent a new challenge to the formal assessment of model relevance because we know that model complexity will only reduce uncertainty to a point and, as explained, will likely increase it past this point [15,23,56].

The integrated modeling paradigm; i.e., the integration of *modules* within a particular model, was adopted relatively early in the history of modeling to promote the reusability and applicability of existing models. Models became more versatile by permitting modules to be turned on or off depending on the needs of the application. An excellent example of the modular approach, and its success, is the now ubiquitous MODFLOW [33], a groundwater flow model in which different aspects of groundwater simulation are handled by modules that may be turned on or off. At the time of its development this approach was compared with the idea of a "component stereo system," as shown in the original model schematic used for the report's cover illustration (Figure 2).

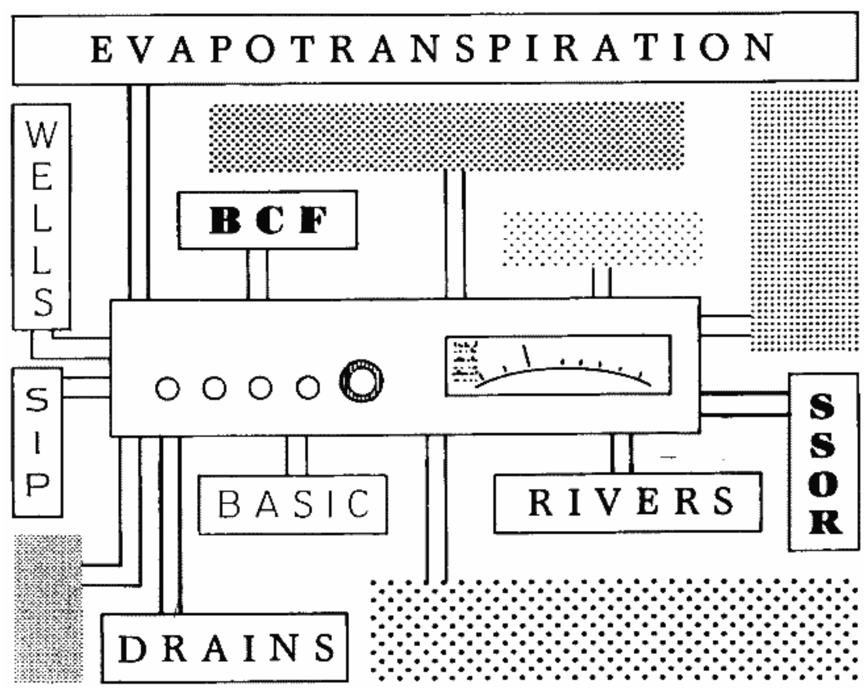

Figure 2. Cover illustration from the original MODFLOW report [32,] depicting the analogy of modules to a component stereo system.

A modern example in the context of climate change assessment is the Integrated Global System Model (IGSM) Version 2 [50], which is composed of several linked models (Figure 3), including the Emissions Prediction and Policy Analysis model; an atmospheric dynamics, physics, and chemistry model; an ocean model; the Terrestrial Ecosystem Model; a Natural Emissions Model; and the Community Land Model.

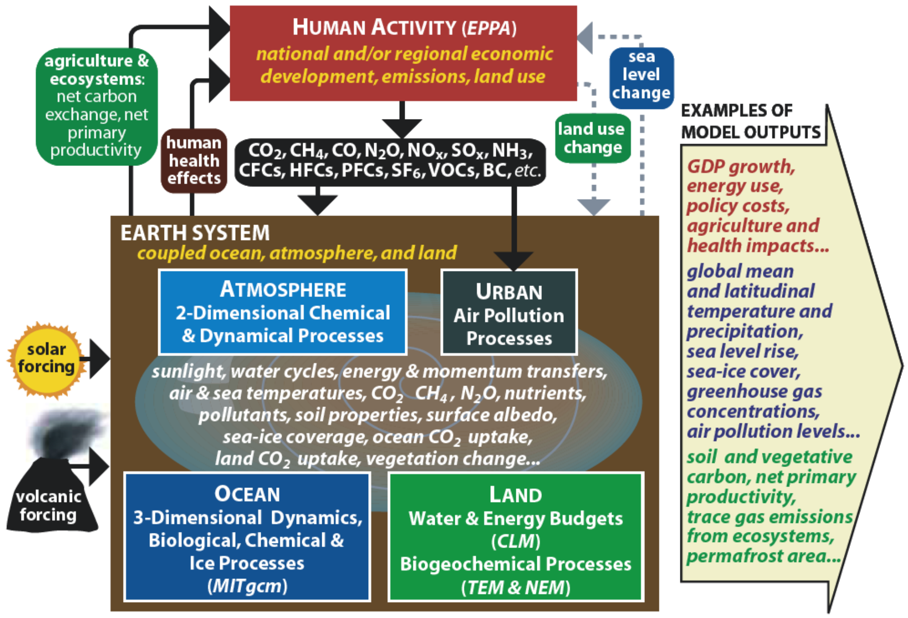

Figure 3. Schematic of the MIT Integrated Global System Model Version 2 [50].

While MODFLOW is considered a complex model of groundwater hydrology, IGSM2 is a self-described earth system model "of intermediate complexity" [50]. A widely used definition of model complexity is a tally of the number of input factors (representing the underlying processes). By this metric, the IGSM2 is by far the more complex, yet it is not considered as such from within its particular community. The implications of this are that notions of model complexity remain unclear and subjective, and change meaning in the context of a particular application. In fact, the MODFLOW system of modules, intended to simulate the integrated processes controlling groundwater, is functionally analogous to the integrated models of IGSM2. However, one is immediately struck by an obvious difference between Figure 2 and Figure 3—the MODFLOW picture looks much less complicated. What's more, in the IGMF case, many of the specified components actually represent full models in their own right [51], themselves each comprised of modules not unlike MODFLOW's. The actual leap in model complexity— i.e., due to the much larger temporal and spatial scales of the integrated model—is even more dramatic than the visual comparison of model structures indicate. In cognizance of this, significant work to assess and address uncertainty in the IGMF has been conducted [13,50,52]. However, this work generally focuses on evaluating the uncertainty of the end model, without consideration of alternative model complexities or their effect on model relevance.

We continue to rapidly increase the complexity of our models driven by external factors like the developer's life cycle (Figure 4), without always acknowledging, rarely studying, and not yet fully understanding the profound implications complexity has for the uncertainty associated with their results.

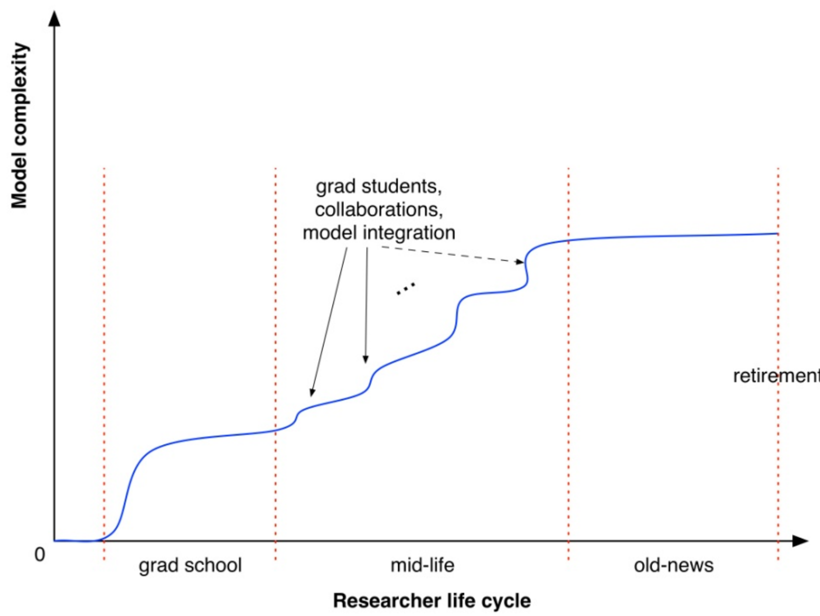

Figure 4. Model complexity and the researcher's life cycle.

Below we propose a methodological framework that serves to formally evaluate the effect of model integration and the relevance of the resulting model to the intended application.

3. A Methodological Framework for Assessing Effects of Model Complexity: A Case Study in the Everglades, FL

A case study for the analysis of the effects of increasing model complexity was carried out as part of a comprehensive testing process during the development of a numerical water quality model, the Transport and Reactions Simulation Engine (TaRSE), developed to simulate the biogeochemistry and transport of phosphorus in the Everglades wetlands of south Florida [17,18].

3.1. MODEL DESCRIPTION: TaRSE

TaRSE is composed of two modules; one that simulates the advective and dispersive transport of solutes [17], and one that simulates the transfer and transformation of phosphorus between biogeochemical components [18]. The term "Simulation Engine" refers to the generic nature of the reactions module, which was designed to be user-definable (by means of XML input files) such that the user specifies the state variables of the model and the equations relating them. State-variables that are transported with flow are termed “mobile”, and those that are not are termed “stabile.” TaRSE employs a triangular mesh to discretize the spatial domain for transport calculations [17] but the reactions module is independent of mesh geometry. Hydrodynamic variables such as depths and velocities can be specified as constant values by the user, as was the case in this work, or must be provided by a linked hydrologic model if variable hydrodynamic conditions are desired.

In addition to the necessary quality control provided by sensitivity and uncertainty analyses, the intention of this work was to study potential effects resulting from TaRSE’s flexible design (i.e., user-defined complexity).

3.2. MODEL APPLICATION

In order to isolate the effects of complexity, an artificial domain was created in which the sources of variability extrinsic to complexity could be controlled and excluded.

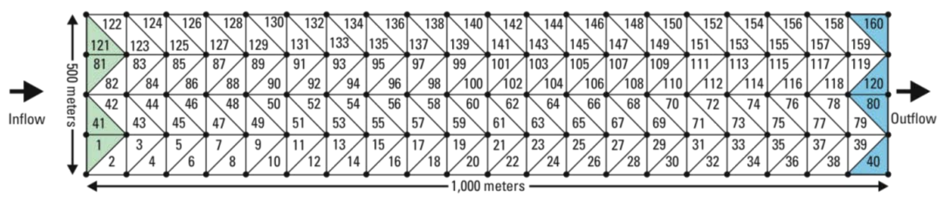

Figure 5. Model domain used for testing of the Transport and Reactions Simulation Engine [18].

A 1,000 × 200-m generic flow domain (Figure 5) was created and discretized into 160 equal rectangular triangles (cells). Flow was set from left to right so that the inflow boundary consisted of cells 1, 41, 81, and 122, and the outflow boundary consisted of cells 40, 80, 120, and 160. A no-flow boundary was applied to the top and bottom (longer) edges of the domain. To exclude the effects of transient flow, steady-state velocity was established, and the effects of heterogeneities were managed by assuming spatially homogeneous conditions. A constant velocity of 500 m/d was established to approximate Everglades flow conditions [25] with a unit average water depth. Simulations were run for 30 days with a 3-hour time-step.

3.3. LEVELS OF COMPLEXITY

Three models of increasing complexity were created (Figures 6a-c) by progressively adding complexity in an organized and step-wise fashion, as recommended in Chwif et al. [9]. One additional state-variable was introduced for each new complexity level. The processes required to integrate the new state-variables into the existing conceptual model were mathematically consistent formulations of biotic growth and loss, and required four additional input factors to characterize.

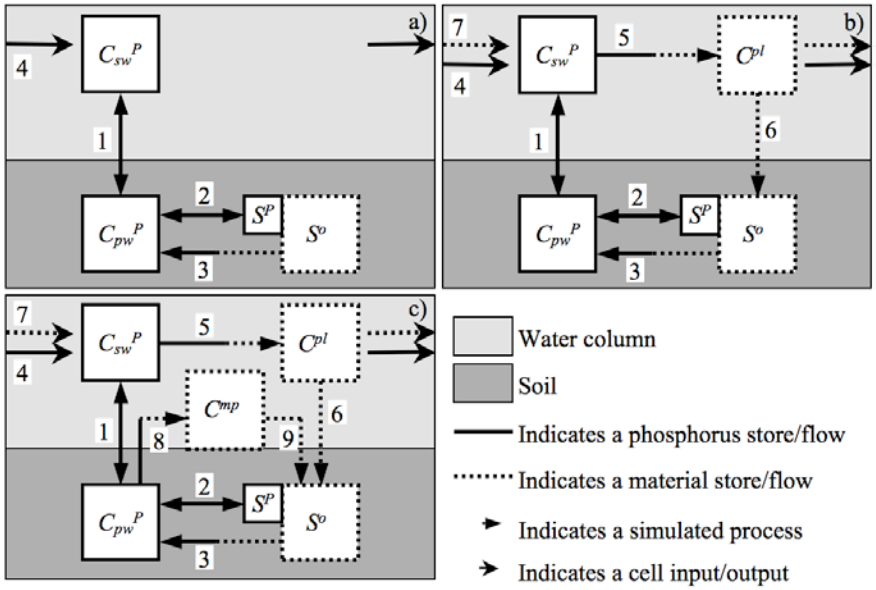

Figure 6. Levels of modeling complexity studied to represent phosphorus dynamics in wetlands. Levels include a) Level 1: interactions between SRP in the water column and SRP in the subsurface; b) Level 2: Level 1 with the addition of plankton growth and settling; c) Level 3: Level 2 with the addition of macrophyte growth and senescence. Notation and details on processes included in each Level are given in Table 1.

The simplest case (Level 1) contained no biotic components (Figure 6a) and eight input factors were tested. The intermediate-complexity case (Level 2) contained surface-water biota in the form of phytoplankton (Figure 6b) and 12 input factors were tested. The most complex case (Level 3) contained additional macrophytes rooted in the soil (Figure 6c) and 16 input factors were tested. Table 1 lists the state-variables and processes that appeared in each complexity level, including the boundary conditions for the mobile state-variables (always quantified in g/m^3) of soluble reactive phosphorus (SRP) in the surface-water (C_{sw}^P) and plankton biomass (C_{pl}). Initial conditions for the stabile state-variables (always quantified in g/m^2) of SRP in the porewater, adsorbed phosphorus, macrophyte biomass, and organic soil mass, were 0.05, 0.027, 500, and 30,000 g/m^2, respectively. Boundary and initial conditions were selected to represent reasonable Everglades conditions. Full descriptions and derivations of the model equations and their numerical implementations can be found in Jawitz et al. [18].

Table 1. Processes and variables used in defining three TaRSE models of increasing complexity.

Process	Levels	Key, Fig 6	Affected variables	Process equation
Diffusion	1, 2, 3	1	Surface-water SRP concentration (mobile), $C_{sw}{}^{P}$ (g/m^3) Soil porewater SRP concentration (stabile), $C_{pw}{}^{P}$ (g/m^2)	$\frac{dC_{sw}^{P}}{dt} = \frac{k_{df}}{z_w z_{df}}\left(C_{pw}^{P} - C_{sw}^{P}\right)$
Sorption-desorption	1, 2, 3	2	Soil porewater SRP concentration (stabile), $C_{pw}{}^{P}$ (g/m^2) Soil adsorbed P mass (stabile), S^{P} (g/m^2)	$\frac{dS^{P}}{dt} = \frac{\rho_b k_d}{\theta}\frac{dC_{pw}^{P}}{dt}$
Oxidation of organic soil	1, 2, 3	3	Soil porewater SRP concentration (stabile), $C_{pw}{}^{P}$ (g/m^2) Organic soil mass (stabile), S^{o} (g/m^2)	$\frac{dS^{o}}{dt} = -k_{ox}S^{o}$
Inflow/outflow of surface-water SRP	1, 2, 3	4	Surface-water SRP concentration (mobile), $C_{sw}{}^{P}$ (g/m^3)	BC: $C_{sw}{}^{P}$ = 0.05 g/m^3
Uptake of SRP through plankton growth	2, 3	5	Surface-water SRP concentration (mobile), $C_{sw}{}^{P}$ (g/m^3) Plankton biomass concentration (mobile), C^{pl} (g/m^3)	$\frac{dC^{pl}}{dt} = -k_g^{pl}C^{pl}\left(\frac{C_{sw}^{P}}{C_{sw}^{P} + k_{1/2}^{pl}}\right)$
Settling of plankton	2, 3	6	Plankton biomass concentration (mobile), C^{pl} (g/m^3) Organic soil mass (stabile), S^{o} (g/m^2)	$\frac{dC_{sw}^{pl}}{dt} = -k_{st}^{pl}C^{pl}$
Inflow/outflow of plankton	2, 3	7	Plankton biomass concentration (mobile), C^{pl} (g/m^3)	BC: C^{pl} = 0.043 g/m^3

Process	Levels	Key, Fig 6	Affected variables	Process equation
Uptake of porewater SRP through macrophyte growth	3	8	Soil porewater SRP concentration (stabile), $C_{pw}{}^{P}$ (g/m^2) Macrophyte biomass (stabile), C^{mp} (g/m^2)	$\frac{dC^{mp}}{dt} = -k_g^{mp} C^{mp} \left(\frac{C_{pw}^{P}}{C_{pw}^{P} + z_{as}\theta} \right.$
Senescence and deposition of macrophytes	3	9	Macrophyte biomass (stabile), C^{mp} (g/m^2) Organic soil mass (stabile), S^{o} (g/m^2)	$\frac{dC^{mp}}{dt} = -k_{sn} C^{mp}$

3.4. MODEL PARAMETERIZATION

The analysis of TaRSE was intentionally performed without prior calibration in order to avoid limiting the potential range of physical conditions (input factor values) the model would be tested over, and through which the effects of new complexity would be expressed. Testing of models across a wide range of possible scenarios is a necessary step in the development process prior to evaluation of model performance for a particular application [43]. Before conducting the global sensitivity and uncertainty analyses it was necessary to specify the range and distribution for each input factor, from which values were statistically sampled using Simlab.

The field-scale ambient variability of many inputs has been reported to be adequately modeled with log-normal or Gaussian distributions [14,19, 26,29]. The (beta) β-distribution can be used as an acceptable approximation when there is a lack of data to estimate the mean and standard deviation for such probability distribution functions (PDFs) [54]. When only the range and a base (effective) value are known, a simple triangular distribution can be used [22].

The input factors used in the analysis of TaRSE (Table 2) were assigned ranges and probability distributions based on an extensive literature review found in Jawitz et al. [18]. The goal of this work was a general model investigation, and not a specific study of its application to a particular site. Consequently, input factor ranges that captured all physically realistic values for the target region were specified. This broad approach encompasses data from a wide range of physical and ecological conditions, and values were derived from relevant literature rather than calculated directly from sets of data. Consequently, the more general β-distribution was used for all biogeochemical input factors. Longitudinal and transverse dispersivity are related to aspects of the physical system that are contingent on site selection rather than natural variation, such as vegetation density, domain dimensions, and velocity. Their probability was therefore considered to be random, and accordingly allocated a uniform distribution.

Table 2. Input factors and distributions tested for using the global sensitivity and uncertainty analysis framework.

Input factor definition	**Symbol (Alternate name in Fig 7)**	**Key, Fig 6**	**Distribution**	**Units**	**Input present in**		
					L1	L2	L3
Coefficient of diffusion	k_{df} (k_df)	1	β (7×10^{-10}, 4×10^{-9})	m^2/s	x	x	x
Coefficient of adsorption	k_d (k_d)	2	β (8×10^{-6}, 11×10^{-6})	m^3/g	x	x	x
Soil porosity	θ (soil_porosity)	2	β (.7, 0.98)	-	x	x	x
Soil bulk density	ρ_b (bulk_density)	2	β (.05, 0.5)	-	x	x	x

Soil oxidation rate	k_{ox} (k_ox)	3	β (.0001, 0.0015)	1/d	x	x	x
P mass fraction in organic soil	X_{so}^{P} (chi_org_soil)	3	β (.0006, 0.0025)	-	x	x	x
Longitudinal dispersivity	λ_l (long_disp)	4	U (70, 270)	m	x	x	x
Transverse dispersivity	λ_t (trans_disp)	4	U (70, 270)	m	x	x	x
Plankton growth rate	k_g^{pl} (k_pl_growth)	5	β (.2, 2.5)	1/d		x	x
Plankton half saturation constant	$k_{1/2}^{pl}$ (k_pl_halfsat)	5	β (.005, 0.08)	g/m^3		x	x
Plankton settling rate	k_{st}^{pl} (k_pl_settle)	6	β (2.3×10^{-7}, 5.8×10^{-6})	m/s		x	x
P mass fraction in plankton	X_{pl}^{P} (chi_pl)	6	β (.0008, 0.015)	-		x	x
Macrophyte growth rate	k_g^{mp} (chi_mp)	8	β (.004, 0.17)	1/d			x
Macrophyte half saturation constant	$k_{1/2}^{mp}$ (k_mp_halfsat)	8	β (.001, 0.01)	g/m^3			x
Macrophyte senescence rate	k_{sn}^{mp} (k_senesce)	9	β (.001, 0.05)	1/d			x
P mass fraction in macrophytes	X_{mp}^{P} (chi_mp)	9	β (.0002, 0.005)	-			x

Outputs were defined for each of the model's state-variables at each complexity level, and are described in Table 3.

Table 3. Definition of outputs and boundary/initial conditions used for the global sensitivity and uncertainty analyses.

Output definition	Description	Nomenclature	Initial/Boundary conditions	Output present in		
				L1	L2	L3
Surface water SRP outflow (mobile)	Average of surface water SRP for outlet cells (boundary cells 40, 80, 120, and 160 in fig. 16) at the final time step	$C_{sw}{}^{P}$ (g/m^3)	0.05 (IC & inflow BC)	x	x	x
Soil porewater SRP variation (stabile)	Difference in averages porewater SRP concentration across the domain (all cells) between initial and final time step	$C_{pw}{}^{P}$ (g/m^2)	0.071 (IC)	x	x	x
Organic soil accretion (stabile)	Difference in average organic soil mass across the domain (all cells) between initial and final time step	S^{o} (g/m^2)	30,000 (IC)	x	x	x
Soil adsorbed P variation (stabile)	Difference in average adsorbed P mass across the domain (all cells) between initial and final time step	S^{P} (g/m^2)	0.027 (IC)	x	x	x
Plankton biomass outflow (mobile)	Average plankton biomass concentration for outlet cells (boundary cells 40, 80, 120, and 160 in fig. 16) at the final time step	C^{pl} (g/m^3)	0.043 (IC & inflow BC)		x	x
Macrophyte biomass accumulation (stabile)	Difference in averages of macrophyte biomass across the domain (all cells) between initial and final time step	C^{mp} (g/m^2)	500 (IC)			x

In the context of this work to investigate the role of complexity, only those outputs that appear in all three complexity levels permit comparison and are presented. Outputs were defined to integrate spatial effects in stabile variables and temporal effects in mobile variables. For outputs of mobile quantities, averages across the outflow domain (cells 40, 80, 120, and 160) were calculated at the end of the simulation period. For stabile quantities, outputs were expressed as the difference between the initial and final value of averages across the entire domain.

Except for structure, all model conditions were consistent across complexity levels, including fixed input factor ranges and distributions; invariant scale, initial, and boundary conditions; and steady hydrodynamics. Any change observed in the uncertainty and sensitivity was therefore attributable to the effects of changes in model complexity.

3.5. GLOBAL SENSITIVITY AND UNCERTAINTY METHODS

Two state-of-the-art methods of global sensitivity analysis were applied: the qualitative method of Morris [35] and the quantitative, variance-based extended Fourier Amplitude Sensitivity Test (FAST) [42]. The latter method employs Monte Carlo simulations and results can therefore be used for uncertainty analysis as well. A brief summary of each method is given below (further details are summarized in Muñoz-Carpena et al. [37] and a thorough treatment of the methods is provided in Saltelli et al. [44]).

The Morris method, extended by Campolongo and Saltelli [8], applies a frugal sampling technique to efficiently explore the full parametric space of the model input factors. A one-at-a-time approach is used such that one input factor is varied while all other input factors are held constant. The change observed in an output, called the "elementary effect," can therefore be attributed to a particular input factor. This approach is analogous to the widely used derivative-based local sensitivity analysis methods, but is globalized by calculating multiple elementary effects after resampling the other input factor values in the model. In this way, the parametric space of the model is comprehensively sampled, and the magnitudes of the elementary effects are averaged to produce a qualitative global sensitivity statistic, μ^*. The magnitude of μ^* indicates the relative importance of each input factor with respect to the model output of interest [7]. The standard deviation of the elementary effects, σ, can be used as a statistic indicating the extent of interactions between inputs. High variability indicates that parametric context (the values of the other input factors) influences the elementary effects produced by varying a given input factor. This indicates that interactions between input factors can contribute to increasing or decreasing the sensitivity, or that output sensitivity to the input factor is non-linear. For each output of interest, pairs of (μ^*_i, σ_i) for each input factor can be plotted in a Cartesian plane to indicate the relative importance (μ^*_i) of each output (distance from the origin on the X-axis), and the prevalence of interaction effects (σ_i) between input factors (distance from the origin on the Y-axis).

The frugal sampling technique used in this approach makes it suitable for assessing the *relative* importance of input factors, sacrificing quantification in lieu of dramatically reduced computational demands. The Morris method is also useful for screening out unimportant input factors before conducting the much more computationally intensive Monte Carlo simulations required for quantitative analysis using the extended FAST method [18,45].

The variance-based extended FAST method provides a *quantitative* measure of the direct sensitivity (S_i) of a model output to each input factor (*i*). It does so by calculating the fraction of the total output variance attributable to a single input input factor. In addition to the calculation of first-order indices, the extended FAST method [42] calculates the sum of the first- and all higher-order indices for a given input input factor (*i*), called the total sensitivity (S_{Ti}) index (Equation 1),

$$S_{Ti} = S_i + S_{ij} + S_{ijk} + \cdots + S_{i\ldots n}, \tag{1}$$

where S_i is the first-order (direct) sensitivity, S_{ij} is the second-order indirect sensitivity due to interactions between input factors *i* and *j*, S_{ijk} the third-order effects to due to interactions between *i* and *k* via *j*, and so forth to the final varied input factor, *n*.

Based on Equation 1, total interaction effects can then be determined by calculating S_{Ti} - S_i. It is interesting to note that μ* of the Morris [35] method is a close estimate of total sensitivity (S_{Ti}) [7]. Since the extended FAST method applies a randomized sampling procedure, it provides an extensive set of outputs that can then be used for the global uncertainty analysis of the model. Thus, PDFs, cumulative probability distribution functions (CDFs), and percentile statistics can be derived for each output of interest with no further simulations required.

3.6. ANALYSIS PROCEDURE

In general, the methodological framework followed six main steps (Figure 7): (1) PDFs were constructed for uncertain input input factors; (2) input sets were generated by sampling the multivariate input distribution according to either the Morris or FAST method; (3) model simulations were executed for each input set; (4) global sensitivity analysis was performed according to the Morris method and then 5) the extended FAST method; and (6) uncertainty was assessed based on the outputs from the extended FAST simulations by constructing PDFs and statistics of calculated uncertainty.

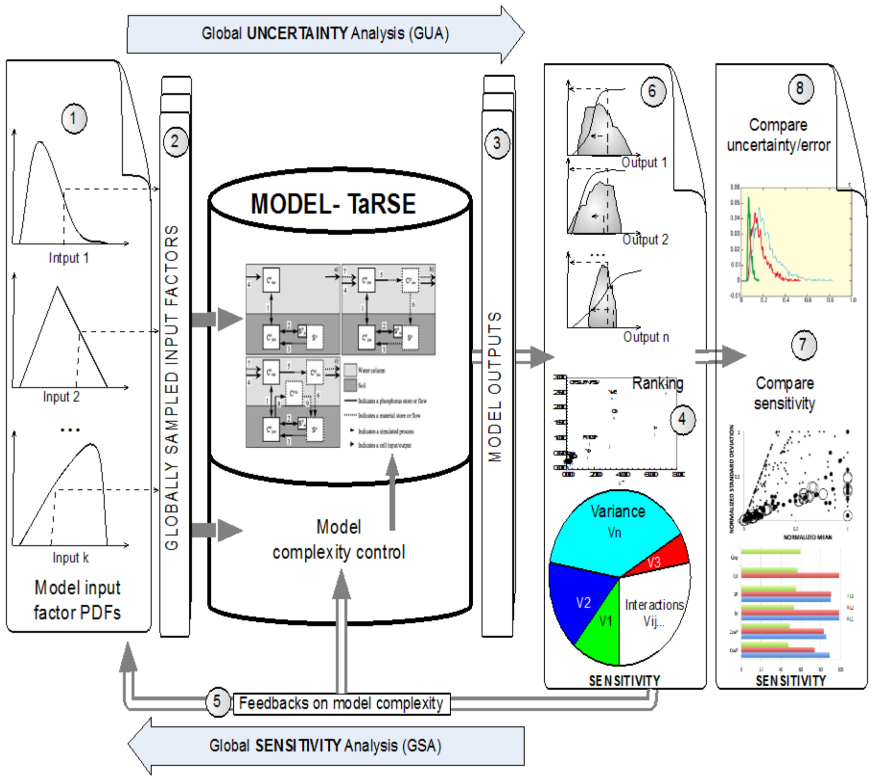

Figure 7. The methodological framework of global sensitivity and uncertainty analysis suggested applied for studying how changing complexity affects the relevance trilemma.

The software Simlab [44] (available at: http://simlab.jrc.ec.europa.eu/) was used for multivariate sampling of the input factors and post-processing of the model outputs. Sample sets were created for all the input factors in each of the complexity levels tested (see subsequent section and Figure 6) and for both methods, resulting in a total of six sets of analyses. The number of model runs was selected based on the number of input factors in each complexity level according to Saltelli et al. [44]. A total of 1,170 simulations were conducted for the Morris method and 45,046 simulations for the extended FAST method.

4. Results

4.1. EFFECTS OF MODEL COMPLEXITY ON SENSITIVITY

In the context of TaRSE's intended use for managing water quality in the Everglades, concentration of SRP in the surface is the most important output because this has a mandated limit of 10 ppb [48]. Figures 8a-c present the Morris method results for this output (C_{sw}^{P}) at each of the three complexities tested.

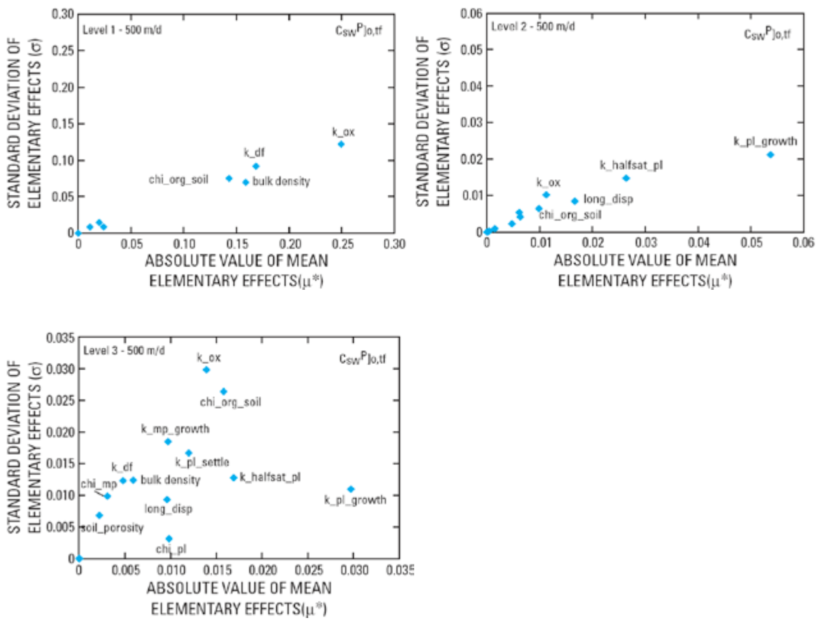

Figure 8. Morris method results for soluble reactive phosphorus in the surface water..

As the complexity increased, the relative location of input factors in the μ*-σ plane changed. At lower complexities (Levels 1-2) input factors were found closer to the μ*-axis. At Level 3, the input factors were generally above the 1:1 line and associated with proportionally higher σ-values. Higher σ-values denote greater variability in the elementary effects, and therefore an increase in the role of interactions between input factors, and a converse decrease in the influence of input factors directly on the output.

As the complexity increased, especially to Level 3, progressively more input factors were drawn out into the μ*-σ plane. Since the important input factors are distinguished from the unimportant by their relative distance from the origin, this result indicates that more input factors became relatively important as complexity increased, or conversely that fewer input factors were uniquely important. The labeled points in Figures 8a-c represent the input factors deemed “important” according to this method. The number of important input factors was found to increase from 4 in Level 1, to 5 in Level 2, and 12 in Level 3. However, the designation of which input factors are deemed important and which are not is subjectively assigned based on being “close” or “far” from the origin. Furthermore, the proportion of important input factors did not increase monotonically: 4 out of 8 is 50 percent in Level 1; 5 out of 12 is 42 percent in Level 2, and 12 out of 16 is 75 percent in Level 3. Quantitative methods are therefore needed to objectively identify the most important input factors, and to characterize these changes in sensitivity more rationally. Nonetheless, the general observation that the number of important input factors in a model, and the way that they influence an output (directly and linearly versus indirectly and non-linearly) were found to be highly susceptible to relatively small changes (four new input factors) in model complexity for tested input factor ranges.

The sensitivity of C_{sw}^{P} to different input factors at different complexities shows how the role of input factors can change as others are added. In Level 1 we found that k_{ox}, k_{df}, ρ_b, and X_{so} were the most important input factors. For Level 2, plankton in the water column was added to the model, and input factors associated with plankton growth (k_g^{pl} and $k_{1/2}^{pl}$) became the most important, though some of the important input factors from Level 1 (k_{ox} and X_{so}) remained germane. With the addition of macrophytes for Level 3 it became difficult to distinguish the most important input factors. Instead, because of the increased role of interactions, the majority of the model input factors became noteworthy. The lack of any consistency in specific sensitivity to input factors among complexities is indicative of important influences contributed by each increase in complexity. While it may be feasible to calibrate a model to fit surface water phosphorus data without a plankton component, the absence of such a component is questionable if it is so clearly important when included. Similarly, the strong influence of a macrophyte component on the results indicates that the omission of this element would have implications for structural uncertainty.

The quantified results provided by the extended FAST analysis permit a more rigorous evaluation of how complexity affects sensitivity. FAST results for first-order (S_i) and interaction (S_T-S_i) effects for all model outputs are presented in Table 4. The input factors of greatest influence to each output are identified with shading. The first-order effects represent the direct responses of an output to each input factor, and the total first-order effect for each output is the percentage of the total variance attributable to direct effects. The remaining percent is that portion of the variance attributable to interactions between input factors. Contributions to variance of particular interactions can be obtained using more rigorous and computationally demanding methods such as the Method of Sobol [50].

Results in Table 4 largely corroborate the sensitivities identified in the Morris analysis, though interpretation of the Morris results would appear to overestimate the role of some input factors. This conservativeness is preferred to a method that might underestimate their role, particularly if the Morris method is to be used as a screening tool prior to quantitative analysis by methods like FAST. Once interactions prevailed, essentially from Level 3, it becomes difficult to identify important input factors in Morris for reasons that became very clear in the FAST results—the interactions are so prevalent that many input factors become comparatively important, hence the confusion in the Morris interpretation.

Table 4. Results from the extended Fourier Amplitude Sensitivity Test.

Output	Complexity level	Input factor																Total
		k_{df}	k_{ox}	X_{so}^{P}	k_{d}	θ	ρ_{b}	λ_{t}	λ_{t}	k_{g}^{pl}	$k_{1/2}^{pl}$	k_{st}^{pl}	X^{pl}	k_{g}^{mp}	$k_{1/2}^{mp}$	k_{sn}^{mp}	X^{mp}	
First order index, S_i																		
C_{sw}^{P}	L1	15.6	36.3	16.1	0.3	0.1	20.3	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	88.9
	L2	0.7	2.2	1.1	0.8	0.1	0.8	1.1	0.1	50.3	16.2	0.1	0.3	0.0	0.0	0.0	0.0	73.9
	L3	2.2	1.4	2.1	3.4	2.3	2.4	2.6	1.6	9.1	6.3	2.8	2.7	2.5	1.6	1.7	2.7	47.3
C_{pw}^{P}	L1	1.9	43.5	20.9	0.4	1.2	17.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	85.6
	L2	1.6	42.4	19.7	0.3	1.8	17.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	83.2
	L3	1.3	4.5	2.3	1.4	1.0	2.2	1.9	1.3	1.5	1.3	1.4	1.1	13.7	2.4	2.5	9.1	48.8
S^{o}	L1	0.0	98.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	98.7
	L2	0.0	98.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	98.6
	L3	2.4	14.2	2.3	3.3	2.3	2.0	2.6	2.0	2.1	1.4	2.9	2.1	2.1	1.6	6.2	4.0	53.5
S^{P}	L1	1.8	51.3	24.7	0.4	0.1	12.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	90.3
	L2	2.5	49.3	25.5	0.6	0.1	12.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	90.5
	L3	1.4	4.5	2.5	1.5	1.0	1.7	1.8	1.4	1.2	1.4	1.4	1.2	20.1	2.2	2.4	10.0	55.5

Output	Complexity level	Input factor																
		k_{df}	k_{ox}	X_{so}^{P}	k_{d}	θ	ρ_b	λ_t	λ_t	k_g^{pl}	$k_{1/2}^{pl}$	k_{st}^{pl}	X^{pl}	k_g^{mp}	$k_{1/2}^{mp}$	k_{sn}^{mp}	X^{mp}	Total
C^{pl}	L2	11.1	31.8	11.8	0.2	0.0	10.6	0.6	0.0	20.8	4.5	0.0	7.3	0.0	0.0	0.0	0.0	98.6
	L3	1.8	2.7	1.9	2.2	2.2	1.7	1.8	1.7	5.5	4.9	8.9	8.8	6.2	1.3	2.4	2.7	56.7
C^{mp}	L3	2.0	6.2	4.7	2.6	2.0	1.4	1.4	1.3	1.4	1.5	2.0	2.3	3.0	1.6	7.8	18.5	59.6
		Interactions, S_{Ti} - S_i																
C_{sw}^{P}	L1	4.4	7.6	7.2	0.6	0.3	4.7	0.4	0.4									
	L2	10.3	12.8	8.0	19.0	25.3	24.9	16.8	16.5	16.8	11.7	18.7	15.7					
	L3	73.2	75.8	78.2	74.8	79.3	73.6	73.9	77.1	72.4	78.2	78.6	76.3	64.7	74.4	74.6	70.6	
C_{pw}^{P}	L1	1.2	9.6	5.4	0.6	0.7	4.2	0.6	0.5									
	L2	1.8	6.7	5.7	0.6	0.9	0.6	0.6	0.6	1.0	5.1	0.7	0.7					
	L3	58.0	66.5	48.5	63.3	63.7	56.7	61.6	74.0	73.7	78.4	61.8	59.4	39.8	54.4	76.9	53.5	
S^{o}	L1	0.2	1.3	0.2	0.2	0.2	0.2	0.5	0.4									
	L2	0.3	1.4	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3					
	L3	75.6	71.6	79.4	78.2	62.6	67.2	81.9	82.2	73.2	78.7	73.1	72.5	59.3	64.5	74.2	68.3	

Output	Complexity level	Input factor																Total
		k_{df}	k_{ox}	X_{so}^{P}	k_d	θ	ρ_b	λ_t	λ_t	k_g^{pl}	$k_{1/2}^{pl}$	k_{st}^{pl}	X^{pl}	k_g^{mp}	$k_{1/2}^{mp}$	k_{sn}^{mp}	X^{mp}	
S^P	L1	0.7	8.1	5.6	0.5	0.4	2.3	0.4	0.4									
	L2	1.0	7.9	6.7	1.2	0.3	0.6	0.7	0.5	0.5	3.1	0.6	0.6					
	L3	57.7	72.7	53.4	72.3	61.6	54.6	60.8	72.2	69.0	77.2	61.1	59.0	39.5	56.3	74.2	52.8	
C^{pl}	L2	4.1	7.5	5.2	0.7	2.9	1.6	0.7	2.1	0.4	5.0	1.2	0.5					
	L3	69.1	67.0	60.1	61.4	59.2	64.3	68.5	72.1	70.6	65.3	65.0	71.4	58.6	58.3	64.6	61.4	
C^{mp}	L3	63.9	60.1	71.6	69.3	52.1	63.1	64.8	72.6	66.8	77.3	66.2	68.0	66.0	69.5	60.9	60.5	

The relative lack of change in overall sensitivity patterns between Level 1 and Level 2 compared with the significant changes seen in Level 3 raise an interesting question: what about the *sensitivity of sensitivity to complexity*? The results of this study appear to demonstrate a nonlinear relationship between sensitivity and complexity, which was also found in Lindenschmidt [27], and drives home the need for more comprehensive global methods to be used when evaluating complex models.

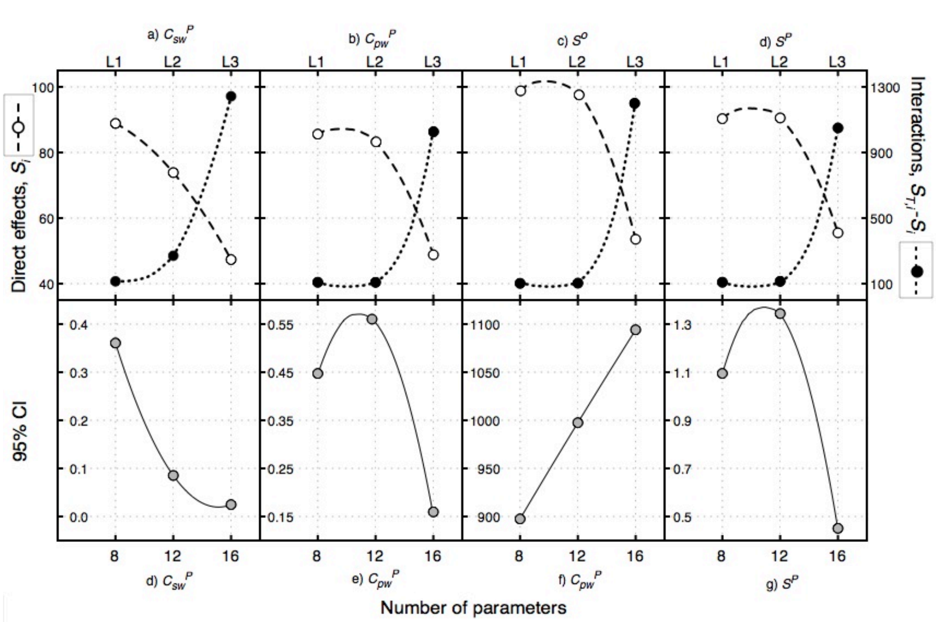

Figure 9. Changes in uncertainty and sensitivity with increasing complexity for state-variables that appeared in all three complexity levels [36].

In general, results for all outputs show that the total percentage of variance that can be attributed to first-order effects decreased with increasing complexity (Figures 9a-d). Conversely, the role of interactions, as was suggested by the Morris method results, rose sharply in the most complex case. Note that for the case of C_{sw}^{P}, the total direct effects decreased from Level 1 to Level 2, but the number of important input factors was also reduced from four to two (k_g^{pl} and $k_{1/2}^{pl}$), and their individual contributions to variance increased. Looking only at the total direct sensitivity for C_{sw}^{P}, one would expect non-identifiability to be a greater risk in Level 2, but the relationship is shown to be more complex when the sensitivities to particular input factors are known.

4.2. EFFECTS OF MODEL COMPLEXITY ON UNCERTAINTY

Some of the uncertainty results (Figures 9e-h), presented here using the 95 percent confidence interval, seem to question the conceptual trends in Hanna [15] (Figure 1a), indicating that these relationships may not be as simple as proposed. In fact, the observed differences are explained by accounting for the fact that some outputs are integrative, meaning that all model components participate in producing their final outcome, whereas others have inherent biases due to the masses and turnover rates of stores. The key output, C_{sw}^{P}, is an example of an integrative output, since it is mechanistically subject to the influence of all other state variables, and the expected reduction of uncertainty holds. By comparison, accreted organic soil (S^{o}) is characterized by a mass that is several orders of magnitude larger than any other outputs or fluxes, and is therefore not integrative. In the case of C_{pw}^{P} and S^{P} we see the uncertainty first rise and then drop, indicating that the relationship between complexity and uncertainty can be non-linear.

Figures 10a-c depict the progression of output PDFs across complexity levels for the same key output, C_{sw}^{P}, from a simpler leptokurtic distribution at the lowest complexity level, through the platykurtic distribution at the intermediate level, to a bimodal distribution at the highest complexity.

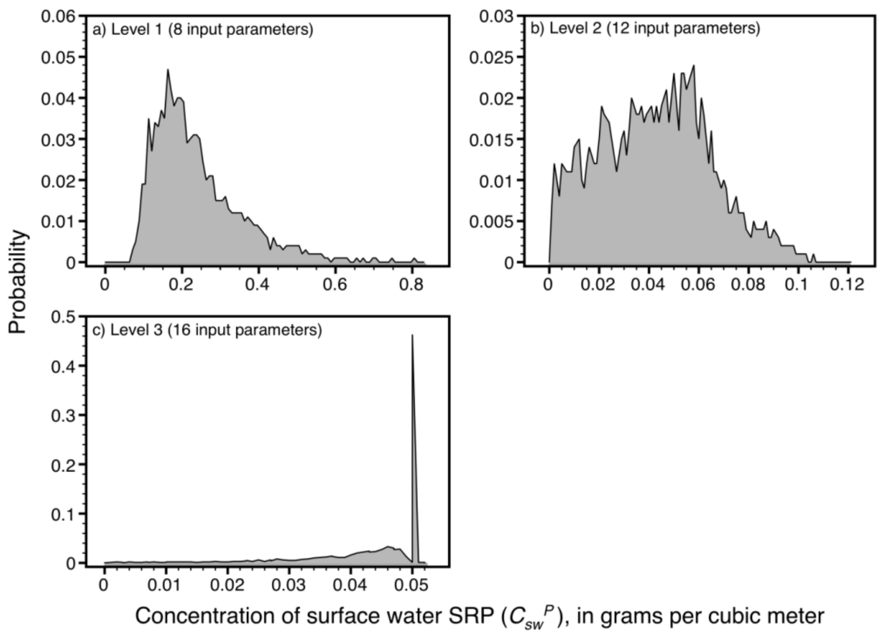

Figure 10. Uncertainty analysis results expressed as probability distribution functions for soluble reactive phosphorus in the surface water using a) complexity Level 1, b) complexity Level 2, and c) complexity Level 3.

The bimodality in Level 3 demonstrates the feasible existence of two stable states within the model. The platykurtic shape exhibited by the Level 2 results remained, but a strongly leptokurtic endpoint was also present, and corresponds to combinations of input factor values that push the simulation out of the original stable-state. In this case, the new stable state (the spike) appears as a single value, and indicates that the complexity at this level was sufficient to capture the existence of a second state, but insufficient to capture any variability within the state.

Mechanistically, the presence of this second state demonstrated that a critical threshold existed for the state previously captured in Level 2. Its presence was caused by combinations of input factor values, working in conjunction with initial and boundary conditions, which resulted in the systemic depletion of the biotic components (plankton and macrophytes). This occurred because the range of values over which the input factors were varied was held constant across complexity levels, yet included values appropriate for both of the known stable-states that shallow water bodies can exhibit in the Everglades [3,46,47]; namely, algae- and macrophyte-dominated systems [2,10]. Testing the full range of plankton-dominated conditions in Level 2 presented no problems to the model because the structure was mechanistically appropriate—there were no macrophytes. However, the incorporation of macrophytes into the model introduced a second potential state, but without the necessary feedback mechanisms (i.e., complexity) in place to resolve the extreme conditions produced by combinations of input factor values simultaneously representative of both algae- and macrophyte-dominated conditions. Without phytoplankton there was no surface-water sink for phosphorus (uptake by phytoplankton), and $C_{sw}{}^{P}$ continuously input at the boundary remained essentially unchanged in these cases, depicted by the spike in outflow values matching the boundary concentration of 0.05 g/m^3.

The platykurtic area represents model conditions under which the input factorization of the system did not catastrophically overwhelm it. The results therefore mimic those of Level 2, where macrophytes were absent and phytoplankton dominated the surface-water phosphorus dynamics. It is noteworthy that the introduction of macrophytes still acts as a phosphorus sink in these cases, stressing the phytoplankton in terms of phosphorus availability and thereby dampening the frequency of lower $C_{sw}{}^{P}$ values (a sign of greater phosphorus uptake due to growing plankton). Macrophytes also prevent the majority of $C_{sw}{}^{P}$ results from exceeding the boundary input concentration (which can only occur when significant diffusion takes place due to high $C_{pw}{}^{P}$, as in Level 2, and as was never the case for Level 3 because of porewater SRP uptake by the macrophytes [18].

5. Conclusions

Modeling is an art because it is an uncertain science. This uncertainty is increasingly attended to by modelers and managers, and is of growing concern to the public [40]. As the complexity of our problems grows we are likely to find ourselves more reliant on more complex models for some modicum of insight into scenarios beyond our ability to experimentally or intellectually assess. Integrated environmental assessment and management in response to climate change must rely on relevant models that can answer the appropriate questions with acceptable uncertainty.

When developing or applying such models there are many important questions to be addressed: What processes should be added? How does this impact uncertainty? Can the real system behavior be modeled? Will the model be usable based on available knowledge of the system? To answer some of these questions in an objective way, and to add transparency and guidance to the process of navigating model development and uncertainty, a relevance framework is suggested based on the trilemma among complexity, uncertainty, and sensitivity. A methodological framework based on global sensitivity and uncertainty analysis proved useful for objectively exploring and characterizing the relevance trilemma.

Application of the proposed framework to a case study allowed for the systematic evaluation of the effect of increasing model complexity on the model relevance. Firstly, in this application direct effects of input factors on output sensitivity were observed to decrease with complexity, while interactions increased. Both the number and identity of important input factors was found to change in complicated ways with the addition of complexity. Uncertainty was found to decrease with increasing complexity for some state-variables, including the key system variables (like surface water reactive phosphorus in the Everglades example), but increased for others, indicating that the relationship between complexity and uncertainty is not as simple as the Hanna et al. [15] conceptual relationship would indicate. Distinct shifts in the output PDFs were observed, including the emergence of bimodal states in the model output. These alternative system states might be a true expression of the ecological system response and therefore desirable (and a driver) of the introduction of the increasing complexity of the model.

From a practical perspective, the proposed GSA/UA tools could inform model development to achieve optimal relevance (R_{opt}), following the pattern presented in Figure 11. From an initial model version (Figure 11a), developers seek a reduction in output uncertainty by refining the description of model components and the inclusion of additional factors; e.g., increased complexity (Figure 11b). In the context of exploring adaptation strategies to climate change, the model is then coupled with other climatic, environmental, or socioeconomic models to create an integrated tool that allows the developer and users to answer some of the pertinent questions. Model coupling thus increases the relevance of the resulting model at the cost of increased complexity and possibly uncertainty (Figure 11c). At this stage, formal GSA/UA informs the developers about opportunities to simplify the model for components that at the scale of integration might no longer be important, or identify important components of the integrated system that require monitoring or experimentation to in turn lead to a better description and a reduction in output uncertainty (Figure 11d). Through user and developer interactions, this path is followed until an accepted model relevance is achieved for the purpose of the problem being studied ($R_{opt.}$) (Figure 11f). Although this is likely an open-ended process, endpoints are achieved through risk analysis, negotiation, and limitations introduced by available resources (e.g., time, model development cost, monitoring and experimentation cost).

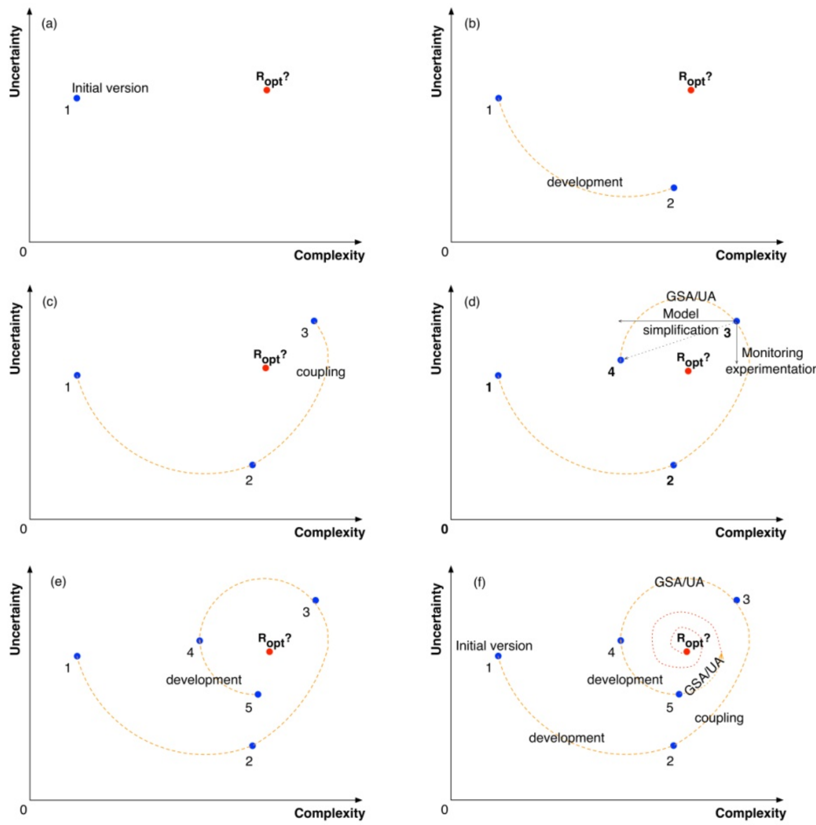

Figure 11. Model development framework to achieve optimal model relevance (R_{opt}) through exploration of sensitivity-uncertainty and -complexity tradeoffs.

One of the motivations for the NATO meeting resulting in this work was recognition of the rapid pace at which conversation has shifted from the question of climate change to the adaptation to climate change, and the "risk of putting the cart in front of the horse" on this issue. The same might be said of our modeling technology in support of these questions. We continue to rapidly increase the complexity of our models without always acknowledging, rarely studying, and not yet fully understanding the profound implications complexity has for the uncertainty associated with their results. In general, the concurrent and systematic evaluation of the global sensitivity and uncertainty of the model during the development process can help elucidate the general patterns introduced by the effects of increasing model complexity, and thus should become a central part of the integrated modeling practice.

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