Deliverable 3.1: WHITE PAPER – METHODS & MODELS FOR ASSESSING POLICY PERFORMANCE UNDER DEEP UNCERTAINTY

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Executive summary

This work presents the first systematic literature review and assessment of uncertainty quantification in Socio-Ecological System (SES) models for water resources management. We review whether and how SES modeling of water resources assess and quantify different sources of uncertainty, including input uncertainty, parameter uncertainty, structural uncertainty, and contextual uncertainty. We note that while most studies consider and to some extent quantify uncertainty (156 out of 198 studies in our sample), the depth and detail of this assessment is far from comprehensive and largely focuses on partial analyses of input uncertainties.

Next, we build on this review to design pathways towards more systematically integrating uncertainty into SES modeling of water resources. We make seven recommendations to mainstream uncertainty quantification into SES modeling of water resources, and potentially into decision-making processes informed by Decision Support Systems, so as to help decision makers identify robust policies with a satisfactory performance under most plausible futures. We also acknowledge the potential limitations of uncertainty quantification and propose strategies to account for them. Finally, we illustrate how a SES model of water resources that accounts for our seven recommendations may look like. We call for hydrologists, economists, agronomists, stakeholders, and other scientists with interest in SES modeling of water resources to join the discussion on how to quantify and assess modeling uncertainties, as well as how to better communicate them to decision makers so that future policies account for unfavorable contingencies and plan strategies to address them.

Contents

1. Introduction: socio-ecological modeling of water resources under deep uncertainty

Worldwide, decision makers and policy approaches for water resources management are increasingly "surprised and overwhelmed" by the systemic nature of water scarcity and climate change, which can trigger or aggravate other ecological (e.g., pests) and socioeconomic threats (e.g., commodity price fluctuations) via feedback loops and cascading impacts across systems that are difficult to foresee (UNDRR, 2021). In this context, planning for the future is characterized by a high degree of uncertainty, or deep uncertainty, a situation where scientists and stakeholders do not know or cannot agree on the external context of the system and its evolution, how systems work and interrelate, or how to value the desirability of alternative and potentially conflicting outcomes (Lempert et al., 2006).

Under deep uncertainty, conventional deterministic modeling based on a complete probabilistic description of future conditions to produce point predictions is no longer adequate, since it artificially reduces uncertainty and thus provides unrealistically precise information that can lead to maladaptation (UNEP, 2021). Reliance on consolidative modeling and point predictions is particularly dangerous where unanticipated nonlinear change emerges (disproportionality of modeling inputs and outputs), which can trigger tipping points with potentially catastrophic consequences (Kreibich et al., 2022). Instead, there is now a growing scientific (Adamson and Loch, 2021; Di Baldassarre et al., 2016; Lempert, 2019; Mustafa et al., 2020) and policy consensus (IPCC, 2021; UNDRR, 2021) that robust policies that deliver a satisfactory socioeconomic and environmental performance under deep uncertainty are needed. Designing and assessing such robust policies necessitates socio-ecological system (SES) models that go beyond conventional consolidative forecasting, and explicitly quantify and represent modeling uncertainty. This is because uncertainty representation and quantification enable decision makers to characterize system and cascading uncertainties across complex SES, and objectively assess performance of alternative policy interventions under alternative plausible futures.

Uncertainty in SES modeling has ontological (due to the inherent variability of the system) and epistemic components (due to the imperfect knowledge of the system; can be reduced) (Walker et al., 2003). Following the taxonomy by Marchau et al. (2019), we can distinguish the following sources of modeling uncertainty (see Figure 1): *Input uncertainty*, the uncertainty associated with data inputs and assumptions; *Parameter uncertainty*, the uncertainty associated with the data and methods used to calibrate the model constants, or parameters; *Structural uncertainty*, which emerges from an insufficient understanding of the system that is object of study; and *Contextual uncertainty,* the uncertainty associated with the boundary conditions of the socio-ecological systems (SES) to be modeled and the completeness of their representation.

Scientific research in SES and other disciplines has developed an expanding toolbox to quantify and represent the different sources of modeling uncertainty. Sensitivity analyses that measure how much each model input is contributing to output variability have been applied to quantify input uncertainty (Bankes, 1993; Lempert et al., 2013) and parameter uncertainties within models (Kwakkel and Pruyt, 2013; Saltelli et al., 2020). Multi-model ensemble forecasting that group multiple alternative models to represent a system have been used to quantify structural uncertainties through the ensemble spread, either within a single system (AgMIP, 2023; HEPEX, 2023) or across multiple systems (cascading uncertainties) (CMIP6, 2023; ISIMIP, 2023). Sensitivity analysis and multi-model ensemble forecasting can be combined in "grand ensemble" experiments that simultaneously quantify input, parameter, and structural uncertainties across systems (IPCC, 2021).

More recently, SES research such as Coupled Human and Natural Systems (CHANS) and socio-hydrology science have developed new modeling techniques that allow for the integration of human and natural components of water systems. These methods link models of multiple systems while accounting for feedbacks (two-way interactions between systems) and heterogeneity (variability in space and/or time) to expand the boundaries and better reproduce the interconnected cross-scale dynamics of complex SES, including nonlinear change that can help understand and anticipate tipping points (Gain et al., 2021). Research has demonstrated the potential to link coupled models of human-water systems with traditional sensitivity analysis and more advanced multi-objective optimization approaches to evaluate robust water management policies under deep uncertainty (Salazar et al., 2017; Schmitt et al., 2021; Gold et al., 2022; Smith et al., 2022; Basheer et al., 2023). However, the majority of the latter research has focused on robustness to future scenario uncertainty (e.g. climate change). In contrast, there remains significant knowledge gaps around how the design of coupled human-water-system models, including input data needs and the need for quantification of human-natural system coupling, and how uncertainties in these areas impact on modeling outcomes (Franzke et al., 2022).

Scientists have repeatedly deemed the integration of uncertainty assessments into SES models for water resources management "insufficient" (Di Baldassarre et al., 2016; Gain et al., 2021; Partida et al., 2023). This assertion has not been substantiated yet by a systematic literature review that assesses to what extent tools for uncertainty quantification are used in SES modeling of water resources, though. Our work aims to address this gap by: i) reviewing whether and how SES modeling of water resources assess and quantify uncertainty; and ii) exploring, building on this review, pathways towards more systematically integrating uncertainty into SES modeling of water resources. The paper is structured as follows: Section 2 maps the sources of modeling uncertainty along the uncertainty spectrum; Section 3 conducts a comprehensive and systematic literature review on the topic of SES modeling of water resources, including i) a detailed account of the methods used to develop the review (sources of information, keywords used, variables studied, types of uncertainty studied) and ii) a discussion of the results; Section 4 offers seven key recommendations to enhance uncertainty quantification in SES modeling of water resources and decision making; and Section 5 concludes.

2. Mapping modeling uncertainty

This section starts by providing a detailed definition of the sources of modeling uncertainty and the different levels of uncertainty along the uncertainty spectrum; and then locates the sources of modeling uncertainty along the uncertainty spectrum (see Figure 1).

Following the taxonomy by Marchau et al. (2019), we can distinguish the following **sources of modeling uncertainty**:

1) *Input uncertainty* is the uncertainty associated with data inputs and assumptions. It is divided in two sub-categories: i) uncertainty emerging from the external driving forces, or *forcings*, that have an influence on the system model, and the magnitude of these forces; and ii) uncertainty on the data inputs that describe the baseline situation and quantify relevant features of the relevant system (e.g., water use data, land use data, economic data).
2) *Parameter uncertainty* is the uncertainty associated with the data and methods used to calibrate the model constants, or parameters. Parameters can be universal constants (such as the mathematical constant π) or well determined by previous investigations (such as the acceleration of gravity), in which case uncertainties are limited and/or controlled. In other cases, though, parameters can be discretionarily fixed to a certain value *a priori*; or calibrated by comparing model outcomes to observed values in historical data series (typically by minimizing the difference). Examples of calibrated parameters are those used to model movement of water through and over the land surface; while examples of *a priori* chosen parameters are those used to model the number of interactions among agents in agent-based models. *A priori* chosen parameters and calibrated parameters are associated with uncertainty that should be assessed and, where possible, quantified.
3) *Structural uncertainty* emerges from an insufficient understanding of the system that is object of study. Structural uncertainty involves uncertainty associated with "the relationships between inputs and variables, among variables, and between variables and output, and pertains to the system boundary, functional forms, definitions of variables and parameters, equations, assumptions and mathematical algorithms" (Walker et al., 2003). Structural uncertainty can compound with technical uncertainty, i.e., the uncertainty generated by software or hardware errors (e.g., typing errors in model coding).
4) *Contextual uncertainty* is the uncertainty associated with the boundary conditions of the socio-ecological systems (SES) to be modeled and the completeness of their representation. In the stand-alone water management models typically used by decision makers to inform policy choices, the contextual uncertainty includes the uncertainty on the external economic, political, social, and technological situation that will have an impact on the water system being examined. Accordingly, deciding on the context framing is a significant part of model design that can result in non-trivial uncertainties.

When collecting and reporting information on whether and how the sources of modeling uncertainty are quantified, the distinction between structural uncertainty and contextual uncertainty is often challenging. This is because system models typically represent a set of key process(es) relevant for that system, but also leave outside other potentially relevant process(es), thus contributing both to contextual and structural uncertainty. In this context, determining how a system model contributes to structural and contextual uncertainty requires a comprehensive and case-by-case analysis to determine what the relevant processes are, and whether they are explicitly modeled or not, which i) necessitates time and other resources that transcend those available for our review and ii) would add subjectivity and potentially biases to our analysis (what are the relevant processes and who decides that?).

A more pragmatic approach is to define structural uncertainty as the uncertainty within each individual system model, and contextual uncertainty as the uncertainty that emerges from cross-scale dynamics and the design of model interconnection protocols (Gain et al., 2021). We adopt this pragmatic definition of contextual uncertainty in this paper. Accordingly, we assess structural uncertainty by looking at issues of "system boundary, functional forms, definitions of variables and parameters, equations, assumptions and mathematical algorithms" (Walker et al., 2003); and contextual uncertainty through those variables referred to the *interconnection* of SES or model coupling (simulation v. optimization, deterministic v. stochastic, dynamic v. static, holistic v. modular, and sequential v. bidirectional interconnections). We consider that a study is quantifying contextual uncertainty where it explores alternative coupling setups instead of opting for a single setup (e.g., testing dynamic and static coupling setups rather than adopting one of the two).

Uncertainty spectrum. Complete determinism (a situation where we know everything precisely) and total ignorance (we do not know that we do not know) act as a limiting characteristic at both ends of the spectrum. Uncertainty levels 1-4 are those relevant for modeling.

Level 1 uncertainty (deterministic uncertainty) describes a situation where the future is clear enough to be correctly modeled and it is possible to obtain a certain estimation of the outcome. There is no absolute certainty, but there is no need or knowledge available to measure uncertainty in any way. The system is assumed to be well known and defined, and decision-makers can confidently rely on consolidative modeling and point predictions to choose one strategy to reach a clear objective. This is the case of some natural phenomena, such as the force of gravity.

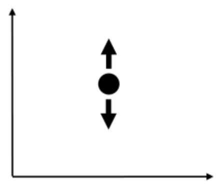
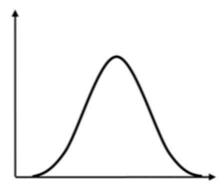
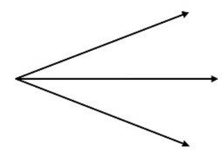
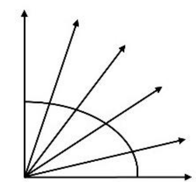
In Level 2 uncertainty (statistical uncertainty) statistics can describe adequately the extent of uncertainty. In this case, it is possible to precisely calculate the probability of every aspect of the problem, from the model to the outcome (Walker et al., 2003). Sampling error, inaccuracy, or imprecision in data measurement is typically associated to level 2 uncertainty. This uncertainty is usually reduced leveraging on the advancement of knowledge to update probabilities using the Bayes' theorem. Thus, the tools of statistics can be used to obtain the associated probabilities to each plausible future and obtain a point prediction via consolidative modeling.

Level 3 uncertainty (scenario uncertainty) describes a situation in which there is a range of plausible futures ("scenarios"), but it is not known, or it is not clear, how the futures were reached and accordingly, it is not possible to assign a probability. We can anticipate how the system can react to some possible inputs, but how, when, and the intensity at which these plausible futures will manifest remains unknown. Scenario uncertainty is typically associated with input uncertainty and can be represented and quantified by simulating the impacts of alternative inputs on each plausible future through sensitivity analysis methods—e.g., exploratory analysis (Bankes, 1993; Kwakkel and Pruyt, 2013).

In Level 4 uncertainty (systemic uncertainty) there is a lack of knowledge or data about the mechanism or functional relationships being studied. Scientists struggle to specify the appropriate models to describe interactions among the system's variables, and cannot attribute probabilities to the model (e.g., parameters) or outcomes. In Level 4 uncertainty, input uncertainty is amplified with parameter, structural and contextual uncertainty. These sources of modeling uncertainty can be represented and quantified through sensitivity analysis (input and parameter uncertainty) (Saltelli et al., 2020), multi-model ensemble modeling (structural uncertainty) (CMIP6, 2023; ISIMIP, 2023), and better/alternative representations of the interconnected cross-scale dynamics of complex SES (contextual uncertainty) (Sivapalan et al., 2012).

An additional level of uncertainty (level 5) is sometimes considered, involving an unknown future with an unknown system model and unknown modeling outcomes. Level 5 uncertainty (unknown future) cannot be represented or quantified via modeling, and therefore is not relevant for the purposes of this work. Under Level 5 uncertainty, "we only know that we do not know", and future events are unpredictable through modeling or other tools (Marchau et al., 2019). These unpredictable events, which can be catastrophic and extreme (black swans), are mostly approached by building adaptive efficiency so that if incumbent adaptive responses prove wrong people and institutions can transition to alternative responses at low transaction costs (Garrick et al., 2013; North, 1994).

Figure 1: Location of the sources of modeling uncertainty along the uncertainty spectrum. Complete determinism (a situation where we know everything precisely) and total ignorance (we do not know that we do not know) act as a limiting characteristic at both ends of the spectrum. The four intermediate levels of uncertainty (level 1-4) are those relevant for modeling. Level 5 uncertainty cannot be modeled and therefore is not relevant for the purposes of this work. Source: adapted from Marchau et al. (2019) and Walker et al. (2003).

			Risk	*Uncertainty*			
	Complete determinism	*Level 1: Determinism*	*Level 2: Statistical uncertainty*	*Level 3: Scenario uncertainty*	*Level 4: Systemic Uncertainty*	Level 5: Unknown future	*Total ignorance*
Context		Clear future 	Alternative futures (with probabilities) 	A few plausible futures 	Many plausible futures 		
System model		A single deterministic system model (consolidative model)	A single stochastic system model (consolidative model)	A few alternative system models	Many alternative system(s) models		
Model outcomes		A point/single prediction	A point prediction, sometimes with a confidence interval	A limited range of plausible futures	A wide range of plausible futures		
Relevant source of modeling uncertainty		NA	(Probabilistic risk)	Input uncertainty	-Input uncertainty -Parameter uncertainty -Structural uncertainty -Contextual uncertainty		
Relevant tools for quantifying uncertainty		NA	(Bayesian inference: update the probability of a future as more evidence or information is made available)	Sensitivity analysis (inputs)	-Sensitivity analysis (inputs and parameters) -Ensemble forecasting -CHANS, socio-hydrology, other SES modeling		

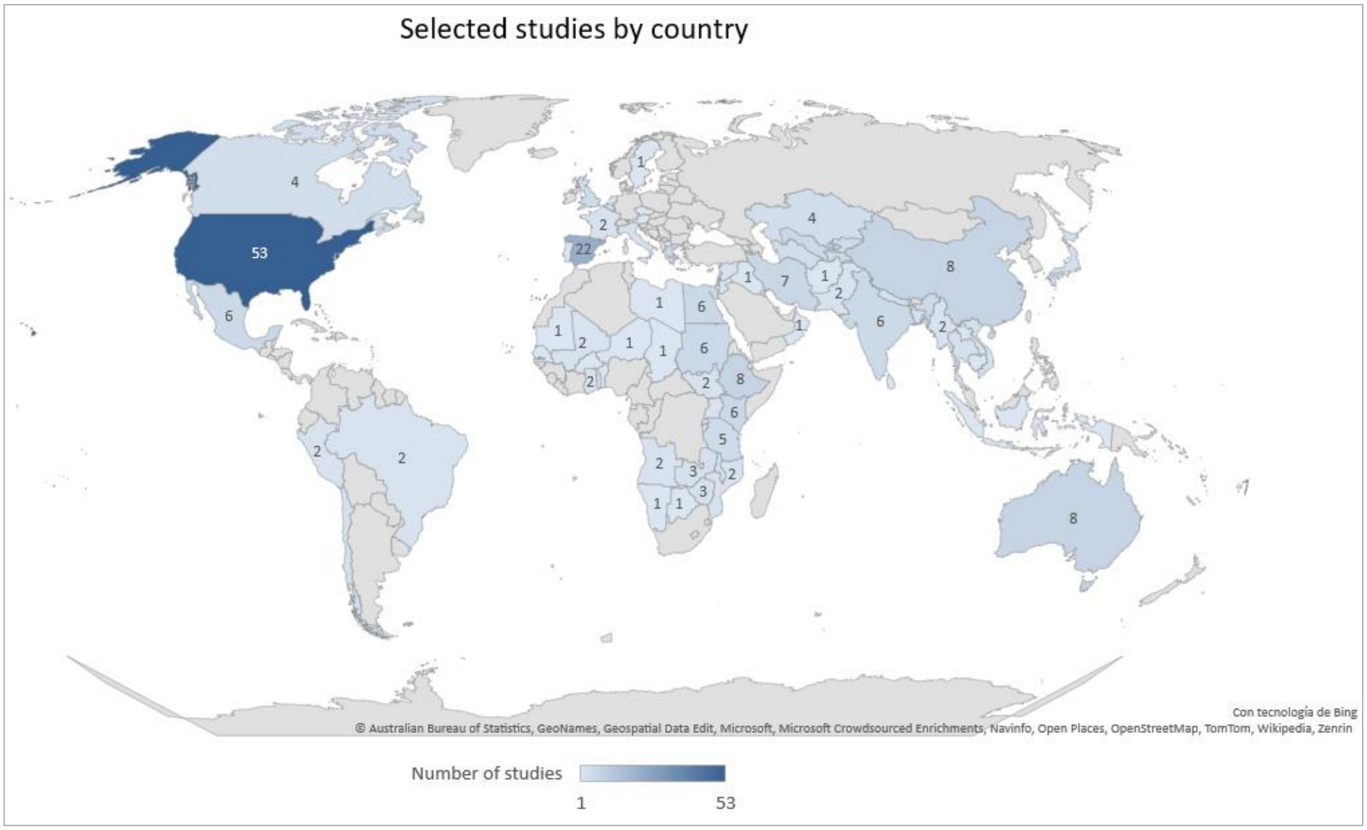
3. Literature review

3.1. Methods

We conducted a comprehensive and systematic literature review on the topic of SES modeling of water resources, identified relevant studies, and assessed the methods used to quantify uncertainty in each relevant study. We searched for relevant scientific papers in Web of Science (WoS) and SCOPUS for the period 1970-2023. The search was implemented by looking for the following terms in the abstract and/or title: "hydro-economic" OR "water-human" OR "human-water" OR "socio-hydrology" OR "Socio-Ecological" AND "model*". This search was complemented with a review of relevant grey literature (technical reports and white papers) in Google Scholar and major repositories on modeling uncertainty research, most notably the RAND repository (https://www.rand.org/), which includes journal articles, reports, books, and research briefs.

2160 papers were identified through this search. This sample of papers was processed further to select those studies that model both human (agent-based, microeconomic, and macroeconomic models of human behavior) *and* water systems (hydrologic and hydrogeologic models, water management models or Decision Support Systems - DSS) quantitatively (i.e., qualitative approaches were excluded) and explicitly (e.g., models that force models of water systems with scenarios of human systems, without using any explicit model for the latter, were excluded). Papers that modeled other systems (e.g., climate system) were also included, provided human and water systems were explicitly modeled as well. This filtering process was applied first by reading the title and abstract; and when this information was insufficient to determine the relevance of the article, by reading the full article. Applying these filters to our original search yielded 198 studies. It should be noted that the depth and detail of the human and water system models used in the sample ranges widely, from piecewise equations that simplify complex systems to full-fledged modeling representations of the system. Most of these studies focus on the US (53 studies), Europe (45 studies) and Australia (8 studies), while the other 92 studies are implemented mainly around Middle East, South America, China and Northwest Africa (see Figure 2). A detailed description of these 198 studies is available in Annex I.

Figure 2: Selected studies by country



For each of the 198 studies in the sample, we provide information on the following variables: author, title, year of publication, location (country and basin/study site), type of water resources assessed (groundwater, surface, other), scale (basin – catchment and sub-basin included, region, district, aquifer, reservoir, state and continent), shock/policy (water allocation, reservoir optimization, aquifer optimization, pricing, water restrictions, flood mitigation policies, dam construction, human response to climate impacts), systems modeled (climate, water, human, agronomic, other), human-water system modeling overview, water system model description, scale of water system model, human system model description, assessment of nonlinearities in human system model (linear v. nonlinear), model coupling (simulation v. optimization, deterministic v. stochastic, dynamic v. static, holistic v. modular, and sequential v. bidirectional), input modeling uncertainty, parameter modeling uncertainty, and structural modeling uncertainty. All this information is available in Annex I.

3.2. Results

Building on our sample of 198 studies, this section discusses the depth and detail in the quantification of modeling uncertainties (input uncertainties, parameter uncertainty, structural uncertainty, and contextual uncertainty) in SES representations of water resources (see Table 1).

Table 1: Summary statistics informing how many studies consider each source of uncertainty

	Input uncertainty	Parameter uncertainty	Structural uncertainty	Contextual uncertainty
Number of studies	156	37	7	0
% of overall sample	78.8	18.7	3.5	0

A first important aspect emerging from our review is that the integration of human and water system models is implemented in 137 out of the 198 studies in the sample through holistic approaches where all systems and processes are coupled in a single model. In the remaining 61 studies, the integration of human and water systems is implemented through modular approaches where water and human systems are developed and run in separate models. Holistic models provide a more effective representation of the causal relationships and feedbacks across systems and reduce computational costs, but increase the complexity of the model, which demands simplifications to be solved (Harou et al., 2009). This is typically done through piecewise equations that simplify the representation of complex systems, so that they can be integrated with other systems into a holistic model that can be solved at once. Due to the "predominance of hydrology" in SES models of water resources (Gober et al., 2017), piecewise equations have been typically adopted to simplify the representation of complex human systems, and thus facilitate their integration into full-fledged hydrological models. For example, irrigation water demands are usually represented in of water resources SES models using piecewise linear or quadratic equations relating water application to economic benefits, which are exogenously generated (Konar et al., 2019). In our review, 97 out of 198 studies in the sample use piecewise equations to represent human systems, while this figure falls to 64 in the case of water systems (see Table 2). It should be noted that hydrology is often very simplified as well: historical or synthetic inflow time series are often adopted as inputs to water management models, without any full hydrological model.

Table 2: Summary statistics informing how many holistic and modular studies consider each source of uncertainty.

	Input uncertainty	Parameter uncertainty	Structural uncertainty	Contextual uncertainty
Holistic models	52%	15.7%	0.5%	0%
Modular models	26.8%	3%	3%	0%

Structural uncertainties. The predominance of piecewise-based holistic approaches has relevant implications for modeling uncertainty, since simplified representations of human and/or water systems tend to amplify structural uncertainties within models (Pindyck, 2017). Moreover, since most of the piecewise representations of human systems are linear (43 out of 97), models cannot anticipate changes in the output that are disproportionate to changes in the input (i.e., nonlinear), which can tell us little about the impacts of "unfavorable surprises" or "tail events", i.e., catastrophic events with a potentially very large impact on key variables of the model (Franzke et al., 2022).

Despite the nontrivial simplifications introduced to water and particularly human system models in holistic studies, only 7 studies in the overall sample of 198 studies (i.e., 3.5%) explore structural uncertainties through multi-model ensemble experiments. Moreover, 6 of these 7 studies are modular. This suggests that mainstream holistic models are ignoring potentially significant biases emerging from model simplification. This would be reasonable if we assumed that the resultant simplified models can accurately represent real-life responses—but evidence has repeatedly shown this is not the case, proving once and again that some of these simplifications, particularly those performed in human systems, are not only inaccurate but also "misleading" (Grafton et al., 2018). Failure to recognize structural uncertainty in model development has led some authors to argue that holistic models "have crucial flaws", and "can create a perception of knowledge and precision that is illusory" (Pindyck, 2017).

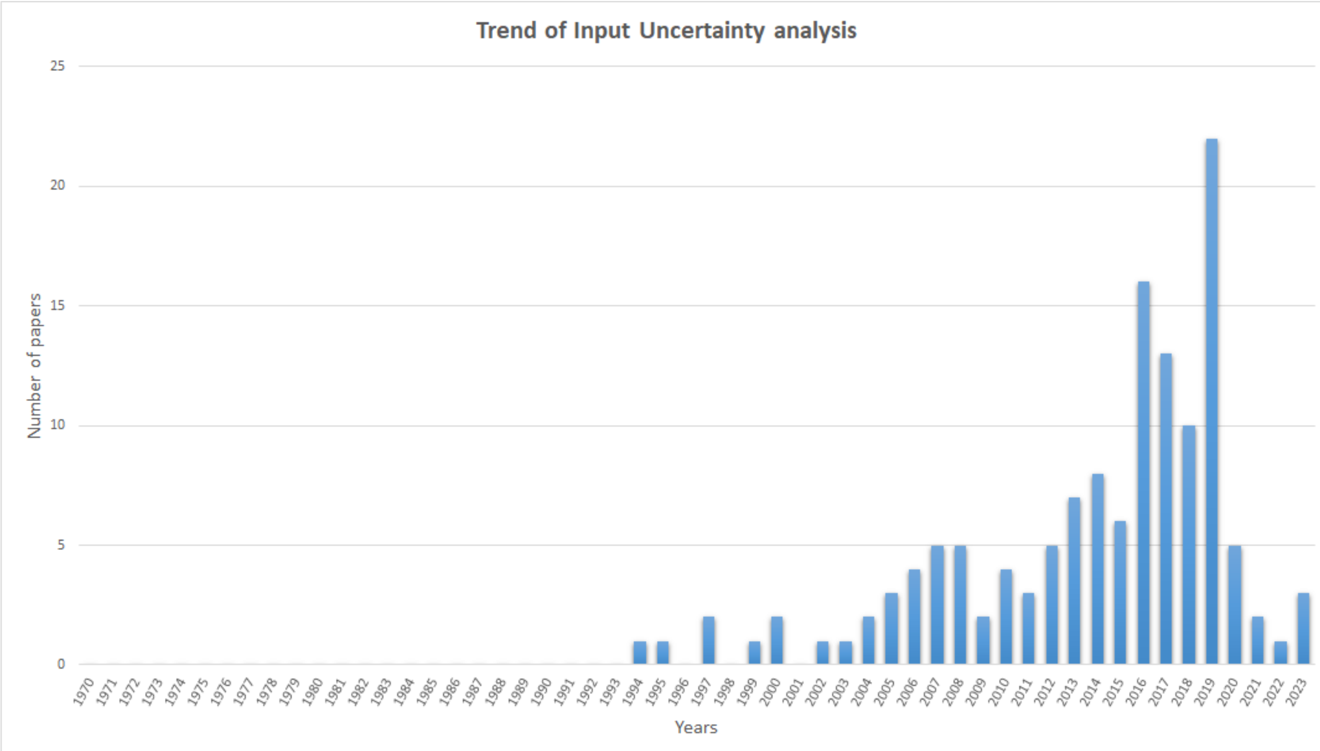
Moreover, it should be noted that the 7 studies that quantify structural uncertainty run multi-model ensemble experiments either on human *or* water systems. To the best of our knowledge, not a single comprehensive multi-model ensemble experiment across human *and* water systems is available in the literature yet. This gap is largely attributable to human systems modeling: while multi-model ensemble experiments have become a fundamental tool to quantify structural uncertainty in ecological (including water) systems research (HEPEX, 2023; ISIMIP, 2023), they are virtually nonexistent in human systems research—which paradoxically are those systems where piecewise equations and other simplifications are more frequently implemented.

Finally, 51 of the 198 studies in the sample employed DSS models that are known to be widely used by decision makers in river basins or other relevant authorities in different regions around the world (including WEAP, MIKE, RIBASIM, LISFLOOD, AQUATOOL, or TOPKAPI). Of these 51 studies, 34 accounted for input uncertainty (87.2%), 2 for parameter uncertainty (5.1%) and 3 for structural uncertainty (7.7%).

Parameter uncertainties are quantified more frequently than structural uncertainties, although their relevance is still limited: 37 out of the 198 studies in the sample conduct some type of sensitivity analysis on the model parameters. Noteworthy, while 41.4% of the studies in the sample of 198 studies are in developing regions, 20 of the 37 studies that quantify parameter uncertainties (54.1%) are implemented in these regions. The relatively higher frequency of sensitivity analyses in developing regions suggests researchers are more prone to quantify parameter uncertainties where data limitations and gaps are more severe, since this can lead to nontrivial calibration errors. In some of these cases, data limitations and gaps may constrain researchers to discretionarily set the value of a parameter, which can further amplify the error. Sensitivity analyses are typically conducted by assigning probability distributions to certain key parameters and then running Monte Carlo simulations. They are more commonly implemented in hydrogeological studies (5 out of 24 studies, 20.8%) than in studies where surface water is the only source (17 out of 82 studies, 20.7%); although this gap is smaller than anticipated by the authors, given that sensitivity analyses are significantly more common in hydrogeology than hydrology studies due to the relevant and largely unexplored heterogeneity of subsurface environments, which results in a discrepancy between the scale and amount of data necessary to accurately calibrate aquifer model parameters and the more limited scale of measurement typically available as a result of resource constraints (Allen and Nott, 2021).

Input uncertainties are the most quantified source of modeling uncertainty in our review, with 156 out of 198 studies conducting some type of sensitivity analysis of model inputs. Most sensitivity analyses assess the impact of a range of plausible forcings, notably by running multiple simulations considering relevant ecological inputs (e.g., climate change futures with alternative greenhouse gas concentrations), and less occasionally socioeconomic inputs (e.g., water prices) (Gorissen et al., 2015; Prudhomme et al., 2010). Some of these sensitivity analyses introduce “policy levers” that dynamically represent input uncertainties through alternative pathways of forcings, building on the Real Options Analysis (Steinschneider and Brown, 2012) and Dynamic Adaptive Policy Pathways methods (Haasnoot et al., 2013). Computational experiments have been also used to systematically explore the input uncertainties emerging from alternative data (e.g., water use data) and forcings, sometimes in combination with parameter uncertainties. For example, info-gap decision theory, which applies sensitivity analysis of the stability radius type to perturbations in the value of a given parameter/input (Korteling et al., 2013); decision scaling, which aims at identifying the inputs/parameters that are most significant to avoid system (catastrophic) failure (Taner et al., 2017); Exploratory Modeling and Analysis (EMA), which uses computational models as generators of plausible futures (Kwakkel and Pruyt, 2013); and multi-objective search methods which link AI-based algorithms to coupled human-water models to identify policy options that perform well across an uncertain range of plausible futures, parameter sets, and/or model setups (Borgomeo et al., 2018; Herman et al., 2020). EMA can be also adopted to systematically explore other sources of uncertainty, including structural and contextual uncertainties, and are a good candidate to develop comprehensive analyses of modeling uncertainty—although thus far their application to quantify these two types of modeling uncertainties has been limited in SES of water resources.

Figure 3. Trend of input uncertainty's analysis over time.



Contextual uncertainties are assessed in our review by looking at the relevant cross-scale aspects that emerge in the interconnection of SES, for which we gather information on the following model coupling setup variables: simulation v. optimization, deterministic v. stochastic, dynamic v. static, holistic v. modular, and sequential v. bidirectional. Cross-scale aspects in SES refer to the feedbacks and interactions between human and water systems, both across time and space, which can be altered by the way the coupling is designed (Gain et al., 2021). Notably, hydrological and SES models of water resources have traditionally focused on the study of systems dynamics over time, while ignoring important socioeconomic dynamics emerging across space, such as social processes driving price formation in markets and the resultant adaptive responses (Konar et al., 2019). When these social processes are represented and integrated into SES models, new adaptive responses may emerge. For example, water scarcity may reduce water availability and yields locally, increase agricultural commodity prices in regional and international markets, and create incentives for illegal water use locally—an effect that can only be anticipated using a bidirectional coupling setup that accounts for spatial heterogeneity in human systems (Castilla-Rho et al., 2017). In another example, a coupling setup that looks for convergence via optimization will yield different results than a setup that adopts a simulation approach (for an illustration of the differences between an optimization v. simulation coupling setup of a model, see e.g., Parrado et al., 2019 v. Pérez-Blanco and Standardi, 2019). We consider that a study is quantifying contextual uncertainty where it explores the consequences of alternative coupling setups (e.g., testing dynamic and static coupling setups rather than adopting one of the two). This can be contrasted with the alternative (and more conventional approach) of consolidating previous knowledge into a single coupling setup. Critically, *all* the studies in our review opt for a single model coupling setup, instead of exploring alternative setups, thus ignoring contextual uncertainties emerging from the choice of the coupling framework.

4. The way forward

Building on the outcomes of our review in Section 3 and recent scientific advances in SES research identified in sections 1 and 2, we propose below seven ways forward to improve uncertainty quantification in SES models of water resources, and thus better inform the adoption of robust policies that deliver a satisfactory socioeconomic and environmental performance under deep uncertainty.

1. Multi-model ensemble experiments should be more systematically adopted to quantify structural and parameter uncertainties. Social and natural sciences have been successful at developing scientifically sound conceptual models capable of representing the essence of critical systems within the human-water SES conundrum. These include microeconomic models to represent the behavior of individuals or firms (Graveline, 2016), Agent Based Models to study spatial interactions of people (Shahri et al., 2022), macroeconomic models to study interrelations among sectors and regions of the economy and their impact on aggregated indicators (Hertel and Liu, 2016), and hydrologic models to study the movement, distribution, and quality of water at different scales (Blair and Buytaert, 2016), among other modeling families. There is consensus in the literature that the combination of scientifically sound prediction methods in perturbed physics and multi-model ensemble experiments (i.e. grouping multiple models and exploring alternative values for critical parameters) can be used to sample parameter and structural uncertainties through the ensemble spread (Athey et al., 2019). This approach has been already used in disciplines such as climate sciences (IPCC, 2014) and hydrology (Cloke et al., 2013), also in combination with initial condition ensembles that explore input uncertainties (Tebaldi and Knutti, 2007). Recent research has combined ensembles of multiple ecological systems sequentially, notably ISIMIP (2022), although the adoption of multi-system ensembles is still very limited as shown by our review. Moreover, the ensemble community still struggles to integrate models of human behavior and responses into these ensemble experiments.

2. Structural and parameter uncertainties in human systems, and the subsequent cascading uncertainties across SES, must be quantified. Existing SES ensemble experiments typically incorporate uncertainties in human systems through sensitivity analysis, notably by forcing ecological models with Shared Socioeconomic Pathways (SSPs) that project the impacts of global socioeconomic changes on ecological systems over time. However, this approach fails to capture human agency and the non-linear adaptive responses by individuals, which are critical to understand and evaluate the feedbacks inherent to coupled human and natural systems and their evolving trajectories, and associated uncertainties. One such feedback phenomena has been introduced as "fixes that backfire", namely the reduction in expected gains from adaptation policies due to behavioral responses, illustrated by floodplain protection (where better protection infrastructures lead to higher exposure of human activities and potentially higher losses) and irrigation modernization paradoxes (where adoption of more technically efficient technologies increases the marginal return of water to farmers, thus increasing rather than decreasing water depletion) (Di Baldassarre et al., 2013; Grafton et al., 2018). In this context, making robust decisions compatible with sustainable and equitable development requires ensemble experiments that are also "people-centric" (UNDRR, 2019), i.e. capable of informing not only the impacts of climate change and other threats on the natural system and the environment, but also their non-linear and often paradoxical reverberations on society and the economy—and vice versa. In this regard, there is a need to explore existing and develop new understanding of human decision-making around water use and responses to water scarcity, which to date have been understudied relative to the physical processes of water movement and storage in the water cycle. This will necessitate increased focus on the collection and analysis of data on human water use and impacts of scarcity, leveraging new technologies for monitoring and data collection (e.g., remote sensing, smart meters, citizen science, etc) and collaborations across social and natural sciences. Alternate 'models' of human water use behavior can also be embedded **within** the modular hierarchy of ecological systems adopted in conventional ensemble experiments such as HEPEX (2023) or ISIMIP (2023) with socioeconomic systems that represent key aspects of human agency and behavior, including the (admittedly still limited) human system ensemble experiments available in the literature (see e.g., Sapino et al., 2020).

3. Contextual uncertainties must be also quantified. Just like ensemble experiments have demonstrated the importance of quantifying modeling uncertainties to formulate robust solutions, recent advances in SES research have demonstrated the importance of accounting for the cross-scale dynamics between human and water systems when seeking to design solutions to complex environmental challenges (Pande and Sivapalan, 2017). Most recently, these two strands of literature have converged into pioneering ensemble experiments that characterize the cascading uncertainties across complex and interconnected SES through two-way feedback protocols. For example, Sapino et al. (2023) interconnect the water management model AQUATOOL with an ensemble of mathematical programming microeconomic models using a recursive modular approach that exchanges information on land use and water withdrawals (from the microeconomic models to AQUATOOL) and water availability constraint (from AQUATOOL to the microeconomic models); while Blanco et al. (2017) force the crop growth model WOFOST using inputs from three General Circulation Models (HADGEM2, IPSL and MIROC) to assess the biophysical consequences of climate change, which are subsequently fed into an integrated recursive economic model to simulate the economic consequences of climate change. These works quantify structural uncertainties while accounting for cross-scale dynamics of SES, but *do not quantify contextual* uncertainties (i.e., uncertainties arising from the discretionary choice of the coupling setup).

We argue that exploring the impact and related uncertainties of alternative coupling setups may be just as relevant as exploring those of alternative model structures, given the relevant impact that the choice of the coupling setup may have on modeling outcomes, as highlighted by the literature on SES models of water resources (Konar et al., 2019; Sivapalan and Blöschl, 2015).

4. Input uncertainties must be more thoroughly assessed and model assumptions systematically revised. Our literature review has revealed that most assessments of input uncertainties available are cast in the same mold and quantify the impact of a range of plausible ecological forcings, notably climate change forcings. We argue that since models are often imported from other locations and applications, their assumptions need to be thoroughly revised with each new location and/or application, including by exploring alternative ecological (climate change and others) as well as socioeconomic forcings and/or data inputs. For example, price volatility of agricultural commodities, which is for the most part irrelevant in determining water and land use in urban catchments, is a critical explanatory variable in agricultural catchments. Moreover, some key model inputs may require values for which there are not reliable estimates. For example, data needed to characterize agricultural water use – the main consumptive use of water in most river basins – is often at best incomplete and at worst entirely absent. Similarly, unexpected events and scenarios by their nature will often be poorly captured, for example the emergence and impacts of a hypothetical conflict that constraints trade (e.g., the Russo-Ukrainian War) cannot be reliably forecasted and may have significant repercussions depending on the inputs/assumptions. Addressing these issues calls for sensitivity analyses that explore alternative forcings and baseline situations (Saltelli et al., 2020). Such analyses can reveal larger uncertainty bounds than initially anticipated, including potential nonlinearities. For example, Puy et al. (2022) show that global water withdrawal estimates can vary fivefold when comparing the results obtained with consolidative applications that use average values of key inputs and parameters values. those obtained with applications that quantify input and parameter uncertainties.

5. Focus on actionable tools to mainstream uncertainty quantification into decision making. A key goal of SES models of water resources is to produce instruments and outputs that can help society navigate the challenges posed by environmental and socioeconomic change. To achieve this objective, scientific research and modeling needs to be actionable, i.e., capable of producing instruments and outputs that can be readily used by decision makers to inform robust strategies (Gil-García et al., 2023). However, as shown by our review, extant SES models of water resources are often disconnected from the DSS adopted by decision makers, which are typically discarded by scientists in favor of more sophisticated approaches. These sophisticated scientific models often disregard key aspects of decision-making processes (e.g., *ad-hoc* algorithms for water allocation perfectioned over time through trial and error) and require the development of new technical skills or capacity amongst decision-making organizations that already face substantial financial, technical, and logistical challenges. This focus on innovation in modeling therefore can face significant barrier when it comes to translating novel science into the adoption by decision makers and other stakeholders (Pérez-Blanco et al., 2021). Producing actionable science that informs robust decisions requires that scientists find ways to mainstream uncertainty quantification and analysis into decision making processes and tools. One way to do that is by integrating cutting edge models and uncertainty assessments into the DSS tools used by stakeholders for water resources planning, such as WEAP, MIKE, RIBASIM, LISFLOOD, AQUATOOL, or TOPKAPI. Linking these DSS with recent advances in socio-ecological science and uncertainty quantification has the potential to deliver a step change in the ability of planners to evaluate the co-evolution of complex SES and related uncertainties, and to identify robust strategies. Accordingly, major national and international players such as the EU are putting efforts into bridging this gap through Horizon research projects such as TRANSCEND or TALANOA-WATER.

6. Balanced stakeholder engagement is critical to thoroughly quantify uncertainty. Stakeholders are the final user of the information provided by models, and their involvement is necessary to make sure all relevant aspects to modeling are considered, including those related to uncertainty. Several stakeholder engagement approaches such as Robust Decision Making (Lempert, 2019), co-creation (Prahalad and Ramaswamy, 2004), or knowledge networks (Eikebrokk et al., 2021) can be adopted to combine heuristic methods (through expert judgement) with mechanistic modeling approaches, identify sensitive aspects, and quantify related uncertainties. In doing so, a critical yet often ignored aspect is to ensure that model predictions do not become "adjuncts to a political cause" (Saltelli et al., 2020). This requires balanced stakeholder engagement and clearly defined science-policy engagement rules, where scientists must be transparent about the assumptions made and related uncertainties, thus constraining stakeholders and particularly decision makers to be accountable of their choices rather than offloading their responsibility to a given model.

7. Balance complexity and usefulness to keep the model relevant. There is a tradeoff between the complexity of a model and its usefulness. As models add new systems and processes, uncertainty is amplified, and boundedly rational individuals may not be capable of processing all sources of uncertainty simultaneously to identify robust decisions. Moreover, at some point forecasting errors and uncertainties can be so wide that forecasts can become nearly useless (Saltelli et al., 2020). Modelers and the stakeholders involved in model development need to be aware that higher complexity does not necessarily indicate better quantification of uncertainties. Particularly in the case of holistic models, the integration of one additional system may come at the expense of reducing detail in some other system that is more relevant in the representation of SES. For example, while macroeconomic modeling of price volatility may be necessary to assess land and water reallocations in basins with a significant share of key agricultural commodities, this system is redundant in urban catchments, and integrating it into a preexisting holistic model will often necessitate to sacrifice detail in other relevant systems.

Admittedly, in some cases the SES under study may be extremely complex with multiple relevant interconnected systems, and demand modelers to account for multiple inputs, structures, parameters and contexts, and their related uncertainties. For example, there is now a growing need to develop SES that represent the impacts of macroeconomic shocks (e.g., Russo-Ukrainian War, mobility restrictions due to COVID-19) on the responses of human agents and water resources locally, and vice versa, as shown by recent research calls. In this context, and particularly where stakeholders are involved, it is important to develop strategies that foster the understanding of complex scientific modeling via experimental learning (Solinska-Nowak et al., 2018). Experimental learning such as serious games and scenathons have been successfully tested as means to 1) deliver scientific knowledge and provide familiarity with complex SES and uncertainty modeling; 2) detect challenges and opportunities in managing human-water SES and identify robust policies under deep uncertainty; and 3) achieve science-based consensus towards the adoption of robust policies that generate collective added value (FABLE, 2020). A comprehensive taxonomy of experimental learning approaches and tools that can be used to support decision making under deep uncertainty, which includes policy architecture, generation of policy alternatives, generation of scenarios, robustness metrics and vulnerability analysis, is provided by Kwakkel and Haasnoot (2019).

A SES modeling chain proposal. Addressing the 7 recommendations above is challenging, but now feasible given recent scientific advances in SES modeling. Particularly promising in this regard are the modular approaches that have been adopted to quantify input, parameter and structural uncertainties, and could potentially be adopted to quantify contextual uncertainties (see e.g., CMIP6, 2023; ISIMIP, 2023). In the area of SES models of water resources, the TRANSCEND Project is set to replicate this approach to the case of human-water systems. To this end, TRANSCEND adopts a modular approach that captures cross-scale spatial and temporal dynamics across systems using alternative coupling setups to interconnect socioeconomic and ecological systems (*contextual uncertainty*). Each system/module is populated with multiple models (*structural uncertainty*), and for each model a sensitivity analysis on the calibrated parameters is performed (*parameter uncertainty*). The resultant multi-system and multi-model SES is used to study the impacts of multiple climatic and socioeconomic forcings including alternative transformational adaptation policies (*input uncertainty*). TRANSCEND SES modeling framework is being tested in 7 laboratories in Europe, SE Asia, South America and Middle East, and includes models of climatic (CMIP6 and downscaled projections in CORDEX), hydrologic (i.a. SUMMA, VIC, HBV, GR4J), agricultural (i.a. AquaCrop-OS, DSSAT, APSIM, WOFOST), microeconomic (econometric and mathematical programming models such as Positive Mathematical Programming, Linear Programming and Multi-Attribute Utility Programming), and/or macroeconomic systems (input-output and computable general equilibrium models, e.g. ICES); as well as other models (see e.g. CMIP6, ISIMIP) and systems deemed relevant by scientists and stakeholders. Moreover, the modeling framework is being integrated into the architectures of the DSS WEAP, AQUATOOL, and TOPKAPI, leveraging on co-creation approach to co-design policies (policy architecture, generation of policy alternatives) and scenarios (generation of scenarios), co-evaluate results (vulnerability analysis) and co-identify robust policies using collectively agreed robustness metrics—all of which supported by continuous monitoring.

5. Conclusions

Our review shows that conventional SES models of water resources rely on a combination of Bayesian inference and consolidative models. Bayesian inference uses observations to estimate event probabilities, which are recurrently updated as new futures are revealed, while consolidative models feed future states and related probabilities into a mathematical representation of the system, and generate point predictions for the identification of optimal actions. When probabilities are well defined and the model seems to reliably relate actions to consequences, the search for optimality is considered as warranted. However, in non-mechanistic coupled human-water SES, where researchers "do not know or cannot agree on the model that relates actions to consequences and/or the future states and probability distributions that feed the model" (Lempert and Groves, 2010), modeling uncertainty is likely to manifest through input, parameter, structural or contextual uncertainties. This calls for models that explicitly and thoroughly quantify model uncertainty.

The literature on SES models of water resources reports significant advances in the quantification of input uncertainties, which are acknowledged but often not quantified (156 out of 198 studies). Albeit the depth and detail of this assessment is far from being comprehensive, studies typically focus on a limited set of forcings rather than comprehensively testing input uncertainties, including those emerging from data inputs. Parameter uncertainties are assessed in a small yet relevant subset of 37 studies (18.7%), often using thorough quantification methods that combine probabilistic approaches and Monte Carlo simulations. On the other hand, structural uncertainties are rarely (7 studies) and only partially quantified, while contextual uncertainties are ignored altogether.

Based on this study, we make seven recommendations to mainstream uncertainty quantification into SES modeling of water resources, and potentially into decision-making processes informed by DSS so as to allow decision makers to identify robust policies with a satisfactory performance under most plausible futures. We also acknowledge the potential limitations of uncertainty quantification and propose strategies to account for them. Finally, we illustrate how a SES model of water resources that accounts for these recommendations may look like. We call for hydrologists, economists, agronomists, stakeholders and other scientists with interest in SES modeling of water resources to join the discussion on how to quantify and assess modeling uncertainties, as well as how to better communicate them to decision makers so that future policies account for unfavorable contingencies and plan strategies to address them.

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