

Author Comment

We would like to express our sincere gratitude for your constructive and thoughtful evaluation of our manuscript. We appreciate your recognition that the manuscript addresses an important and timely challenge in water-energy-food (WEF) nexus modelling.

We have carefully considered the two fundamental concerns you raised: (1) **the treatment of uncertainty**, and (2) **the absence of a numerical proof-of-concept application**. We agree that both aspects are important for demonstrating the practical applicability, transparency, and credibility of an integrated WEF nexus modelling architecture.

We believe that both concerns can be addressed through **substantial but focused revisions** that build directly upon the existing theoretical architecture and our ongoing empirical work on its implementation. We respond to the two concerns in reverse order, as the numerical implementation provides the computational foundation for the subsequent analysis of uncertainty.

Response to Major Concerns

1. **Comment:** The second concern is about the presentation of the architecture in the manuscript: It remains on a conceptual level throughout, describing the state variables and their interactions by interaction diagrams, closure relations and dynamical equations, but not a single proof-of-concept application is provided, nor any code or data sets for test application. To assess the realism and the competitiveness of a new model architecture, test applications with comparison against observations and benchmark models are indispensable.

Response: We sincerely thank you for this important comment. We fully understand your concern that theoretical architecture should ultimately be able to support real-world decision-making rather than remain solely at the conceptual level. Indeed, this was also our motivation underlying the development of the proposed theoretical model.

The original manuscript was deliberately focused on the theoretical development of the proposed WEF nexus architecture. Building on our systematic review of 834 WEF nexus studies (Li, Ward, and van Wesenbeeck 2025), we identified important limitations in existing nexus modelling approaches and therefore positioned the primary contribution of this manuscript around the development of **a theoretically integrated and mathematically solvable architecture**.

At the same time, we agree that a numerical implementation would substantially strengthen the manuscript by demonstrating that the proposed architecture can be translated into an operational computational model. **This concern is also closely related to the issues of empirical testing, calibration, and validation raised by Reviewer #1.** To address your concern without diluting the primary methodological focus of the present paper, while keeping the revised manuscript focused and tractable, we propose three focused revisions:

1. Add **a small but structurally complete numerical proof-of-concept application** based on a hypothetical region and synthetic data;
2. Add **an explicit implementation roadmap** showing how the proposed architecture can be taken from theoretical formulation to full empirical application; and

3. **Temper and reframe the claims** throughout the manuscript to distinguish clearly between what is demonstrated in the present methodological study and what requires subsequent empirical development and validation.

1. Numerical proof-of-concept application

We will add a small but structurally complete numerical proof-of-concept application based on a hypothetical region with synthetic but physically meaningful data. The purpose of this example is not to replace full empirical validation against observations or benchmark models. Rather, it is intended to demonstrate that the proposed architecture can be translated from its theoretical formulation into a finite-dimensional computational model and solved numerically, thereby providing a transparent first test of its operational feasibility.

We believe that a controlled synthetic application is particularly appropriate for this purpose. The primary novelty of this paper lies in the proposed theoretical architecture and its integrated representation of WEF resource interactions. A synthetic numerical application allows these structural features to be examined without the substantial additional complexity introduced by a large empirical dataset, heterogeneous observations, and case-specific calibration choices. It also allows the internal cascading mechanisms of the proposed architecture to be examined under controlled conditions, for example, by varying resource availability.

The numerical application will **retain the six-dimensional architecture** proposed in the manuscript, including the dimensions, (h) , (s) , (t) , (l) , (m) , and (c) , together with a minimal set of consumer types (i) and firm activities (j) . The number of elements within each dimension will be intentionally kept small so that the relationships between assumptions, numerical inputs, constraints, resource balances, and model outputs remain transparent.

A tentative structure is as follows:

Parameter	Definition	Set in the numerical example
i	Consumer type	Urban residents
j	Firm activity	Agricultural planting, thermal power generation, wastewater treatment, and conversion of straw into electricity
h	Resource quality	Pure water, COD, homogenous food quality, homogenous energy quality
s	Region	One hypothetical region
t	Time step	Winter, summer
l	Soil layer	Firm activity, natural layer
m	Resource commodity	Water, corn, electricity, fertilizer, coal
c	Water temperature	Low, high

In the hypothetical region, there will be one type of consumer, namely urban residents, and one agricultural crop, corn. Crop water requirements will be supplied by rainfall and surface water. Corn will be planted in winter and harvested in summer. The two seasons will also allow us to distinguish between different water-temperature conditions. The region will have one representative water

pollutant, COD, caused by agricultural fertilizer application. The thermal power plant will use coal as its sole energy source and surface water as cooling water. Its discharged water will affect water temperature but will not introduce additional water pollutants.

These assumptions are deliberately simplified, but the simplification concerns the **number of elements and the degree of parameterization, rather than the fundamental structure of the proposed architecture**. The example is designed to retain the core structural features corresponding to the six objectives of the proposed model to the extent appropriate for a transparent and computationally tractable proof-of-concept. More specifically:

- **Objective 1: Resource security in both quantity and quality.**

The numerical example will represent both the quantity and quality dimensions of water **resources**. Water availability and use will be explicitly represented, while water temperature and COD will provide a simplified representation of resource quality. Thus, the example will retain the core distinction between resource quantity and quality rather than treating water as a single homogeneous commodity.

- **Objective 2: Return flows and resource circularity.**

A simplified human water-consumption process and associated return flow will be incorporated into the numerical example. Although the number of return-flow pathways will be much smaller than in a full real-world implementation, the example will explicitly demonstrate how post-consumption flows can be returned to the integrated resource-balance system and subsequently become available for further treatment or use.

- **Objective 3: Transferability across spatial, temporal, and geographic contexts.**

The numerical example will retain explicit spatial and temporal dimensions. This demonstrates that the proposed mathematical structure is not intrinsically tied to a particular empirical case and can accommodate different spatial and temporal configurations. We will nevertheless avoid interpreting this single numerical example as empirical evidence of transferability across geographic contexts; rather, it demonstrates the structural extensibility of the architecture that would allow such transferability to be investigated in subsequent empirical applications.

- **Objective 4: Comprehensive representation of WEF interactions.**

The numerical instance will explicitly retain the six mutual interactions among water, energy, and food, as follows:

- **Water → Energy:** cooling water use for thermal power generation;
- **Water → Food:** irrigation water for agricultural production;
- **Energy → Water:** energy use for wastewater treatment;
- **Energy → Food:** fertilizer inputs for agricultural production;
- **Food → Water:** COD pollution associated with agricultural fertilizer application;
- **Food → Energy:** conversion of agricultural by-products, such as straw, into electricity.

- **Objective 5: Integration of economic, environmental, and societal considerations.**

The optimization objective of the numerical example will focus on the core resource-balance constraint, namely minimizing the discrepancy between the resource sources and uses such that the resource-balance gap approaches zero. The proof-of-concept will therefore demonstrate how resource allocation can be operationalized within an integrated optimization framework while retaining environmental considerations. It does not attempt to fully operationalize the societal-welfare component of Objective 5, nor does it claim to provide a calibrated representation of economic preferences. These require additional behavioral assumptions, preference information, and empirical parameterization, which need substantial resources even for a stylized example and are beyond the purpose of this illustration.

- **Objective 6: Theoretical rigor and empirical solvability.**

This objective is addressed directly by the numerical implementation itself. The full finite-dimensional instance will be formulated from the proposed theoretical equations, implemented in GAMS, and numerically solved. **The complete synthetic dataset and GAMS code will be provided as supplementary material**, allowing the numerical implementation to be independently inspected and reproduced.

A real-world empirical application would **retain the same mathematical formulation while expanding the index sets and replacing the synthetic inputs with empirically derived data**. A large-scale empirical application of the proposed framework is being developed separately for Beijing-Tianjin-Hebei (BTH) region of China. That study involves substantially greater empirical detail and requires case-specific calibration and validation. We therefore regard it as a separate empirical application rather than an appropriate substitute for the controlled proof-of-concept in the present methodological manuscript. Incorporating the BTH application into the present manuscript would substantially broaden its scope and length and could blur the distinction between the methodological contribution of this paper and the separate empirical study. It would also introduce a large amount of case-specific empirical detail before the theoretical architecture itself has been demonstrated in a transparent and controlled numerical setting.

The numerical example is therefore not intended as a substitute for empirical validation, but as a **transparent computational bridge between the theoretical architecture and its subsequent real-world implementation**. We believe this provides an appropriate balance between structural completeness and computational transparency for a theory-oriented proof-of-concept.

2. Implementation roadmap

In addition to the proof-of-concept, we will add a clear roadmap for the practical implementation of the proposed model (Fig. 1 below). The purpose of the roadmap is to make explicit which stages are addressed in the present manuscript and which stages require subsequent empirical work.

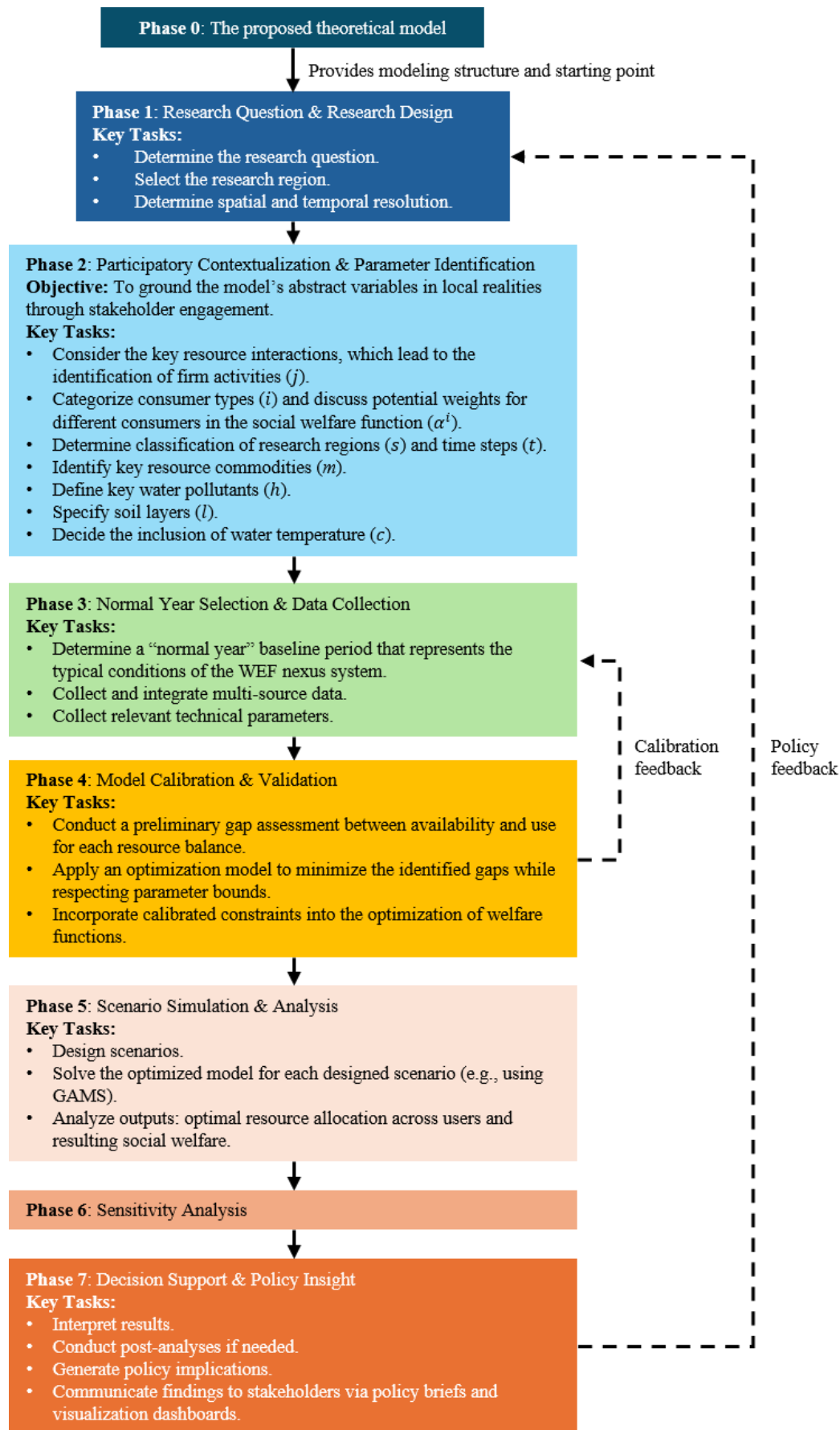


Fig.1. Roadmap for practical implementation of the proposed theoretical model.

The present manuscript focuses primarily on Phase 0, namely the development of an integrated WEF nexus architecture and its mathematical formulation. Phases 1-3 are illustrated conceptually in the manuscript through the BTH region to demonstrate how future empirical applications could identify relevant system components, resource interactions, and data requirements.

The proposed proof-of-concept above does not constitute empirical model calibration or validation. Rather, it shows that the proposed theoretical architecture can be translated into a **solvable integrated model** and can reproduce the intended interactions among water, energy, food, and related system components under controlled assumptions. It should therefore be understood as a preliminary computational demonstration that prepares the model for the subsequent calibration and validation stage in empirical applications. The synthetic example also includes **limited illustrative sensitivity analyses** for selected assumptions and parameters. These analyses are intended to demonstrate the model's response to uncertainty and to identify aspects that warrant attention in future applications; they do not replace a comprehensive sensitivity analysis based on empirical data.

Accordingly, comprehensive calibration and validation (Phase 4), scenario simulation and analysis (Phase 5), comprehensive sensitivity analysis (Phase 6), and decision support and policy analysis (Phase 7) are beyond the scope of the manuscript. These stages require case-specific data, calibration choices, and stakeholder-informed assumptions, and are being pursued in a separate empirical study.

3. Tempering and reframing claims

Finally, we will carefully **temper and reframe the claims throughout the manuscript**. A numerical proof-of-concept should not be interpreted as empirical validation, nor should a theoretical architecture be presented as empirically established before it has been calibrated and tested against observations.

Accordingly, the revised manuscript will clearly distinguish between three levels of contribution:

- the **theoretical contribution**, namely the development of an integrated and mathematically solvable WEF nexus architecture;
- the **numerical proof-of-concept**, which demonstrates that the architecture can be operationalized and solved computationally while retaining its key structural features; and
- the **subsequent empirical implementation**, through which the model can be calibrated, validated against observations, compared with benchmark approaches, and evaluated under real-world scenarios.

We will revise relevant statements throughout the manuscript to avoid implying that the present study has already established empirical validity, transferability, or superiority of the framework. Instead, such claims will be framed as questions to be investigated through subsequent empirical implementation.

Summary

We greatly appreciate your observation that the manuscript should demonstrate more clearly how the proposed architecture can move from theoretical formulation toward practical application. In response, we will add a **small but structurally complete numerical proof-of-concept using synthetic data, together with reproducible GAMS code**, introduce an **explicit implementation roadmap**, and **temper and reframe claims** to distinguish operational feasibility from empirical validation.

We believe that these planned revisions provide a rigorous and transparent numerical test of the proposed architecture while preserving the methodological focus of the manuscript. It also establishes a clear pathway from the theoretical framework presented here to the full empirical calibration, validation, benchmark comparison, and real-world application that you rightly identify as important next steps.

References

Li, Wei, Philip J. Ward, and Lia van Wesenbeeck. 2025. "A Critical Review of Quantifying Water-Energy-Food Nexus Interactions." *Renewable and Sustainable Energy Reviews* 211: 115280. doi:10.1016/j.rser.2024.115280.

2. **Comment:** The first is about the modeling framework itself: Any sectoral model in the water-energy-food nexus is afflicted with substantial predictive uncertainty. For hydrological predictions (as an example), this has been recognized more than a century ago (see Krzysztofowicz, 2001, and references therein), and it is still true today. If this is true for sectoral models, it is even more so for integrated models. Any ambitious model architecture in the water-energy-food nexus therefore needs to be inherently probabilistic. Such probabilistic predictions are not only an honest account of what is known (and what not), they also provide practical advantages for end users and decisionmakers (Buizza, 2008).

Response: Thank you for highlighting the importance of uncertainty in an integrated WEF nexus modelling framework. We fully agree that uncertainty becomes particularly important when multiple sectoral models and resource interactions are brought together within an integrated architecture. Uncertainty in one component may propagate through the coupled system and affect other components, potentially amplifying or attenuating uncertainty through cross-sectoral interactions (Gao, Chen, and Memon 2024). **The importance of uncertainty has also been increasingly recognized in the WEF nexus literature, although explicit treatment and propagation of uncertainty remain relatively limited** (Albrecht, Crootof, and Scott 2018; Muhammad et al. 2026; Zeng et al. 2023).

Drawing on the uncertainty literature and WEF nexus studies (Gao, Chen, and Memon 2024; Krzysztofowicz 2001; Yung et al. 2019), we focus on two sources of uncertainty that are particularly relevant to the proposed WEF nexus model: **(a) uncertainty in empirical inputs**; and **(b) uncertainty in model parameters**. We clarify how these two forms of uncertainty can be represented and examined within the proposed architecture below.

(a) Uncertainty in empirical inputs

Uncertainty in empirical inputs may arise from measurement, data availability, spatial and temporal aggregation, secondary calculations, and differences in source reliability. **This is particularly relevant to WEF nexus applications because the nexus integrates information from multiple sectors, disciplines, and administrative sources** (Gao, Chen, and Memon 2024; Yung et al. 2019).

The original manuscript already incorporates uncertainty in empirical inputs through **a classification of input-data reliability, although this treatment was not made explicit**. Directly reported quantities from authoritative statistical or administrative sources are assigned to higher confidence, whereas quantities requiring secondary calculations are associated with greater uncertainty. Inputs that require indirect inference from qualitative information, such as policy targets or guiding principles, are subject to a higher degree of uncertainty.

Based on this information hierarchy, plausible lower and upper bounds can be assigned to uncertain inputs, with narrower intervals for more reliable information and wider intervals where uncertainty is greater. In this sense, the proposed model **does not assume that empirical inputs are deterministic point estimates**; rather, uncertain inputs are represented as **bounded or interval-valued quantities**, with the width of the interval reflecting the reliability of the input.

This treatment is consistent with the nature of the proposed model. The WEF nexus model is formulated as a **deterministic optimization framework** in which, for any given set of empirical input values within their admissible bounds, the model identifies the corresponding optimal solution subject to the specified resource-balance equations and system constraints. Uncertainty is therefore not incorporated by making the core optimization problem itself probabilistic; instead, uncertainty in the empirical inputs can be examined by solving the deterministic model repeatedly under alternative plausible input values.

More specifically, the sensitivity of the model to an individual uncertain input can be examined by varying that input while holding the other inputs constant. Alternatively, several uncertain inputs can be varied jointly when there is a substantive basis for considering their uncertainties together. Repeated solutions under such alternative input configurations generate a set of corresponding model outcomes, which can be compared to **assessing the sensitivity and robustness of the integrated WEF outcomes** to plausible variation in empirical inputs. These procedures can be implemented in GAMS by repeatedly solving the model under alternative admissible intervals of the uncertain inputs.

We recognize your point that **probabilistic treatment is particularly important in predictive modelling, such as hydrological forecasting**, where the objective is to characterize uncertainty in future states or predictions (Krzysztofowicz, 2001). However, the primary purpose of our proposed framework is different. **It is a system-level equilibrium and optimization framework, rather than a probabilistic predictive model**. The model uses empirical information to establish resource-balances and then identifies optimal resource allocations subject to these resource balances and other model constraints. When uncertain empirical inputs are represented by admissible lower and upper bounds, the model can be solved over these admissible values to examine how uncertainty in the inputs affects the resulting system solution. **Probabilistic uncertainty may therefore be**

incorporated as an extension where appropriate, but it is not imposed as a prerequisite for the core resource-balance architecture. Future scenario analysis could subsequently be used, but probabilistic forecasting is not the primary purpose of the current architecture.

The proposed architecture itself does not require empirical inputs to be represented in a particular probabilistic form. In many cases, the available empirical information may justify a plausible interval for an input but may not provide sufficient evidence to specify a defensible probability distribution. Imposing probability distributions in such cases could introduce additional assumptions that are not adequately supported by the evidence. **We therefore consider that interval bounds provide a more transparent representation of what is known and what remains uncertain.**

Where sufficient empirical information is available to justify probability distributions for particular inputs, the same modelling framework can instead **be extended to probabilistic uncertainty analysis**, for example through Monte Carlo sampling. This would require no change to the underlying WEF resource-balance and optimization structure; the probability distribution would determine how input realizations are generated, after which the same model can be solved repeatedly for those realizations. **We regard this as a possible extension for future empirical applications rather than a necessary component of the present theoretical formulation.**

In the revised manuscript, we will **make the current uncertainty treatment explicit and use the numerical proof-of-concept described above** to demonstrate how uncertainty in empirical inputs can be represented and propagated through the resource-balance equations to affect the resulting integrated system solution. Specifically:

1. **Uncertainty representation:** empirical inputs in the synthetic database will be assigned different levels of reliability to mimic the heterogeneity of empirical information encountered in real-world applications. Inputs assigned higher reliability will be associated with narrower plausible variation intervals, whereas inputs with lower reliability will be assigned wider intervals, where appropriate.
2. **Deterministic optimization:** for any given set of input values within these admissible intervals, the proposed WEF nexus model will be solved to obtain the corresponding optimal solution. In the numerical example, this will first be demonstrated using the initial set of synthetic input values and their associated uncertainty bounds.
3. **Sensitivity analysis:** alternative plausible input values will then be examined through repeated model solutions. Depending on the specific uncertainty being investigated, we may vary one uncertain input while holding the others constant or vary several uncertain inputs jointly where such a joint variation is substantively meaningful. The resulting alternative model solutions will be compared and, where appropriate, visualized as distributions or ranges of outcomes to assess the sensitivity and robustness of the model results to uncertainty in empirical inputs.
4. **Scope of probabilistic uncertainty:** we will also explicitly acknowledge that the present formulation does not impose a probabilistic treatment of uncertainty. Where empirical evidence is sufficient to justify probability distributions, probabilistic uncertainty analysis could be incorporated in future empirical applications without changing the fundamental system-level architecture.

5. **Tempering claims:** we will also temper our use of the term “ideal model” and clarify that the present formulation represents uncertain empirical inputs primarily through reliability-based bounds. **This is an uncertainty-representation choice rather than a structural restriction of the proposed architecture:** where sufficient empirical evidence is available, probabilistic input distributions can be incorporated into the same framework through repeated model solutions without changing the underlying WEF resource-balance and optimization structure.

We believe that these revisions more accurately reflect the role of uncertainty in the proposed architecture while avoiding the introduction of unsupported probabilistic assumptions. They also provide a clear basis for extending the framework to probabilistic uncertainty analysis in future empirical applications where the necessary empirical information is available.

(b) Uncertainty in model parameters

Some technical, conversion, or efficiency coefficients may be uncertain and may not be directly determined by empirical observations. An important characteristic of the proposed architecture is that its core parameters, including the A , B^{oi} , and B^j matrices, are **deterministically derived from empirical inputs within the model**. We therefore do not treat such internally derived quantities as independent sources of uncertainty within the proposed formulation. Their uncertainty is inherited from the uncertainty of the empirical inputs from which they are calculated.

The same principle applies to **genuinely exogenous parameters** used to construct empirical inputs. These parameters are not directly entered into the integrated model as independent uncertain quantities. Instead, they are used to transform, disaggregate, or otherwise construct the empirical inputs required by the model. Their uncertainty is therefore already reflected in the reliability of the resulting empirical inputs. For example, if annual crop production is directly reported but monthly production is required by the model, an externally specified monthly allocation profile is needed to disaggregate the annual total into monthly values. If the allocation profile is supported by limited evidence and is therefore considered less reliable, the resulting monthly production input is assigned a wider uncertainty interval. The uncertainty associated with the exogenous allocation profile is thus captured through the uncertainty bounds of the empirical input that ultimately enters the model. Accordingly, we do not introduce a separate layer of uncertainty for such exogenous parameters when their uncertainty is already reflected in the empirical inputs they are used to construct. This avoids **double-counting uncertainty**.

In the revised manuscript, we will clarify this distinction between parameters that are deterministically derived within the model and exogenous parameters used to construct empirical inputs. Their uncertainty is represented consistently through the reliability-based uncertainty bounds assigned to the final empirical inputs that ultimately enter the integrated model.

References

Albrecht, Tamee R, Arica Crootof, and Christopher A Scott. 2018. “The Water-Energy-Food Nexus: A Systematic Review of Methods for Nexus Assessment.” *Environmental Research Letters* 13(4): 043002. doi:10.1088/1748-9326/aaa9c6.

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Concluding response

We greatly appreciate your valuable comments, which help us identify two important areas in which the original manuscript required further strengthening: the **demonstration of computational applicability** and the **explicit treatment of uncertainty**.

In response, we plan the following focused revisions:

1. Add a **small but structurally complete numerical proof-of-concept** based on a hypothetical region and synthetic data, implemented and solved in GAMS, with the synthetic dataset and code provided as supplementary material.
2. Add an **explicit implementation roadmap** clarifying the pathway from the theoretical architecture to numerical operationalization and, subsequently, full empirical application.
3. Make the treatment of **input uncertainty and parameter uncertainty** explicit, using reliability-based bounds and repeated model solutions for the present numerical demonstration, while clarifying that probabilistic representations can be incorporated where sufficient empirical evidence supports them without changing the underlying model architecture.
4. **Temper and reframe claims**, including the use of the term “ideal” and clearly distinguish the theoretical contribution and numerical proof-of-concept from empirical calibration, validation, benchmark comparison, and full real-world application.

We believe these revisions will substantially strengthen the manuscript and provide a clearer account of both its computational feasibility and treatment of uncertainty, while preserving its central theoretical contributions. We respectfully hope that these focused revisions will address the concerns you raised substantively and provide a sufficient basis for **reconsideration of the manuscript as a major revision**.

Yours Faithfully,

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