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Integral modelling for water security beyond the water cycle

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Water pollution is a critical constraint to water security, impacting natural environment and reducing the resilience of infrastructure. Conventional approaches, often focused on modelling the hydrological cycle, struggle to capture the wider interactions between natural and engineered systems in which water is embedded. However, water systems are closely linked with transport, food and energy, creating feedback that remains poorly understood. In this Perspective, we propose that advancing water security requires integral modelling frameworks that move beyond water-cycle-only approaches. Such frameworks provide a modular, graph-based representation capable of linking physical systems with human behaviour and decisions. We illustrate this conceptually through the Water Systems Integration Modelling framework, showing how its modular development can extend modelling beyond the water cycle. As an example, we outline how tyre wear pollution can be conceptualised through pathways that connect water and food systems. We conclude by highlighting three priorities for future work: developing interdisciplinary processes for cross-sectoral integral modelling, evaluating systemic portfolios of interventions, and extending applications to sectors such as energy, all of which will shape the next generation of integral modelling for water security.

KEYWORDS

integral modelling, modular development, tyre wear pollution, water quality, water security

1 Introduction

Water security is increasingly recognised as a multidimensional challenge that goes beyond the availability of freshwater resources. Water quality has become a major constraint to sustainable outcomes, as pollution undermines ecosystem services and reduces the resilience of infrastructure (Gunda et al., 2019). These pressures are further compounded because water systems are not independent. They are embedded in wider socio-technical networks that include land use, food production and infrastructure (Mijic et al., 2024b). These wider interactions govern both the movement of water and pollutants as well as more complex dynamics that are difficult to analyse but essential for future planning and the effectiveness of interventions.

Modelling complex water systems is critical for future planning across a wide range of uncertainties (Mijic et al., 2024a). Modelling water quality in these systems is particularly challenging because it requires capturing multiple dynamic interactions between natural and engineered domains, as well as feedback driven by both physical and societal processes. Although integrated modelling has been recognised as essential, existing approaches often fall short in representing these interdependencies (Razavi et al., 2025). Models are usually developed within disciplinary silos and, while they may include some coupled components, they rarely provide

a unifying framework that can dynamically link processes beyond water systems while accounting for key process representations.

In recent years, a new generation of models has been developed that can simulate multiple components within a unified framework, which we refer to as integral models. These models link physical processes in ways that support both observation-based evaluation and intervention analysis (Voinov and Shugart, 2013). Water Systems Integrated Modelling provides one such framework for building integral water system models (Dobson et al., 2024). It represents systems using a node–arc structure, where nodes capture physical components such as rivers, treatment plants or urban areas, and arcs govern the flow and transformation of water and pollutants. The model's orchestration, which defines system operations, can be customised to adjust structure without altering the code. This flexibility creates opportunities to simulate impacts beyond the water cycle (Mijic and Dobson, 2025). Within this structure, feedback between physical system states and human decision-making are represented through rule-based and scenario-driven simulations, including urban water abstractions and use (Whaley et al., 2024) and rural–urban discharges (Liu L. et al., 2022).

This Perspective introduces an integral water system modelling approach that addresses the challenge of going beyond the water cycle in water security. It sets out an expanded paradigm designed to incorporate cross-sectoral processes in a modular and extensible way. We outline the framework and its modular development, illustrate its application through pollution propagation across transport, water and food domains, and explore implications for future research and application.

2 Integral modelling of water cycle interactions

The integral modelling theory has been proposed to enable seamless exchange of information within a simulation model (Voinov and Shugart, 2013). Integral model coupling, which defines the configuration of components and their interactions, can be broadly characterised in two ways: (1) tight coupling, with pre-defined equations and interactions, as in most traditional numerical and conceptual models,

and (2) flexible coupling, in which components remain easy to configure and users can define their arrangement, with different configurations suited to different applications. This process is known as model orchestration (Dobson et al., 2024). An illustrative example of flexible coupling is the integration of a sub-daily dynamic water use generator developed to assess changes in urban water demand during the COVID-19 pandemic (Dobson et al., 2021). This generator captured shifts in water use associated with working from home behaviour and was seamlessly incorporated into the existing model orchestration without altering any other components of the water system model. This enabled the assessment of impacts on flows and water quality under rapidly changing demand patterns, demonstrating how flexible coupling can support timely exploration of emergent system behaviour that would be difficult to achieve through tightly coupled model formulations. We suggest that flexible coupling provides the most effective balance and represents the most promising pathway for advancing integral water system modelling beyond the water cycle.

The Water Systems Integration Modelling framework has been developed as an application of integral modelling theory to simulate the terrestrial water cycle (Dobson et al., 2024). In its baseline version, the framework defines seven water system domains that mutually interact (Figure 1A), which are called nodes. Each node is represented by a domain model. The interactions between domains are enabled by connecting arcs, which can simply move water and pollutants across the system or define more complex exchanges, such as information on available capacity or abstraction volumes. All elements of the framework are explained in detail in Dobson et al. (2024).

2.1 Modular development within integral frameworks

We define modular development as the systematic refinement or extension of an integral water system baseline model shown in Figure 1A. Two main approaches can be distinguished: (1) internal refinement and (2) structural extension. Internal refinement replaces one or more domain models with alternative representations. The refined model serves the same overall function but introduces additional detail or process specificity. This allows the framework's structural coherence to be maintained while selectively enhancing parts of the system to reflect new scientific understanding, data availability, or

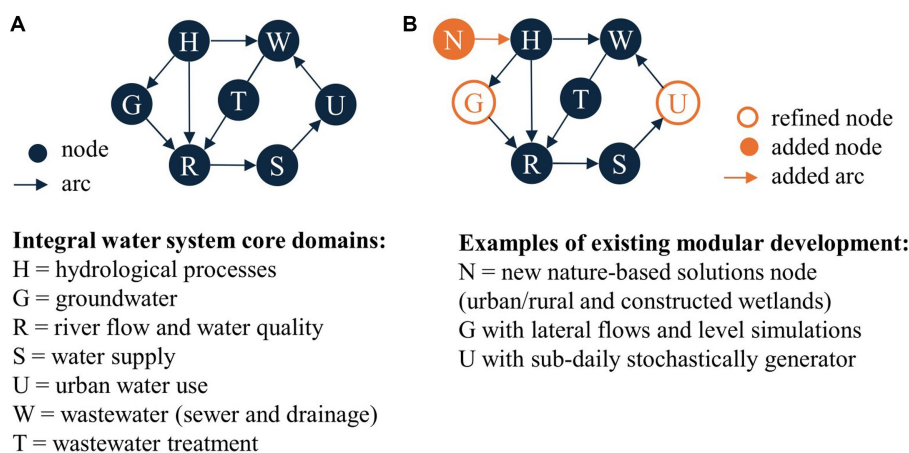


FIGURE 1

Example of modular development in Water Systems Integration framework. The baseline model (A) represents core water system domains (nodes) and their interactions (arcs). Modular development (B) can refine existing nodes, add new nodes, and introduce new arcs to extend system representation.

domain-specific needs. Structural extension introduces new domains or components (e.g., processes or interactions) by adding nodes and arcs to the baseline model. Both refinement and extension can be achieved using the baseline store–flux conceptual paradigm or through higher-resolution numerical or data-driven methods, including statistical models and AI. We refer to these latter approaches as multi-fidelity or hybrid modelling (Razavi et al., 2025).

We illustrate modular development with four examples drawn from our previous work (Figure 1B). Two involve internal refinement. First, the baseline groundwater domain model was refined to simulate groundwater levels and lateral flow (Liu et al., 2024). Second, a detailed urban water use generator was developed to improve the representation of baseline per capita demand (Dobson et al., 2021). Structural extension has been used to represent water management interventions in the baseline model. One example shows how urban and rural nature-based solutions can be added (Liu et al., 2023), while other focuses on constructed wetlands (Peng et al., 2025). These examples also demonstrate the range of modelling approaches. The groundwater refinement and nature-based solutions used the baseline conceptual approach, while the water use generator showed how a domain model can be replaced with a stochastic generator running at a different spatial and temporal scale than the baseline framework.

3 Extending integral modelling beyond the water cycle

While current examples demonstrate the potential of modular development for integral water system models, extending these principles to systems beyond the water cycle has not yet been addressed. We use tyre wear pollution (TWP) as an example to show how integral frameworks can support model development across interconnected systems. Globally, an estimated six million tonnes of TWP are produced each year (Kole et al., 2017), a figure expected to rise with the shift towards heavier electric passenger cars (Timmers and Achten, 2016). We first outline the environmental pathways of the TWP system, then map it onto the integral framework, and finally discuss initial directions for integral model development.

Evidence shows that TWP is a dominant source of microplastics in riverine ecosystems and represents a significant but poorly understood form of freshwater pollution (Baensch-Baltruschat et al., 2020). TWP can enter rivers through multiple potential pathways (Zheng et

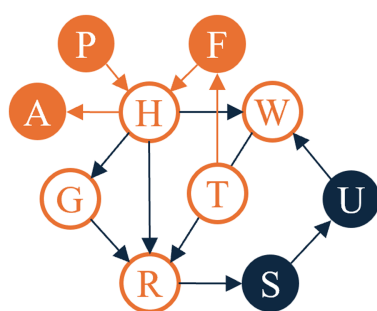
al., 2025). Analytical studies indicate that up to 40% will reach urban rivers directly from wastewater networks during rain events (Wagner et al., 2018), which will become more pronounced with increased surface runoff under climate change (Chan et al., 2022). However, TWP can also enter rivers indirectly, as particles retained in wastewater treatment plants are incorporated into sewage sludge, around 24% of which is applied as fertiliser on agricultural land, from where rainfall and runoff can mobilise them into surface waters (Baensch-Baltruschat et al., 2021). Recent reviews further show that this pathway links water and food domains, as TWP in sludge-amended soils can alter soil properties, affect crop performance, and potentially transfer pollution through the food chain (Kang et al., 2025).

In integral modelling, including TWP introduces a new pollutant state variable that must be represented in model development. This requires simulating TWP load generation, extending baseline transport processes to capture its movement through the water system, and adding new processes for sludge production, fertiliser application, and impacts on food systems. We present this as a modular development challenge in Figure 2.

3.1 Towards a tyre wear pollution integral model

The conceptual representation of the new TWP model (Figure 2) suggests that modular development will likely combine structural extensions (e.g., load generation, sludge reuse and food systems) with internal refinements (e.g., TWP propagation through the water system). We propose a two-step process for selecting modelling approaches. First, baseline model users should define the requirements for new representations. Second, a team of domain experts should be convened to identify specific models that meet these requirements. We next outline the requirements for TWP modular development, which will provide the basis for engagement with domain experts in future work.

To simulate the TWP load generation, a new transport domain model can be designed in two ways. The first option is to add a model that outputs pollutant mass directly (e.g., kilograms of TWP per road segment), which can be used as input to the wastewater node. The second option is to use a transport domain model that provides traffic data (e.g., vehicle counts per day per road segment), which then requires a conversion model to estimate tyre wear per vehicle, deposition on roads, wash-off dynamics, and other processes that determine pollutant mass entering the wastewater system. Such a conversion model may include parameters such as vehicle type distribution,



Conceptual representation of tyre wear pollution integral model development:

P = new tyre wear pollution generation
 H and W with detailed pollution transport
 T with sludge generation
 F = new sludge transport
 A = new food system
 R and G with sediment transport

FIGURE 2

Conceptual modular development of a tyre wear pollution model within the baseline framework with new (orange) and refined (orange outlines) nodes. Arrows indicate added arcs for pollutant transport and interactions across water, land, and food domains.

rainfall-dependent wash-off, and pollutant accumulation rates (Liu Y. et al., 2022). In addition, transport domain models may represent behavioural aspects of vehicle use, including acceleration and braking intensity, cornering behaviour, and driving speed distributions. These factors influence tyre abrasion rates and therefore pollutant generation at source, reflecting how human behaviour contributes directly to pollution generation rather than only influencing responses at the receiving end of the system (Liu Y. et al., 2022). To generate a complete TWP profile, load generation data must be combined with information on TWP properties, including tyre composition and wear rates, to estimate emission factors for different particle sizes, chemical components, and toxicity as a function of vehicle type and traffic conditions (Bae et al., 2024).

Propagation of TWP through the water system requires internal refinement to represent pollutant transport from roads to wastewater (i.e., surface processes), which is highly sensitive to both current and past hydrological and temperature conditions. This calls for a new theoretical formulation of TWP mobilisation, for example, by building on empirical studies of wash-off during precipitation events and partitioning of runoff between wastewater and natural (Baensch-Baltruschat et al., 2020). In addition, a representation of in-network behaviour is needed, where smaller particles can be assumed to traverse the entire network, while larger particles may deposit in low-velocity sections but can be remobilised. Implementing this in the baseline model will require adapting sediment transport equations and offers an opportunity to integrate hybrid modelling with machine learning (Montes et al., 2021).

The current representation of processes in the wastewater treatment baseline module needs to be upgraded to capture the integration of TWP into sludge. Candidate models should include activated sludge for biological treatment and anaerobic digestion for sludge treatment, and they should support time-resolved simulation to study transient behaviours such as daily load variations and operational disturbances (Hauduc et al., 2010). Once sludge generation is represented, fertiliser use can be added by defining a new node linking the improved treatment plant module to the land module, where fertiliser application is already included in the baseline representation. This will require data on sludge transport, which can be derived from estimations (Willén et al., 2017) or obtained directly from water companies through engagement.

The new TWP model should be extended with a food system representation that can capture nutrients and farmer behaviour and simulate the impact of TWP on crop yield. A new model would need to represent how TWP alter soil properties, including reductions in porosity, slower rates of organic matter decomposition, and disruptions to soil microbial communities such as declines in nitrogen-fixing bacteria. It could also capture phytotoxic effects on plants, including root blockage and oxidative stress linked to zinc release (Kang et al., 2025).

The development of such representations also requires structured collaboration across disciplines, including social sciences, to capture human decision-making processes such as farmer behaviour and the economic feasibility of intervention portfolios (O'Keeffe et al., 2016). These interdisciplinary interactions must explicitly consider differences in temporal and spatial scales across model components. For example, hydrological processes are often simulated continuously at basin scales, whereas food systems and land management decisions may operate at plot, district, or national

scales and over discrete decision horizons (Sivapalan and Blöschl, 2015). Addressing these scale mismatches through appropriate model orchestration and coupling strategies is therefore essential for the development of an integral TWP modelling framework.

Finally, the river module should be refined beyond classic mass-balance to account for the size and density of TWP particles. Unlike passive tracers, these particles may sediment, move slowly near the bed at low flows, or attenuate dispersion at higher flows (Russell et al., 2023). The module therefore needs simple physics-based expressions to estimate sedimentation rates, travel times, and possible infiltration into the hyporheic zone, the region beneath and alongside a riverbed where surface water and groundwater mix.

4 What next: future directions for integral modelling

Based on the examples presented in this paper, we identify three directions for advancing integral modelling beyond traditional water system applications: developing interdisciplinary processes, designing systemic intervention portfolios, and expanding integration across sectors.

First, developing interdisciplinary processes is essential to capture inputs and outputs and to model exchanges across domains. While Section 3 highlighted technical requirements for modular development of TWP models, the next step is to translate such requirements into a formalised process for model building and testing. This requires structured collaboration between hydrologists, water, transport and environmental engineers and soil scientists to ensure that inputs and outputs are defined consistently across domains and that model exchanges reflect both physical and chemical processes. Interdisciplinary methodological approaches can help design and execute truly interdisciplinary research by aligning conceptual and technical designs across disciplines (Tobi and Kampen, 2018). Embedding such frameworks into integral model development would provide a systematic pathway for incorporating new pollutants or cross-sectoral challenges into models, enhancing both their scientific credibility and practical utility.

Second, in complex systems, the key challenge is defining the most effective combination of measures across domains to maximise co-benefits and minimise unintended trade-offs (Dobson and Mijic, 2020). Options for TWP management range from upstream measures such as changes in tyre design and production, to midstream measures like nature-based solutions for runoff control and upgraded wastewater treatment, and downstream measures such as limits on sludge reuse or improved soil remediation. Each has benefits and limitations, and integral modelling can help compare these options under different conditions to identify robust portfolios of interventions that are both effective and feasible in practice.

Finally, while this paper focuses on transport-related pollution, expanding integral modelling beyond the given example is essential to capture cross-sectoral drivers of water security. Other sectors also exert indirect but significant pressures on water systems. For instance, the transition to renewable energy will alter water demand and infrastructure operation, from hydropower scheduling to cooling requirements in solar thermal and bioenergy production (Zakariazadeh et al., 2024). Extending integral modelling to systematically explore such

cross-sectoral linkages will help anticipate unintended consequences, identify co-benefits, and design strategies that advance water security alongside broader sustainability goals.

5 Conclusion

This Perspective set out how integral modelling can evolve from established water cycle applications towards addressing broader cross-sectoral challenges. Using tyre wear pollution as an example, we demonstrated how modular development enables new pollutants and processes to be incorporated, while maintaining a coherent system representation. The discussion outlined three priorities for future work: formalising interdisciplinary processes, identifying systemic combinations of interventions, and expanding integration across sectors such as transport, energy, and food. Taken together, these directions position integral modelling as a practical and extensible approach to advancing water security in the face of growing complexity and change.

Data availability statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author.

Author contributions

AM: Visualization, Writing – original draft, Conceptualization, Writing – review & editing. WB: Formal analysis, Writing – review & editing. BD: Writing – review & editing, Formal analysis, Conceptualization. EK: Formal analysis, Writing – review & editing. MS: Formal analysis, Writing – review & editing. DV: Data curation, Writing – review & editing.

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