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Bridging global, basin and local-scale water quality modeling towards enhancing water quality management worldwide

Ting Tang[1], Maryna Strokal[2], Michelle TH van Vliet[2], Piet Seuntjens[3,4,5], Peter Burek[1], Carolien Kroeze[2], Simon Langan[1] and Yoshihide Wada[1,6]

Global water quality (WQ) modeling is an emerging field. In this article, we identify the missing linkages between global and basin/local-scale WQ models, and discuss the possibilities to fill these gaps. We argue that WQ models need stronger linkages across spatial scales. This would help to identify effective scale-specific WQ management options and contribute to future development of global WQ models. Two directions are proposed to improve the linkages: nested multiscale WQ modeling towards enhanced water management, and development of next-generation global WQ models based-on basin/local-scale mechanistic understanding. We highlight the need for better collaboration among WQ modelers and policy-makers in order to deliver responsive water policies and management strategies across scales.

Addresses
[1] International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria
[2] Water Systems and Global Change group, Wageningen University & Research, Wageningen, Netherlands
[3] Unit Environmental Modeling, Flemish Institute for Technological Research, Mol, Belgium
[4] Institute of Environment and Sustainable Development, University of Antwerp, Antwerp, Belgium
[5] Department of Environment, Ghent University, Ghent, Belgium
[6] Department of Physical Geography, Utrecht University, Utrecht, Netherlands

Corresponding author: Tang, Ting (tangt@iiasa.ac.at)

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Water quality modeling at different spatial scales: the missing linkages

The world's water resources are under increasing threats from a wide range of pollutants, resulting in deteriorating water quality in rivers, lakes, aquifers and seas [1–4]. Deteriorating water quality limits water availability for various human uses and ecosystem functioning [5,6]. Moreover, global water demand has increased considerably in the past decades and the trend will continue into future decades due to population and economic growth, resulting in increasing water and food demands [7,8]. The combination of deteriorating water quality and increasing water demand poses increasing challenges to address water scarcity and water resources management under future socioeconomic and climate changes [9]. Water quality (WQ) modeling plays an important role in better understanding the magnitude and impact of WQ issues and in providing evidence for policy-making and implementing measures to mitigate water pollution.

WQ modeling of surface water takes place at different spatial scales, ranging from individual field-stream to global modeling of land surfaces and water bodies (examples in Table 1, and see [10–17] for comprehensive reviews) with diverse modeling purposes and approaches. WQ modeling in rivers dates back to the 1920s [16,17], while it evolved by including point sources and landscape transport of non-point source (NPS) pollutants in the 1970s [12,13]. With most global WQ models developed in the past two decades [18], global WQ modeling is an emerging field compared with basin/local-scale WQ modeling. In this article, the term "scale" refers to the designed spatial coverage of a model, while the finest model discretization is referred to as "resolution" (e.g., grid). We take "local-scale" modeling to refer to point-scale, field-scale, instream transport modeling and modeling of technical components (e.g., BNRM2 [19] for wastewater treatment plants, WWTP). "Basin-scale" modeling refers to WQ simulation for a single river basin, including both landscape and instream WQ modeling.

Local-scale WQ models (e.g., [20,21]) are often developed to quantify and better understand the

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Table 1

Example models[a] of different spatial scales discussed in this article

Spatial scale	Example models	Simulated water quality parameters	References
Global	Global *NEWS*-2 (Global Nutrient Export from WaterSheds 2)	Different forms of carbon, nitrogen & phosphorus	[33,48]
Global	IMAGE-GNM (IMAGE-Global Nutrient Model)	Total nitrogen and phosphorus	[40]
Global	VIC-RBM (Variable Infiltration Capacity - River Basin Model for water temperature)	Water temperature	[38,39]
Basin	BASINS (Better Assessment Science Integrating point & Non-point Sources), with watershed (basin) sub-models: • HSPF (Hydrological Simulation Program - FORTRAN), • SWAT • SWMM (Storm Water Management Model) • PLOAD (Pollutant Loading Estimator), etc. and instream sub-models • AQUATOX, • WASP (Water Quality Analysis Simulation Program)	Dissolved oxygen, biological oxygen demand, sediment oxygen demand, pH, alkalinity, nutrients, algae, zooplankton, coliform bacteria, etc.	[25]
Basin	SWAT (Soil and Water Assessment Tool), with sub-models: • EPIC (Erosion-Productivity Impact Calculator) for sediment yield, • CREAMS (Chemicals, Runoff, and Erosion from Agricultural Management Systems) for chemical runoff from agriculture, • adapted QUAL2E (Enhanced Stream Water Quality Model) for instream nutrient routing • adapted GLEAMS (Groundwater Loading Effects on Agricultural Management Systems) for pesticide transport and fates, etc.	Sediment, different forms of nitrogen and phosphorus, algae, biological oxygen demand, pesticides, bacteria and heavy metals	[24,26]
Basin	HYPE (HYdrological Predictions for the Environment)	Organic carbon, total nitrogen and phosphorus & water temperature (as a tracer)	[23,55]
Basin	SimplyP	Sediment and phosphorus	[57]
Local: Field to small watershed	APEX (Agricultural Policy Environmental Extender)	Sediment, different forms of nitrogen and phosphorus, and pesticides	[20]
Local: Field(s)	DAISY	Carbon, nitrogen and pesticides	[21]
Local: Wetland	WETSAND (Wetland Solute Transport Dynamics)	Different forms of nitrogen and total phosphorus	[72]
Local: WWTP	BNRM2 (Biological Nutrient Removal Model No. 2)	Nitrogen and phosphorus (removal in WWTP by biological processes)	[19]

[a] For comprehensive reviews of WQ models, see [10,11]) for global WQ modeling, [12–15] for basin-scale and local-scale WQ modeling and [16,17] for instream WQ modeling.

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biogeochemical processes for given WQ parameters on land and in water bodies, and to assess the effectiveness of management measures [12,19]. They are often either mechanistic or empirical with parameters reflecting local biogeochemical characteristics (e.g. temperature, organic matter content). Empirical models have limited associations to or assumptions for the underlying biogeochemical mechanisms (e.g., Freundlich equation for pollutant adsorption onto soil [22]), which are often data-driven, and can be statistical when statistical relationships are constructed. Mechanistic models describe system behaviors using biogeochemical parameters and attempt to incorporate known mechanisms of system behaviors underlying the observational data. In principal, they can predict system behaviors under changes to the modelled system. Understanding of the underlying biogeochemical mechanisms and processes (mechanistic understanding) and their mathematical descriptions from local-scale models (e.g., pH/temperature-dependent first-order denitrification) are the basis for basin-scale modeling. The aim of basin-scale modeling is diverse, but could be largely considered as to better understand underpinning sources, transformations and transport mechanisms in order to manage the targeted system in an integrated manner. Contemporary basin-scale WQ models typically incorporate local-scale modeling and experimental approaches in simplified manners [13], and are therefore often (semi-)mechanistic (i.e., mechanistic or hybrid of empirical and mechanistic approaches) and process-based (e.g., [23–26]), namely with explicit descriptions of dominant individual processes based on mechanistic understanding.

Global and multi-basin (e.g., continental-scale) WQ models typically aim to understand the state (e.g., pollution hotspots and their causes) and spatiotemporal trends of WQ issues in a consistent manner under multiple interactive drivers. Global WQ models are necessary because water pollution is an increasing global concern and globally consistent WQ assessments are needed to identify global WQ hotspots and trends, especially in regions where WQ data is insufficient for a detailed assessment. Furthermore, global WQ models can account for large-scale drivers that are difficult to capture in basin-scale models. Hoekstra [27] stressed that water pollution is so heavily intertwined with the global economy that it cannot be dealt with independently from global economy. Global WQ models can elucidate the interplays among drivers [e.g., 28], such as climate change and virtual water and pollution transfer related to international trade [27,29,30] and assess their impacts on water quality. For example, studies highlighted the importance of international trade of food and animal feed on global nutrient cycling [29,31] and river organic pollution [32].

Due to practical constrains, such as data availability and computational costs, global WQ models (e.g., [33–36]) rely on heavily simplified relationships (e.g., export coefficient approach to estimate landscape nutrient retention). These relationships are often of empirical nature because they are derived from basin/local data and associated relationships in data-rich regions, and do not necessarily reflect the underlying biogeochemical processes due to the heavy simplifications. Global WQ modeling are currently moving towards hybrid approaches. However, this is limited to WQ parameters with relatively simple drivers, sources or processes and with good data availability, such as water temperature (i.e., PCRGLOB-WB [37] and VIC-RBM [38,39]) and nutrients (i.e., IMAGE-GNM [40]). The selection of empirical or mechanistic approaches depends on the modeling purposes and the associated data availability. With the increase of spatial scale, generally simplified relationships with less relevance to the underlying processes are more often used accompanied by lower spatiotemporal resolutions and model complexity (Figure 1). On one hand, such simplicity or empirical nature is justified because global-scale models are intended to identify hotspots and long-term trends, which are in relative terms and hence arguably require lower quantification accuracy. Empirical methods have merits in their limited data requirements, while still being frequently characterized by high levels of model accuracy [41]. On the other hand, model developers need to make sure the approaches are sufficient for the intended purposes of global WQ models, especially when potential effects of changes to the modelled system are of interest.

Missing linkage 1: Global WQ models need sufficient consideration of basin/local-scale mechanistic understanding

The heavily simplified relationships in global WQ models result in difficulties to satisfy their designed modeling purposes in some cases. Such relationships are often developed using historical data of specific locations and climate conditions. For example, nutrient loss/retention fraction along the river network in Global *NEWS-2* (L_F) is estimated either using a constant or as a function of channel drainage area, which were derived from observations in the United States [33]. The global Cryptosporidium model (GloWPa) estimates NPS Cryptosporidium runoff fraction from manure using a method developed for Europe [34]. The critical question here is, are the relationships transferrable from data-rich to data-scarce regions and to future conditions under global changes (transferability issue)? The transferability issue is not unique to global models or WQ modeling. It has widely been discussed in, for example, ecological modeling [42,43]. Although we do not have a concrete example to demonstrate the issue in global WQ models, one should not rule out its potential existence and impacts. Basin/local-scale mechanistic understanding helps to understand and potentially address the issue. However, a lot more efforts are needed to properly incorporate basin/

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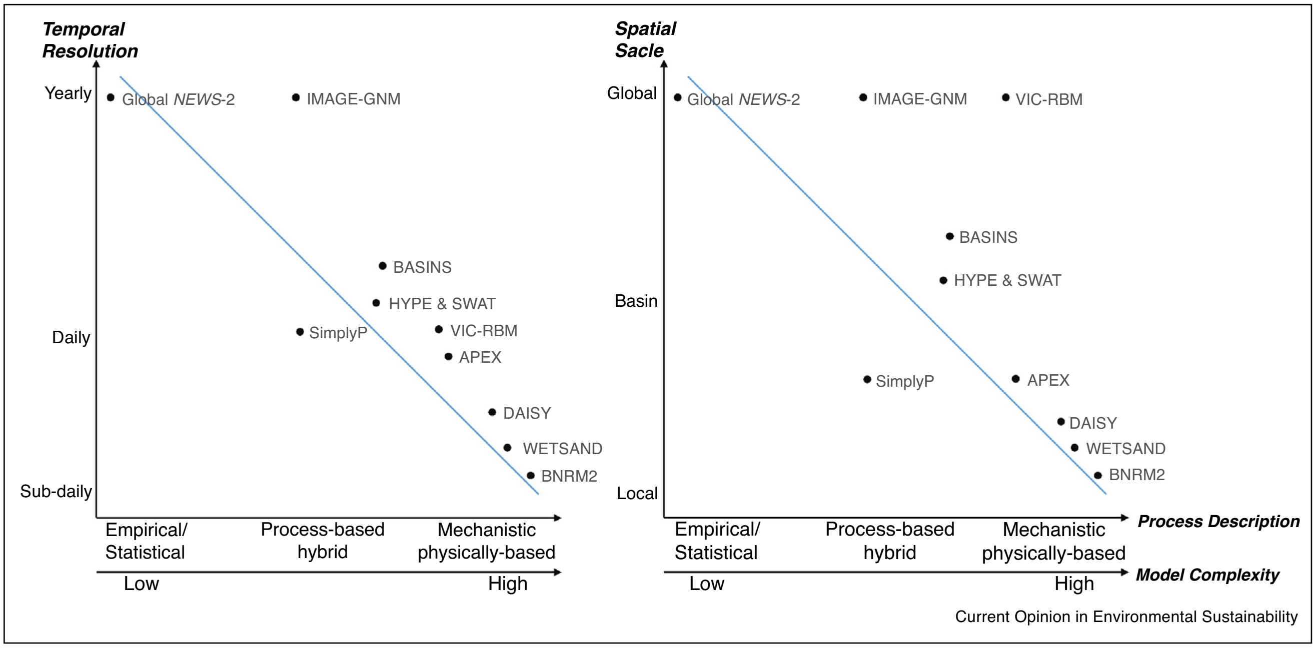
Figure 1



Illustrative overview of the continuum of WQ model types based on process description and the corresponding model complexity and spatiotemporal scale, with example WQ models from Table 1. All axes are continuous with two endpoints and important mid-points discussed in the paper are added for process description, temporal resolution and spatial scale. Partially based on Bouwman et al. [67]. Note that "spatial scale" herein refers to the designed spatial coverage of a model rather than its spatial resolution.

local-scale knowledge into global WQ models, in order to have a reasonable balance among model complexity, data demand and availability. Kroeze et al. [44] called for mechanistic global nutrient export models and combining the strengths of basin-scale models. Global (semi-)mechanistic models already exist for water temperature and nutrients, but the efforts should extend towards other WQ parameters, such as oxygen demand, pathogens and pesticides. Although we do not argue for highly complex mechanistic global WQ models, global WQ models should incorporate mechanistic understanding from basin/local-scale WQ models to tackle the transferability issue.

Missing linkage 2: Global WQ models are rarely considered in water-related policy-making or water management

Water quality management and water governance are multiscale issues [45], ranging from local measures (e.g., vegetated filters to control erosion [46]) to river basin plans (e.g., Danube [47]), international policies (e.g., EU Water Framework Directive) and global policy agenda (e.g, Sustainable Development Goals, SDGs). Models need to mirror this policy need for multiscale management. Global models, such as Global *NEWS*-2 [33,48], WorldQual [49] and IMAGE-GNM [40], account for a wide range of pollutant sources (e.g., agricultural, domestic and industrial), associated socio-economic and climate drivers. These models are therefore appropriate tools to pinpoint the dominant drivers and pollutant sources, which guides policy-making for pollution abatement at the highest administrative level (e.g, international guidelines and national policies). However, the actual use of global WQ models in policy-making is rare, except for one case where WorldQual provided an assessment of WQ status in South America, Africa and Asia for the United Nations Environment Programme (UNEP) [1]. Policies at the highest administrative level need to be implemented at the basin or lower administrative (e.g., provincial or national) level, wherein basin-scale models are more appropriate. Implementation of mitigation measures or infrastructural development are at even smaller scales, which requires local-scale models. Linking global WQ models with basin/local water management models is therefore ideal to facilitate management, but is very rare to our knowledge, although basin/local-scale models are often coupled for management purposes. Meanwhile, local management measures and basin-scale management plans are expected to influence water quality dynamics and therefore should be considered as feedback into large-scale policy-making and WQ modeling. WQ models should therefore be actively linked across spatial scales and support each other to ensure responsive policy-making and effective WQ management.

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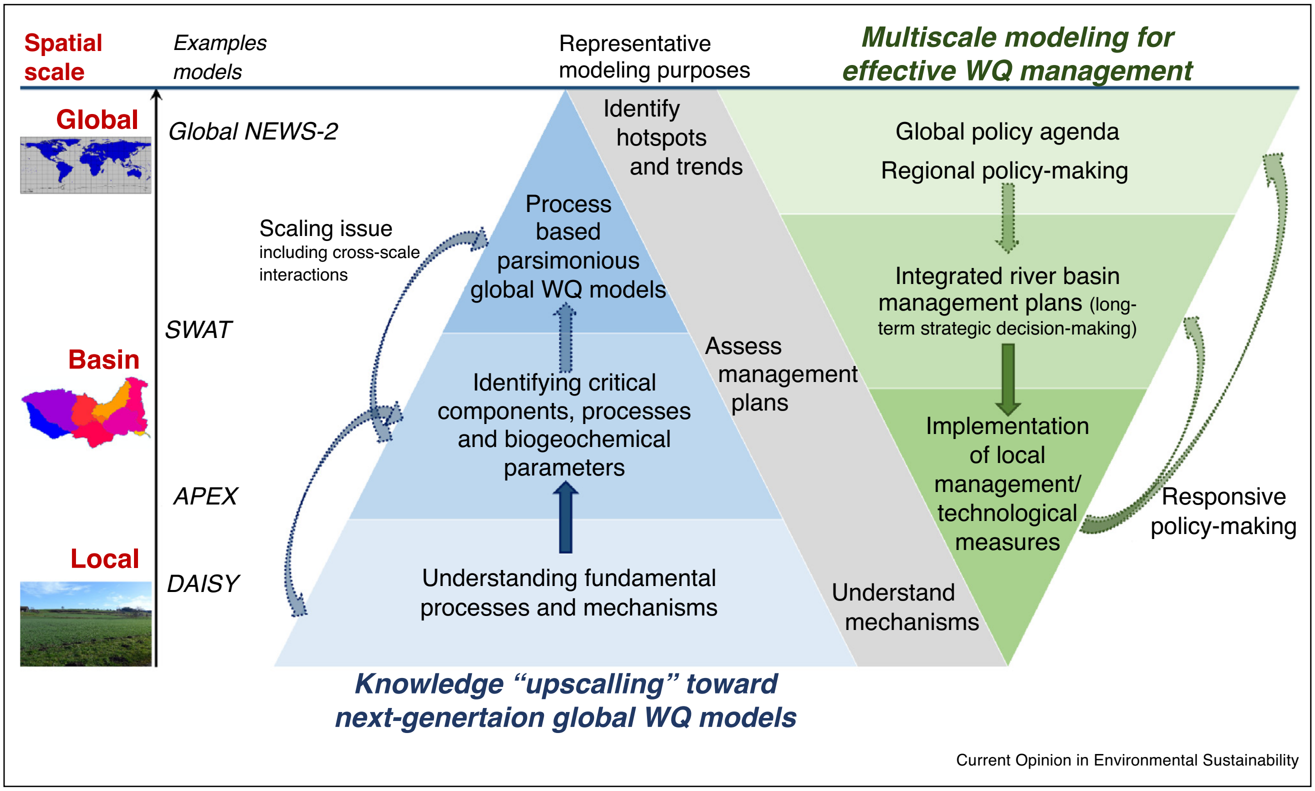
Figure 2



The proposed framework to improve the linkages of WQ modeling at different spatial scales, from a global WQ model development (left triangle) and water quality management (right triangle) perspective. Examples of WQ models at different scales are presented.

Filling the gap: a proposed framework to bridge WQ modeling across scales

The framework

We propose a framework with two directions (Figure 2) to address the missing linkages outlined in Section 1. Firstly, we argue that a nested multiscale WQ modeling approach is needed for WQ management, wherein global modeling is actively accounted for in long-term policy-making, river basin management and local measures, and the latter two are considered as feedback in policy-making and WQ models at the global scale. The multiscale approach therefore also considers the interactions and linkages among multiple spatial scales. Secondly, considering the simplicity and potential implications of current global WQ modeling approaches, we argue that mechanistic understanding from basin/local-scale models should be better used to develop the next generation of global WQ models. Improvements of the current modeling approaches are needed to ensure the reliability of model predictions under long-term changes and to include feedbacks from local and basin management practices. Therefore, the next-generation WQ modelling is not only about improving global WQ models, but also about bringing models of different scales together to develop flexible frameworks with scaling issues (e.g., non-linearity and interactions among scales) considered. The latter can facilitate nested multiscale modeling for WQ management. We note that the proposed directions are demonstrations of important linkages beneficial for water management and are therefore not intended to represent the full spectrum of possible linkages.

Nested multiscale WQ modeling towards enhanced water quality governance and management

The SDGs represent one policy agenda at the largest (i.e., global) scale. SDG6 (clean water and sanitation) Target 6.3 sets out to improve ambient water quality of the world's water bodies. Global WQ modeling comes into play here and provides a globally consistent assessment of spatial hotspots, source attribution and underpinning drivers of the status and future projections under different climate and socioeconomic scenarios. This is currently not possible using approaches such as global monitoring due to limited data and capacities in least developed countries [50]. Such assessment from global WQ models helps international organizations, such as the World Health Organization and UNEP, to develop international frameworks and set global agendas (e.g., SDGs), which provide potential entry points for management. Thanks to close contacts with different countries, international

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organizations should use this knowledge as a strong message to push heavily polluting countries, especially of transboundary basins, to address the pollution issues, and to better advice national or regional (e.g., multi-national or transboundary basins) policy-makers on implementing environmentally sound policies and management practices.

Basin/local-scale models provide more detailed assessments of WQ issues, based on better local data and context wherein the issues needs to be managed. From this, detailed management strategies can be designed and implemented. For example, Cools et al. [51] coupled the basin-scale WQ model SWAT with an economic optimization model to select the most cost-effective measures to reduce instream nitrogen concentration from a larger pool of measures in the draft management plan for the Scheldt basin in Belgium. BASINS [25] was developed to assist in basin-scale management e.g., by developing the total maximum daily loads for each pollutant into impaired water bodies, which is legally required by the United States Clean Water Act [52,53]. These types of information call for implementation at the local scale, to either specific areas (e.g., vegetated filters [46]) or technological improvement (e.g., WWTPs). Whether it is best management practices in agricultural settings or low impact development measures in urban environments, local models are most appropriate to evaluate the potential effects of such measures and therefore contribute to implementing the most cost-effective measures to fulfill basin or global-scale targets.

Basin/local-scale mechanistic understanding for next generation of global WQ models

Basin-scale WQ models, such as SWAT and HYPE, have successfully been applied at the continental scale [54,55]. In principal, they can be applied at the global scale in a similar manner. However, a few challenges may hinder direct upscaling. Firstly, many basin-scale (semi-)mechanistic WQ models are over-parameterized with at least some not-readily measurable parameters (e.g., nutrient percolation coefficients in SWAT), and have been criticized as overly-complex compared with the available observations to parameterize the models [56,57]. Even if sufficient local monitoring data are available, over-parameterization easily leads to large model uncertainties [58,59]. Secondly, current applications of basin-scale models to the continental scale are limited to data-rich regions (e.g., Europe). WQ monitoring data and model input data (e.g., fertilizer/pesticide application data) are, however, scarce in many other regions (e.g., Africa and south Asia) [1]. This complicates the assessment of global model reliability in these regions. Lastly, the increasing need to holistically address climate-water-land-food-ecosystem nexus issues drives the development of integrated modeling frameworks (e.g., IMAGE), which further increase complexity and propagate uncertainties [60]. Consequently, it is hardly justified to directly employ basin-scale (semi-)mechanistic WQ models at the global scale.

Similar constrains exist for global hydrological models (GHMs), wherein basin-scale models are rarely used for global applications [61], although mechanistic hydrological models are available for mesoscale catchments and currently being upscaled to basin and continental scales [62]. After several iterations of developments, current GHMs have similar processes to basin-scale hydrological models, but differ considerably in their complexity, ranging from bucket-type empirical approaches to hybrid approaches [61,62]. To increase model accuracy, GHMs are moving towards higher spatiotemporal resolution [61,62] and more mechanistic representations of important processes, such as reservoir operations [63], groundwater routing [8] and floodplain processes [62]. Model inter-comparison of GHMs is used to expose uncertainties in input data and model structure (i.e., representation of processes) [64,65], and therefore help to improve relevant processes based on mechanistic understanding. Such improvements are accompanied by the improved data availability, especially from Remote Sensing (RS) products (e.g., for evapotranspiration, terrestrial water storages and their changes) [61]. Similar to current GHMs, we argue that process-based parsimonious approaches should be the basic principle in developing the next generation of global WQ models by balancing modeling purposes and data availability while making use of basin/local-scale mechanistic understanding. A parsimonious approach uses the simplest approach that fits the modeling purpose and available data.

A flexible next-generation global WQ modeling framework by building a process-based parsimonious model

Process description in a process-based global WQ model can be empirical or mechanistic, but should include system responses to altered environmental conditions to capture future global changes. A process-based model is therefore generally hybrid and modular (Figure 1). With sufficient good quality data, it can offer more robust predictions under global changes than empirical models [42], while avoiding issues of mechanistic models. The modularity means the model can be highly flexible and a modeling framework can be easily constructed with multiple descriptions of each process or for multiple pollutants. One can therefore navigate among different model structures and optimize the structure to her/his own data/needs. Given the complexity of WQ-related processes, prioritization of components and processes in the modelled system becomes essential to ensure model parsimony.

Parsimonious global WQ models through prioritization, simplification and parameter regionalization

One way of achieving parsimony is to simplify basin/local-scale WQ modeling approaches with a stepwise

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prioritization. With basin/local-scale models, one can follow three steps: 1) identify basin-scale main components influencing pollutant transport (e.g., river channels, lakes, riparian wetlands), 2) assess dominant processes within the main components influencing pollutant dynamics (e.g., sedimentation, biodegradation), and 3) identify critical biogeochemical parameters (e.g., pH, soil organic carbon) for the dominant processes.

With this procedure, one can prioritize and narrow down to the critical components, processes and parameters for global WQ models. Noteworthy, a relative term is needed in component and process prioritization (Steps 1&2). River basins have different pollutant sources and physical characteristics (e.g., extent of wetland, length of river network). These characteristics should be normalized when identifying dominant components and processes that are relevant at spatiotemporal scales appropriate for global WQ modeling. The spatiotemporal resolution of global WQ modeling is typically lower than basin/local-scale WQ models (Figure 1 & [11]). Consequently, care should be taken during component and process prioritization in order to identify the predominant processes relevant at the global scale and account for scaling issues (e.g., non-linearity and interactions among scales). Further discussions on the scaling issue are available elsewhere for landscape pollutant modeling [12,66] and instream transport modeling [67]. Statistical, empirical or simplified mechanistic relationships can thereafter be constructed for dominant processes using either existing large-scale observations or existing basin/local-scale relationships. Sensitivity analysis is one of the effective means to identify critical parameters (Step 3). One important consideration in Step 3 is to use easily-accessible measurable biogeochemical or hydro-climatic parameters or their measurable proxies whenever possible. This reduces the challenge to parameterize the model and partly compensates the transferability issue for empirical or statistical relationships. Parameter regionalization is another opportunity to parameterize data-scarce regions in global WQ models, although it is currently mainly used in hydrological modeling [68]. The regionalization approach attempts to transfer information from data-rich areas to data-scarce areas based on similarities among the areas or statistical relationships between model parameters and basin attributes (e.g., topography, soil) [68,69]. For example, based on climatic and physiographic similarities, calibrated parameter sets from 674 basins by a GHM were transferred to another 1113 basins, resulting in global parameter maps for follow-up hydrological simulation [68].

As an example for the whole procedure, riparian wetlands efficiently remove or retain pollutants (sediment, nutrients and heavy metals, Step 1) [70]. Denitrification is the main nitrogen removal process in wetlands (Step 2), which is controlled by sediment oxygen content, retention time, nitrate loading, pH and temperature, among others [70,71]. IMAGE-GNM estimates denitrification by riparian wetlands using 8 parameters, including pH, temperature, riparian zone thickness, travel time, flow rate and soil properties [40]. These parameters are relatively easy to obtain or estimate, compared with highly spatial-variable biogeochemical parameters (e.g., denitrification rate). However, for a process with no global data to calibrate, the number of parameters seems to be rather high. Step 3 (identifying critical biogeochemical parameters) using sensitivity analysis of IMAGE-GNM or wetland models (e.g., WETSAND [72]) could be the next step to avoid over-parameterization and simplify the model.

Challenges and future outlook

This paper proposes that a nested multiscale approach of global WQ models based on mechanistic understanding is needed in order to provide reliable results that can be actively used in policy-making and water management across scales. Two main challenges exist in providing reliable results and translating them into policies.

Data availability remains the biggest challenge for global WQ modeling and management

Good quality, freely available and easily accessible global datasets are essential for global WQ modeling in terms of model inputs (e.g., pollutant sources, sanitation and treatment level) and monitoring data for model evaluation. Global databases exist on socioeconomic drivers and their future projections (summarized in [10]). However, large uncertainties exist in estimating pollutant sources (e.g., discharge from human waste) from the drivers. Available global monitoring datasets have limited data for many developing regions (e.g., Africa) and limited temporal coverage (e.g., http://www.worldwaterquality.org/ and http://portal.gemstat.org/). Significant efforts are still in need for data-scarce regions to develop their monitoring capacity. An emerging opportunity to address data limitation is high-resolution hyperspectral RS techniques, which are used for large-scale monitoring of optically-active WQ parameters such as turbidity, salinity, *chlorophyll*-a and dissolved oxygen [73,74]. RS data can potentially improve data availability at the global scale that is consistent with basin/local-scale data for optically-active WQ parameters.

Active collaboration among communities is critical to advance water quality management across scales

Several critical questions may arise due to data limitation in global WQ modeling. Firstly, how can model reliability and the associated model uncertainties be assessed without sufficient input or observational data? Secondly, to what extend can policy-makers make decisions based on the modeling results and associated uncertainties? While improving model reliability is fundamental for using global WQ models in policy-making and WQ

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management, active communication and collaboration are also required among policy-makers and modeling communities.

Due to the propagation of prediction errors from climate and hydrological models and high variability of biogeochemical processes, WQ models are subject to relatively large uncertainties [60]. The global WQ modelling community needs to be explicit on model uncertainties, explore the different sources of uncertainties and address them accordingly to facilitate the use of global WQ models in evidence-based policy-making. One example is to conduct model inter-comparison to reveal and address model structural uncertainties [11], which is often used in climate science and GHMs [64,75,76]. Work is needed at the interface of research into policy to better portray uncertainties so that they are understandable by decision-makers and can be properly considered in global agendas and national/regional policies [e.g, 77]. In addition, WQ modelers need to fully recognize that modeling purposes differ depending on the spatial scales, leading to different modeling approaches and advantages. Such differences are the reasons why a nested multiscale approach benefits water management. We therefore call for active knowledge exchange and collaboration among different modeling communities despite the seemingly different questions addressed by WQ models of different spatial scales.

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