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To cite this article before publication: Maryna Strokal *et al* 2025 *Environ. Res.: Water* in press https://doi.org/10.1088/3033-4942/adf571

Advancing water quality model intercomparisons under global change: Perspectives from the new ISIMIP water quality sector

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Abstract

Water pollution poses widespread risks to ecosystems, human health, and water users more broadly. Furthermore, the interplay of future hydroclimatic changes and socioeconomic developments will strongly impact the quality status of freshwaters across the globe. Innumerable pollutants are increasingly entering water bodies, potentially creating hotspots at various spatial and temporal scales and with implications for different water-dependent sectors. While it is recognized that proactive solutions to protect and improve water quality are key for the achievement of Sustainable Development Goal 6.3 (clean water for all), deficiencies in our understanding of the current and future quality status pose significant challenges. Water quality models help bridge the gaps in our understanding of water quality due to limited observations, but they vary in terms of pollutants, spatial-temporal resolution, and structure. While such diversity poses various challenges, it also presents an opportunity to design a multi-dimensional framework for water quality model intercomparison projects (WQ-MIPs) that focus on three distinct aspects: multi-pollutant, multi-scale, and multi-sector. The water quality sector has been launched within the ISIMIP initiative to help facilitate these multi-dimensional WQ-MIPs. In this paper, we present community insights on WQ-MIPs. We first synthesize the diversity found among water quality models and then propose an ISIMIP intercomparison framework aimed at enhancing our understanding of uncertainties in pollution levels and identifying robust pollution hotspots, sources, and impacts across multiple sectors, pollutants, and scales. To this end, we use four illustrative examples of WQ-MIPs. Finally, we outline a future agenda for advancing WQ-MIPs that are essential for developing effective solutions to preserve future water quality under global change.

Keywords: multi-pollutant, multi-scale, multi-sector, model intercomparison, water quality

1. Introduction

Society and nature rely on clean water, which is not always available [1]. This has been increasingly recognized with the integration of water quality into water scarcity assessments [2-3], with a diverse set of newly emerging pollutants (e.g., plastics [4-5], pesticides [6-7], antibiotics [8]) further exacerbating water quality issues worldwide (Figure 1). Water pollution has multiple impacts, including domestic (drinking water), recreation, industry, agriculture, and aquatic ecosystems (Figure 1; [9]). For example, high nitrate levels in drinking water can cause "blue baby syndromes" [10]. Recreational activities and ecosystems can also be negatively impacted by high nutrient loads. Such high levels can initiate eutrophication [11-12] and harmful algae blooms [13-14] leading to the release of toxins that are dangerous to humans and can alter the food web composition [15-16]. Other examples are the impacts of multiple pollutants on human health (e.g., pathogens [17-18]), on agriculture (e.g., salinity [19], pathogens [20]), and on ecosystems (e.g., antibiotic resistance [21], emerging contaminants [22], plastics [23-24]; Figure 1).

Pollution can originate from various environmental and societal sources [25], resulting in cross-sectoral impacts, e.g. impacts on agriculture, groundwater, and lakes ([3, 26]; Figure 1). For example, urban wastewater contains elevated levels of emerging pollutants such as pesticides, antibiotics, and microplastics [27]. Agriculture is one of the main sources of nutrients [28-29], plastics [30], antibiotics [31], pesticides [32], and pathogens [28]. Industrial wastewater from mining and resource extraction releases organic compounds, chemicals, heavy metals, and total dissolved solids (TDS) [33-34]. Thermoelectric power generation requires water for cooling and then discharges warmer water back into water systems [35-36]. Mismanaged solid waste is a key source of plastic pollution [37]. However, solutions that could address common sources of multiple pollutants and reduce their cross-sectoral impacts are lacking. These issues hinder meaningful progress towards Sustainable Development Goals (SDGs) 6.2 (sustainable access and supply) and 6.3 (clean water) (https://sdgs.un.org/goals/goal6).

Despite scientific efforts, water pollution remains widespread [38]. This is due to the complex interplay of hydroclimatic change and socioeconomic developments, collectively representing global changes. Floods and droughts influence water availability, whereas [39] unsustainable socioeconomic developments [1] can result in additional pollutant emissions to the environment. Together, they change the availability of clean water for sectors that are confronted by too little, too much, or too dirty water [3, 26]. Consequently, the United Nations Environment Assembly (UNEA) calls for water quality assessments (www.unep.org). Although Intergovernmental Panel on Climate Change (IPCC) reports focus on the impact of climate change within socioeconomic development scenarios, and mention water temperature and oxygen levels, there remains a lack of quantitative assessment of global change-related risks of water pollution [40].

Model intercomparison projects for water quality (WQ-MIP) are therefore urgently needed to foster process understanding and model development, in addition to supporting large-scale UNEA and IPCC assessments. While monitoring data, especially for emerging pollutants, is often limited in time and space, models could fill these (data) gaps and offer forward-looking scenarios [41]. A diverse set of water quality models exists, with large differences in modeling approaches (e.g. steady state versus dynamic), water quality constituents (pollutants), type of water resources (lakes, rivers, groundwater, coastal waters), and spatial and temporal resolutions (see Section 2 for more details), which poses challenges for WQ-MIPs [42]. On the other hand, it creates some valuable opportunities [43]. For example, the diversity in models could help to identify robust (i.e., consistent) multi-pollutant hotspots, their sources, and trends, which are crucial to prioritize areas for actions and monitoring to achieve SDG 6.3 [42]. WQ-MIPs also help to improve our scientific understanding of model uncertainties, supporting future projections of water quality under climate change and socioeconomic developments.

To facilitate WQ-MIPs, a new "Water Quality" sector in the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP) platform has been launched (https://www.isimip.org/). The ISIMIP platform is comprised of multiple sectors. Examples are the Agricultural, Energy, Forest, Water (Global and Regional), and Lakes sectors. ISIMIP nomenclature therefore defines sectors not only as water users (agriculture, energy, forest) but also types of water bodies (lakes, groundwater). ISIMIP provides sector-specific protocols to support modelers in the harmonization of model inputs and outputs to enhance the consistency of multi-model assessments. Although the ISIMIP Water Quality sector is new, its community has been built over the past years through collaborations and interactive workshops (SI Table A.1 in Appendix A) that started with the UN World Water Quality Alliance (UN-WWQA, https://wwqa.info/) workshop in 2017. This led to a special issue of 2019 [44] calling for large-scale water quality MIPs [42] and eventually to the construction of multi-model and multi-constituent scenarios [45] and to formalizing modelling protocol and steps (https://protocol.isimip.org/#/ISIMIP3a/water_quality). The first WQ-MIPs focused on nutrients and water temperature at the global [42, 46] and continental [47-48] scales. Although MIPs are an established modelling practice that exists for global hydrological [49] and climate impact model communities [50], limited attention has been paid to water quality, especially to multi-pollutant hotspots, their sources, and trends at multiple scales and across sectors [25, 42]. The current "Focus Issue"- where this work is submitted – uses mostly the future scenario data generated by the WQ-MIP community over the past few years [49].

We have undertaken three important new steps in developing WQ-MIPs. First, building on previously identified challenges and opportunities for developing WQ-MIPs [42], we harmonized storyline scenarios across several global water quality models to keep internal consistency for multiple pollutants and sectors [45]. Second, we expanded WQ-MIPs with more models and now focus on multiple dimensions characterizing multi-pollutants, multi-sectors, and multi-scales. In this regard, we make connections to other ISIMIP sectors (Figure 1). For instance, the Agricultural ISIMIP Sector provides input to our WQ models and benefits from our outputs (e.g., instream nutrient concentrations) to support the impact assessment of water quality on food production. Similarly, river water temperature simulations inform quantifications of powerplant water demands and usable capacity in collaboration with the ISIMIP Energy sector. Other examples emphasizing cross-sectoral connections lie in exchanging expertise, data, and model simulations with the Lake sector, Groundwater sector, and Global Water sector within ISIMIP. Third, we have identified new types of WQ-MIPs that leverage the diversity in our models as a strength for WQ assessments. To this end, we go beyond the common MIPs in which models are compared using their ensembles for one output (see Examples in Section 3 as well as studies in the current "Focus Issue").

In this paper, we first summarize the five main types of model diversity [42] and our interactions over the past years (Section 2). Then, we present the community effort towards building a WQ-MIP framework (Section 3). This framework builds on the generic aspects of the ISIMIP framework (https://www.isimip.org/protocol/) but expands it to encompass the diverse aspects of water quality models, considering multiple pollutants, sectors, and scales. We provide four examples of water quality model intercomparisons to illustrate lessons, challenges, and limitations of different types of WQ-MIPs, with a focus on large-scale water quality models. Finally, we outline a future agenda for new opportunities in cross-scale and cross-sectoral multi-pollutant assessments of water quality (Section 4).

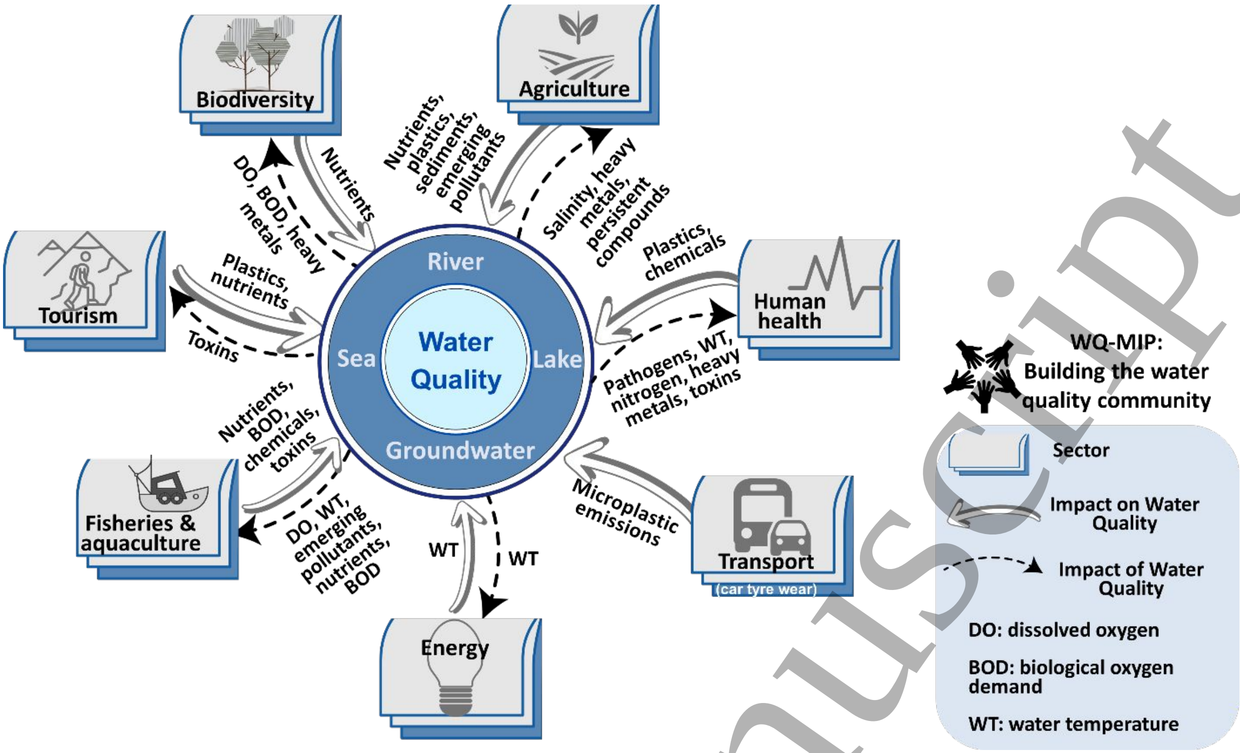

Figure 1. Water quality cross-sectoral linkages for selected water quality constituents. The figure does not aim to be exhaustive, but simply illustrates important cross-sectoral aspects of water quality identified by the large-scale water quality community. Sectors are defined according to the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP; https://www.isimip.org/). ISIMIP is comprised of multiple sectors that are topic-oriented: e.g., Agriculture, Fisheries (here "Fisheries and aquaculture"), Biodiversity, Energy, Lakes, Coastal systems (here "Sea"), Health (here "Human health"), Water Quality, and Groundwater. Rivers are included in the Water (Global) and Water (Regional) sectors of the ISIMIP platform. WQ-MIP is short for water quality model intercomparisons. Source: examples were collected by the large-scale water quality community during the workshops (SI Table A.1 in Appendix A).

2. Methodology

The primary aim of this paper is to share initial, community-wide insights from the intercomparison of water-quality models. This study presents a synthesis of existing knowledge assembled from previously published and independently validated simulations from various teams. This approach lets us highlight both the challenges and the opportunities of multi-model intercomparisons and establishes a foundation for a larger coordinated community effort. Accordingly, this phase deliberately leverages existing runs to demonstrate the multi-pollutant potential of water-quality model intercomparison projects (WQ-MIPs). Looking ahead, during ISIMIP Phase (3a/3b and beyond, https://www.isimip.org/), all participating water quality models will be required to rerun their simulations with a fully harmonized model input dataset, following the standardized and commonly adopted modelling protocols (https://www.isimip.org/).

Here, we briefly outline the models underlying our illustrative examples of WQ-MIPs presented in this study. While a detailed description of the participating models is outside the scope of this study, interested readers can refer to cited literature. Instead, we highlight diversity, challenges, and opportunities.

2.1 Diversity in Large-scale Water Quality Models

We identified five main types of model diversity: (1) modeling approaches, (2) spatial, and (3) temporal resolutions and extents, (4) types of water resources, and (5) water quality constituents (Figure 2 as an example; SI Table A.2 and Figure A.1 in Appendix A). These diversity types apply to both large-scale and regional water quality models [51] and are reflective of the model's original purpose and target users [51]. Modeling approaches differ, for example, in underlying process description, implementation and assumptions. The spatial resolution and extent of the large-scale model differ from hydrological response units to grids of different sizes, basins, or sub-basins (see Table 1). Similarly, the temporal resolution and the periods over which processes are modeled and output can vary widely from daily and monthly up to annual scales (e.g., [52-53]). The types of water resources considered range from groundwater to surface waters with distinct shapes, sizes, and dynamics (e.g., streams to rivers [17, 54], lakes, and/or reservoirs [55], and coastal areas [11, 52]). Models may focus on different water quality constituents (Table 1): e.g., chemicals [8, 56-58], pathogens and microorganisms [17, 59], nutrients [11], or plastics [60-61]. Furthermore, models may differ in terms of output units, including concentrations [53] and loadings [52].

Representative nine models illustrate the model diversity (Figure 2, SI Figure A.1):

1. MARINA model family (Model to Assess River Inputs of pollutaNts to seAs); it consists of the models for nutrients (MARINA-Nutrients [26]), antibiotics (MARINA-Antibiotics [66]), plastics (MARINA-Plastics [60]) and multiple pollutants (MARINA-Multi [52, 67]),
2. SWAT+ (Soil and Water Assessment Tool [62-63, 68-69]),
3. GloWPa (Global Waterborne Pathogen [17]),
4. GREEN (Geospatial Regression Equation for European Nutrient losses [70-71]),
5. IMAGE-GNM (IMAGE-Global Nutrient Model [11]),
6. WorldQual (water quality model embedded in the WaterGAP3 modelling framework) [54, 72-73],
7. DynQual v1.0 (dynamical surface water quality model [53]),
8. mQM (multiscale Water Quality Model) [74-75], and
9. Wflow-DWAQ [76].

Some of the selected models take a time-invariant (steady) approach (e.g., MARINA and GREEN), while others are dynamic (e.g., IMAGE-GNM, mQM, DynQual v1.0, WorldQual, and Wflow-DWAQ) (Diversity type 1). SWAT+ is based on a hydrological response unit, whereas five out of nine models (GloWPa, IMAGE-GNM, DynQual v1.0, WorldQual, and Wflow-DWAQ) run at a grid scale. Wflow-DWAQ aggregates 30x30 arcsecond results to the HydroBasin delineations (level 7, [77]). In contrast, GREEN and MARINA adopt basin and sub-basin scales (Diversity type 2). . Simulation time-step spans from daily (DynQual v1.0, Wflow-DWAQ) to monthly (e.g., GloWPa, WorldQual, and SWAT+) and annual (e.g., MARINA, GREEN, IMAGE-GNM, and mQM) (Diversity type 3). Most models focus on rivers and/or seas, whereas SWAT+, mQM, and IMAGE-GNM include a groundwater component (Diversity type 4). Notably, most of the WQ models include nutrients, though the dimensions differ between loadings and concentrations (Diversity type 5). The WorldQual and DynQual v1.0 models represent similar water resource types (Diversity type 4), and both include water temperature and concentrations of fecal coliforms, organic pollutants, and salinity, but they differ in whether they include nutrients as well (Diversity type 5). Among the selected models, only Wflow-DWAQ simulates toxic effects: the impact of the mixture of toxic substances on biodiversity. Despite this diversity, certain spatial coverages, constituents, and water systems remain underrepresented.

To illustrate the opportunity that WQ-MIPs offer, seven large-scale models are used from the list of Figure 2: MARINA (versions: MARINA-Multi and MARINA-Nutrients), SWAT+, GREEN, IMAGE-GNM, WorldQual, DynQual v1.0, and mQM. Most of them have internal consistencies in hydroclimatic forcings (the same ISIMIP2b global climate models are used) and socioeconomic storylines (e.g., SSP5 is often used for future analysis). Yet, some inconsistencies in model inputs exist. For example, different hydrological models underpin the water quality simulations. The WorldQual model is coupled with the WaterGAP3 framework, that provides hydrology [1], whereas SWAT+ generates its hydrology [62-63], IMAGE-GNM [11] and DynQual v1.0 [53] are coupled with the PCR-GLOBWB2 hydrological model [78], the MARINA [67] and GloWPa [17] models take hydrological outputs from the VIC (Variable Infiltration Capacity) model [79], and the GREEN model uses hydrological outputs from the LISFLOOD model [80]. These hydrological models differ in their approaches and may introduce uncertainties in model intercomparisons [81]. Other uncertainties may arise from the aggregation procedure of model results to a harmonized spatial and temporal resolution [82]. All examples are based on available datasets (e.g., model inputs) that are either published or provided in the ISIMIP repository (https://data.isimip.org/). Details on model inputs are given in references to the model (Table 1).

Table 1 Summary of the large-scale models that are included in Figures 2-3 of this study. BOD, TDS, and WT are short for biological oxygen demand, total dissolved solids, and water temperature, respectively. *Model runs up to 2100, simulations up to 2050 are available in the ISIMIP repository. Diversity types are summarized in Figure 2.

Name	Full name	Approach – Diversity type 1	Spatial details of model inputs and outputs – Diversity type 2		Temporal details of model inputs and outputs – diversity type 3		Main output – Diversity type 4	Constituents – Diversity type 5	Main output – Diversity type 5	Hydrological model used	Details in
			Resolution	Extent	Resolution	Extent					
MARINA	Model to Assess River Inputs of pollutaNts to seAs	Static, uncalibrated	Sub-basin	Global	Annual	Up to 2100*	Surface waters, seas	Nutrients, plastics, chemicals	Loading: Inputs to rivers and river exports to seas by source and sub-basin	VIC: Variable Infiltration Capacity (soft coupling)	[67, 83]
SWAT+	Soil and Water Assessment Tool	Dynamic, calibrated	Hydrological response units	Africa	Monthly	Varied	Surface waters, groundwater	Nutrients	Concentration of nutrients in rivers and groundwater	Generate itself	[62-63, 68-69]
GREEN	Geospatial Regression Equation for European Nutrient losses	Static	Sub-basin	Europe	Annual	Up to 2050	Surface waters, seas	Nutrients	Loading: river exports by source to seas	LISFLOOD	[70-71]
IMAGE-GNM	IMAGE-Global Nutrient Model	Dynamic	0.5°grid cell	Global	Annual	Up to 2050	Surface waters	Nutrients	Concentrations of nutrients in surface waters	PCR-GLOBWB2	[11]
WorldQual	-	Dynamic	5 arcminutes grid cell	Global	Monthly	Up to 2100	Surface waters	Nutrients, pathogens, BOD, TDS, and WT	Loadings and concentrations of pollutants in rivers	WaterGAP3 framework	[54, 72-73]
DynQual	Dynamical surface water quality model	Dynamic	5 arcminutes grid cell	Global	Monthly	Up to 2100	Surface waters	Pathogens, BOD, TDS, WT	Concentrations of pollutants in rivers	PCR-GLOBWB2	[3, 53]
mQM	multiscale Water Quality Model	Static	0.5°grid cell	Europe	Annual	Up to 2050	Surface waters	Nutrients	Concentration of nutrients in rivers	mHM	[74-75]
Wflow-DWAQ	-	Dynamic	30 arcseconds	Global	Daily	Flexible	Surface waters	Anthropogenic chemicals	Concentration: Toxic effects in surface waters	Wflow	[76]

2.2 Challenges and Opportunities in Large-scale Water Quality Models

Model diversity poses some challenges for creating harmonized model ensembles for comparative analysis [42]. For example, differences in spatial and temporal resolution (Diversity types 2-3) may create (technical) barriers for model intercomparisons, particularly in terms of pollutant concentrations. Several approaches and frameworks in related fields have been developed over the past decade that can help to overcome such technical barriers (e.g., [84]). Moreover, conceptual and (computer) programming language barriers (i.e. coding, software) must be reconciled to establish a common ground for interdisciplinary model comparisons when models are designed for different purposes [42]. Additional conceptual challenges arise from differences in pollutants (Diversity type 5) and water resources (Diversity type 4). Furthermore, models often have different units, requiring processing steps to compare model simulations (Diversity type 5). A protocol is therefore helpful to harmonize spatial and temporal levels of details among models and ensure consistency in model inputs and outputs.

On the other hand, model diversity creates opportunities for water quality model intercomparisons, WQ-MIPs [45]. Combining or comparing models with varied spatial resolutions, temporal settings, and pollutant types (Diversity types 2, 3, and 5) can provide new insights into multi-pollutant assessments and cross-scale scales. For example, combining outputs of the DynQual v1.0 [53] and MARINA-Multi [67] could represent different (seven) water quality variables of concern (Figure 2). Overlapping features of model outputs can help identify spatial consistencies or uncertainties. For example, one can contrast riverine concentrations of nutrients from IMAGE-GNM or WorldQual and pathogens from DynQual v1.0 or GloWPa, and thereby examining changes over time can reveal (robust) hotspots of multiple pollutants under global changes. Another opportunity to highlight uncertainties is by looking at the variation in water quality projections due to varying climate model forcings. In Section 3, we illustrate four examples of insights that can be gained from WQ-MIPs.

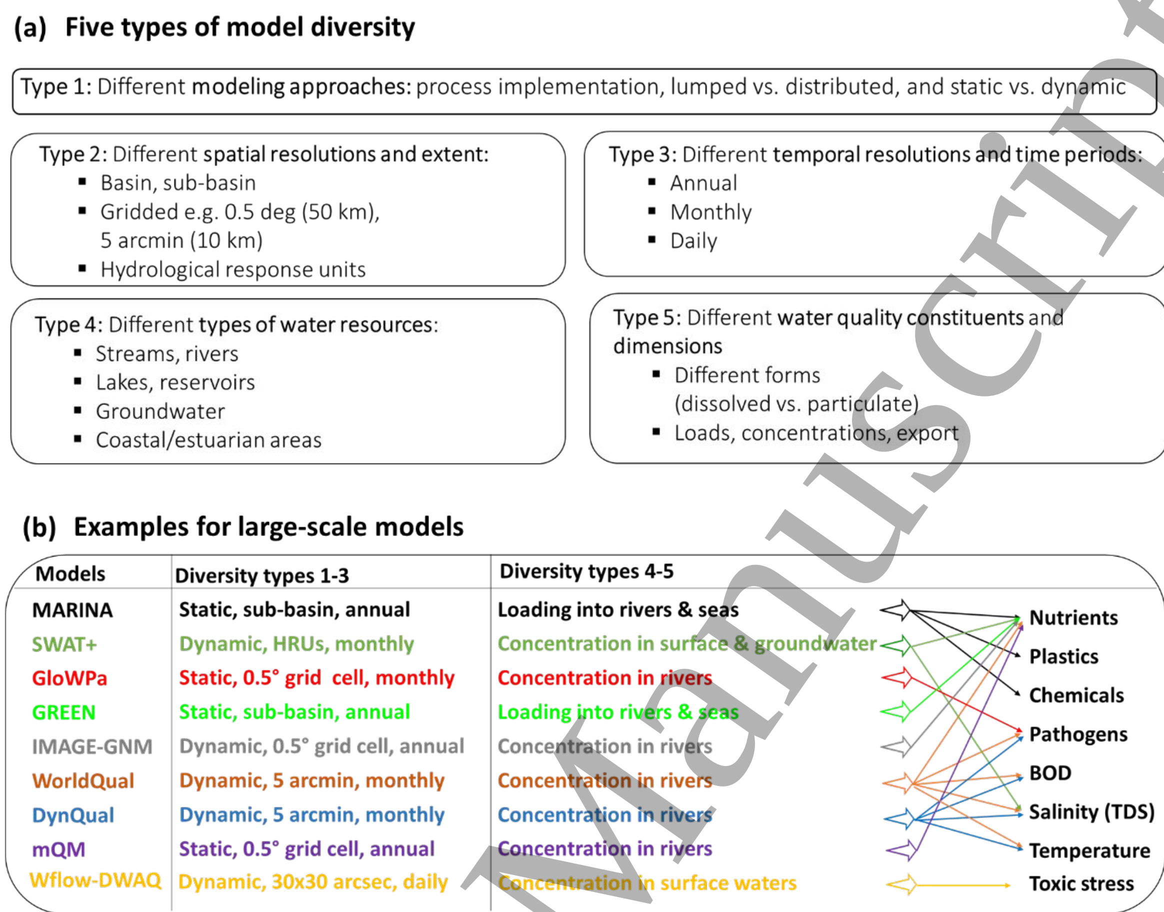

Figure 2. Five main types of model diversity (a) and their examples for the selected nine large-scale water quality models (b) included in the water quality model intercomparisons. TDS is total dissolved solids. Section 2 and Table 1 provide references. Sections 3 and 4 provide a framework for model intercomparisons of water quality and examples. DynQual refers to the first version (v1.0). DynQual and WorlQual models operate on 5 arcminutes (arcmin) and aggregate their results to 0.5° grid cells for model intercomparisons. MARINA refers to the family of the models on multi-pollutant assessments [85]. IMAGE-GNM includes the groundwater component in simulations of nutrient flows from land to surface waters. Source: The overview is based on the UN-WWQA and ISIMIP workshops over the past years (SI Tables A.1-A.2 in Appendix A).

3. Results and Discussion

3.1 Multi-dimension Model Intercomparison Framework for Water Quality

We propose a framework for model intercomparisons of water quality (WQ-MIPs, Figure 3). The framework encourages WQ-MIPs to take multiple aspects into account, covering multiple water quality constituents, sectors (e.g. agriculture, forests), and scales. While multiple sectors and scales are also common in other impact model MIPs (e.g., [49, 86-87]), multiple pollutants are specific to WQ-MIPs. Considering the three dimensions - pollutants, scales, and sectors - makes WQ-MIPs more comprehensive and offers a view of current and future water quality assessments. In advocating the multi-dimension framework for WQ-MIPs, we elaborate on two building blocks: (1) identified (four) objectives for WQ-MIPs and (2) the ISIMIP protocol, which facilitates data harmonization for achieving the WQ-MIP objectives (Figure 3). Below, we focus on large-scale models of surface freshwaters, acknowledging the opportunities that exist to further incorporate other water systems (e.g., lakes, reservoirs, groundwater, and seas).

WQ-MIP objectives

Building on previous, smaller WQ-MIPs [42], we identified four main objectives to enhance WQ-MIPs concerning pollutants, scales, and sectors (Figure 3b). Comparisons among models are valuable not only to identify areas of agreement (e.g., finding robust levels, hotspots, and impacts) but also for elucidating disagreements. For example, disagreements between the models provide an opportunity to further improve modeling approaches to reduce uncertainties and support large-scale modeling of water quality. The following (four) objectives of WQ-MIPs are aimed towards facilitating the learning process and enhancing our knowledge.

Objective 1 is to better understand differences in modeled pollution levels and their associated processes among models (Figure 3a). It aims to look into one water quality constituent (e.g., water temperature) or pollutant (e.g., microplastics) but spans across multiple spatial and temporal scales. Harmonized results can build trust in model outputs, while discrepancies can highlight areas of further scrutiny, e.g., for improving modelling assumptions (learning from each other). In this way, we build upon the strengths of the diverse modelling approaches to simulate water pollution levels. Although few examples exist for this objective [45-46], they cover only a limited number of water quality constituents.

Objective 2 is to identify robust hotspots and their sources (Figure 3a). Prioritizing areas (e.g., hotspots) and pollutants of concern is important for management purposes. Spatially explicit modelled pollution levels are compared to thresholds (e.g., [88]), national water quality targets (e.g., [26, 89]), or environmental policy strategies (such as the Green Deal and Farm-to-Fork [90-91]). Such thresholds are often pollutant-specific and based on the impact on ecosystems or human health [45, 68]. Pollution hotspots occur when pollution levels exceed the identified limits. Again, agreements between models build trust for management intervention, whereas disagreements may spark in-depth analysis to understand their causes, leading to new insights and model improvements [92]. Not only can pollution levels be compared. Also, modelled sources of pollution in the hotspots can be explored. For example, IMAGE-GNM and MARINA models simulate nutrient loadings to coastal waters by source. The analysis can be extended to multiple pollutants [67] or to the temporal dimension, looking at how pollution levels change over time (increases or decreases).. Identifying multi-pollutant hotspots, the exceedance of the thresholds (in space) and trends (increases in pollution in time) helps to define priority areas for pollution management or for improved monitoring needs. Monitoring is often time and resource-consuming and cannot cover all water systems in the world [41]. Some examples of multi-model comparisons exist for hotspots of individual pollutants [42, 45], but are still limited for multiple pollutants.

Objective 3 is to identify robust pollution impacts of water quality on sectors (Figure 3a; e.g., [45]). Impacts can be determined in various ways. One of them is to compare pollution levels of today and in the future to sector-specific thresholds (building on the first objective), focusing on the most impactful. For example, pathogens pose risks to recreation and human health, nitrate threatens drinking water safety, nutrients affect aquatic ecosystems, and salinity impacts agricultural irrigation (see Section 1 for references). Robust impacts are indicated when models tend to agree on the exceedance of the thresholds across space and time. Hence, the WQ-MIP can help identify the most impacted sectors and prioritize solutions for them. Few WQ-MIPs addressed this objective. Some studies assessed global water quality using concentrations of constituents that have the potential to impact irrigation [93], human health [94], and ecosystems [18]. However, an explicit link to the impact of water pollution on sectors is still lacking. Indicator-based methods, such as water scarcity indices [3, 26] offer promising avenues to integrate water pollution into impact assessments.

Objective 4 is to better understand uncertainties in the effects of management strategies under global change (Figure 3a). WQ-MIPs for multiple pollutants, sectors, and scales can build on the previous three objectives. Scenario analyses are particularly valuable for examining how different management or policy choices influence future pollution levels. The ISIMIP experiments can support impact assessments of climate change and socioeconomic developments on water pollution (https://www.isimip.org/). These experiments are based on the combined scenarios of the Shared Socioeconomic Pathways (SSPs) [95] and the Representative Concentrative Pathways (RCPs) [96]. Together, they reflect global change, including population growth, economic developments, urbanization, and climate change extremes. These scenarios can be further developed for future water quality assessments and can incorporate specific environmental strategies (e.g., [27, 97]). Comparing model outputs with and without these strategies helps build greater confidence in projected pollution reductions. Although several studies have evaluated the effectiveness of environmental policies at global [38, 51] and regional [82, 98] scales, multi-model, multi-pollutant, and multi-sector comparisons remain limited.

ISIMIP protocol

ISIMIP is a global platform for climate change impacts and thus aims to support international assessments such as the IPCC. The platform consists of modelers who are organized around sector-specific topics. Today, more than 15 sectors exist: e.g., Water (global), Water (regional), Groundwater on hydrological aspects; Agriculture, energy, and Peat sectors on human activities; Health and Biodiversity sectors on aspects related to impacts on people and nature (https://www.isimip.org/about/#sectors-and-contacts).

The Water Quality sector is relatively new in ISIMIP. Over the decades, numerous large-scale water quality models have been developed independently (see Figure 2). This started in the 20th century primarily for nutrients [72, 104] with a focus on the sources of pollution and eutrophication [105]. Since then, a variety of new global models that address a range of water quality constituents, such as organic and microbial pollution, emerging contaminants, and plastics, have been developed (Figure 2).

We adapted the standard ISIMIP protocol to fit our four WQ-MIP objectives (Figure 3b). In doing so, we considered the diversity in our models (Figure 2), recognizing that not all models simulate the same water quality constituents and thus require different inputs. For example, the modeling of microplastics requires a different set of inputs [60] than modelling nutrients [11] or pathogens [17], or emerging contaminants. This implies that some model inputs in the protocol could be pollutant-specific. Yet, the large number of water quality constituents, not all of which are currently modeled, makes their selection for the protocol difficult. Therefore, in developing the (first in-kind WQ-MIP) protocol, we prioritize a subset of constituents that are currently addressed by large-scale WQ models. We illustrate six broad water quality groups and indicate some representative constituents:

- (1) Nutrients (nitrogen and phosphorus in different forms),
- (2) Organic pollution and Salinity (biochemical oxygen demand and total suspended solids),
- (3) Chemicals and Emerging Contaminants (arsenic, diclofenac, glyphosate, and triclosan),
- (4) Plastics (nano-, micro- and macroplastics),
- (5) Microorganisms (fecal coliforms and *Cryptosporidium*), and
- (6) Temperature.

Other aspects of the protocol include harmonized units and spatial and temporal aggregations for reporting model results. We prioritize model results in annual loads for the nutrients and plastics groups (e.g., kg/year) while also welcoming simulation output results in other units as well. For the chemicals and microorganism groups, we focus on concentrations (e.g., mg/L, oocysts/L). The common spatial resolution of the ISIMIP protocol requires 0.5° grid cells to allow for consistency and cross-sectoral analyses. We follow this to be able to connect to other sectors and perform cross-sectoral impact assessments of water quality.

Integrating and synthesizing existing model outputs under the framework of the ISIMIP protocol can already offer valuable insights. Hence, this initiative aims to acknowledge the community efforts over the past years and empower large-scale modelers in WQ-MIPs. In this way, we establish more connections between the water quality modelers and their communities and engage them in joint activities. Model intercomparisons are, therefore, largely based on existing knowledge and model simulations that predominantly rely on ISIMIP2b simulations of hydroclimate forcings [99]. In this WQ-MIP, we acknowledge inconsistencies in model inputs and approaches, learn from them (Section 3), and provide a platform to improve future WQ-MIPs (Section 4).

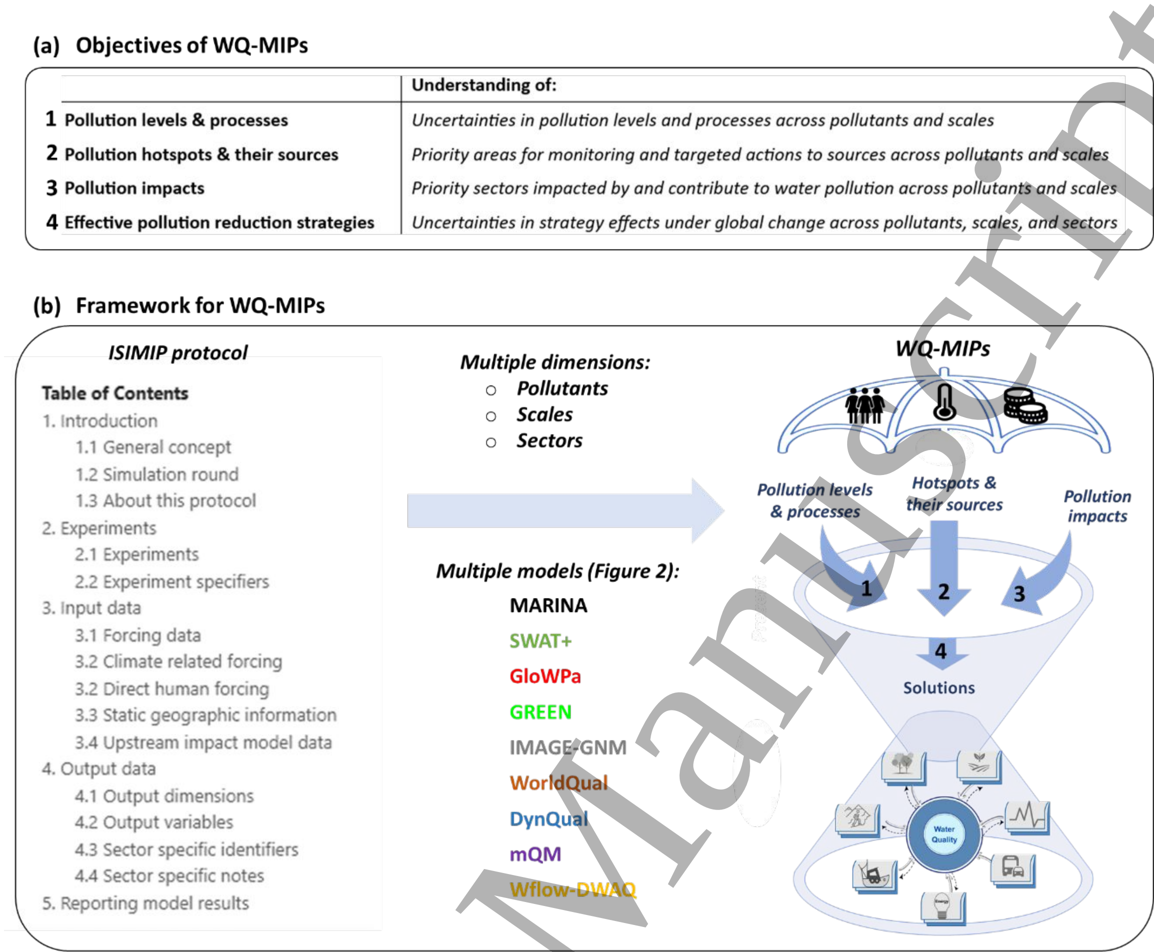

Figure 3. The identified four main objectives of WQ-MIPs (a) and the associated framework (b) taking the large-scale models from Figure 2 as an example. WQ-MIPs are water quality model intercomparison projects focusing on pollution levels & processes, pollution hotspots & their sources, and pollution impacts to identify solutions across pollutants, scales, and sectors under global change (e.g., socioeconomic developments, climate change). ISIMIP is the Inter-Sectoral Impact Model Intercomparison Project. The proposed framework is based on the WQ ISIMIP protocol to consider cross-sectoral aspects (Figure 1) and model diversity (Figure 2).

3.2. Illustrative Examples

We provide four practical examples related to the four WQ-MIP objectives (Figure 3). **Example 1** focuses on pollution levels at multiple scales (Objective 1, Figure 3), comparing nitrogen concentrations in Africa and Europe as simulated by IMAGE-GNM, mQM, and SWAT+ models (Figure 4). **Example 2** is related to Objective 2 (hotspots; Figure 3), identifying robust multi-pollutant hotspots under future climate-induced hydrological uncertainties. Here, one model (MARINA-Multi) is used to simulate trends of several pollutants (e.g., nitrogen, plastics, diclofenac) driven by five different Global Climate Models (GCMs), which influence the hydrological inputs (Figures 5 and 6). Here, we define robustness based on the multi-GCM agreement on pollution trends. **Example 3** is overarching between Objectives 2 and 3 (Figure 3). This example focuses on the robustness of concentration-based water quality trends and reflects the potential impact on sectors (Figure 7). Similar to Example 2, the comparison concerns the GCMs for one model (e.g., DynQual v1.0). Finally, **Example 4** is related to Objective 4 on solutions (Figure 3), focusing on the effects of pollution reduction options and environmental policies on water quality (Figure 7). Here, two models of similar spatial and temporal resolutions (e.g., MARINA-Nutrients and GREEN) are used to simulate nitrogen and phosphorus loadings into European seas under management scenarios.

Our examples focus on the Shared Socioeconomic Pathway 5 (SSP5) and the Representative Concentration Pathway 8.5 (RCP8.5) scenario for 2050. SSP5 has high challenges for mitigation and low challenges for adaptation [95]. This scenario assumes a world with high economic development, moderate population growth, and low environmental awareness [95]. Specifically, in the first half of the century, the population is expected to increase in all regions around the world except the reforming economies. RCP8.5 assumes high global warming and represents a “high emissions” scenario dominated by fossil fuels [96].

Below, we present the examples, followed by their comparison in terms of lessons, strengths, and limitations.

Example 1: *Model intercomparisons across spatial scales – Europe vs Africa*

- Purpose: to better understand uncertainties in pollution levels and their hotspots across scales in the future (2050);
- Water quality constituent: total nitrogen (TN) in surface waters;
- Models: IMAGE-GNM [11], mQM [74-75] and SWAT+ [68];
- Scales: Europe (Figure 4a) and Africa (Figure 4b);
- Hotspots definition: mean annual TN concentration exceeds the threshold of 2.5 mg/L following [45] and [88];
- Comparisons: among the outputs of the two separate models (annual at the grid of 0.5°) while acknowledging variations in their model inputs and structures.

For Europe (Figure 4a), TN pollution results are compared between the IMAGE-GNM (integrated, global terrestrial nutrient model) and mQM (dynamic travel-time augmented water quality model). The results indicate a strong overall agreement in identifying TN pollution hotspots – regions where mean annual TN concentrations exceed the 2.5 mg/L threshold. Around 77% of the total grid cells where both models have agreement. The consistency among the two models encompasses more than two-thirds of the projected critical areas to be at risk in 2050 (Figure 4a). Models also show a high level of agreement (across 80% of the area) in classifying non-critical areas. This high level of agreement corroborates the robustness in capturing major future trends in TN pollution across the European landscape. However, some regional discrepancies exist. For example, in some parts of southern Ukraine and central Italy were identified as critical by only one model but not the other. These differences are likely structural, including different model parameterizations and embedded processes. For example, in mQM, the excess (diffuse) nutrients are partly allowed to build up in a source region, a soil pool, as opposed to such considerations in IMAGE-GNM. Such output discrepancies emphasize the models' specific characteristics that deserve further analysis to understand the factors driving them.

For Africa (Figure 4b), the TN river pollution results for 2050 projected by the IMAGE-GNM and SWAT+ models are compared. The overall agreement between the models is, once again, high; over 70% of the area is consistently classified as either critical or non-critical. Both models project that approximately 27% of African river reaches will exceed the critical threshold of 2.5 mg/L by 2050. The models also agree on over 72% of the non-critical areas, showing their ability to simulate a broad range of pollution levels. This good level of spatial agreement indicates the robustness of both models in representing major future trends in TN pollution across the African continent. Nevertheless, regional discrepancies are evident, especially in parts of the Okavango and Orange basins in Southern Africa, where the models diverge in their classification of critical areas. These discrepancies may be attributed to differences in model inputs, structural configurations, parameterization, and scale of application. For example, the IMAGE-GNM model is run at 0.5° grid cells, while the SWAT+ model is run at a hydrological response unit (HRU). Investigating these model-specific characteristics can help clarify the factors influencing divergent outputs and improve our understanding of model strengths and limitations. It is also important to note that the application of a binary threshold (e.g., ≤2.5 vs. >2.5 mg/L) simplifies the classification of critical areas but may introduce classification errors in model intercomparisons. Small inter-model differences near the threshold can be exaggerated, increasing disagreement despite numerical proximity. Range-based classifications would better preserve the continuous nature of the data and reduce the risk of misclassification bias. In conclusion, while the global and continental models offer robust and largely consistent projections for future TN pollution across Europe and Africa, regional

227 disparities underscore the importance of using different models, e.g., global and regional, to better capture a range of potential outcomes. This could better inform comprehensive nitrogen management strategies for continents.

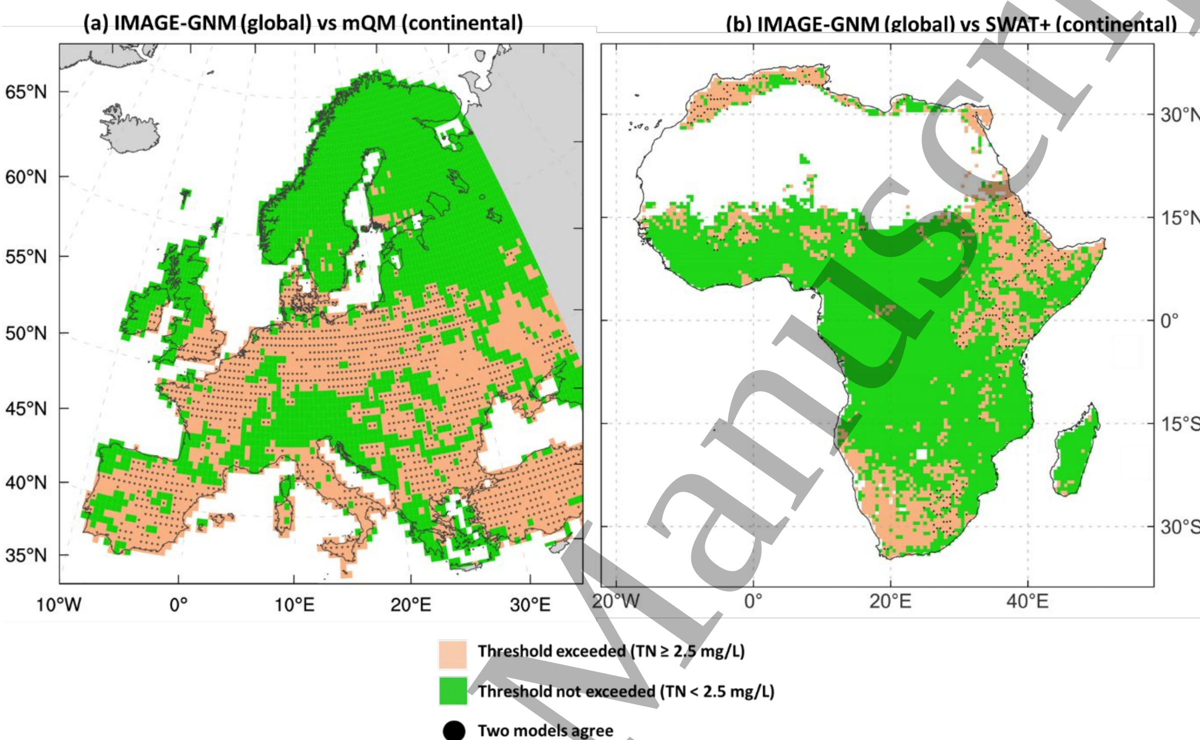

Figure 4. Model intercomparisons of nitrogen pollution hotspots in rivers across spatial scales (global vs continental models) for 2050 following the combined Shared Socioeconomic Pathway 5 and Representative Concentrative Pathway 8.5 (SSP5-RCP8.5). Two examples are for Europe (a) and Africa (b). Nitrogen pollution hotspots are defined as total nitrogen (TN) mean annual concentrations in rivers exceeding the threshold of 2.5 mg/L, according to Schulte-Uebbing, Beusen [88] and Bouwman, Bärlund [45]. The hotspots are compared between the global (IMAGE-GNM) and continental models (mQM and SWAT+). Note that, for clarity, the dots represent model agreement only for grid cells exceeding the threshold limit (orange). Model agreement in safe areas (green) is also significant but not shown in detail here. Source: IMAGE-GNM [11], mQM [74-75] and SWAT+ [68].

Example 2: ***Model intercomparisons across pollutants – Global analysis***

- Purpose: to better understand uncertainties in future multi-pollutant hotspots and their uncertainties due to projected future hydrology;
- Water quality constituents: river exports of total dissolved nitrogen (TDN), microplastics (MIP), macroplastics (MAP), and diclofenac (DCL, painkiller);
- Models: MARINA-Multi [67], which is part of the MARINA model family [85] whose hydrology is based on five GCMs [100];
- Scales: Global and sub-basins (Figures 5 and 6);
- Hotspots definition: river exports of pollutant loads exceed 20% of the increase from 2010 to 2050 SSP5-RCP8.5, following existing approaches [27, 67];
- Comparisons: among the river exports of pollutants and five GCMs with the consistent socioeconomic model inputs and structure.

All four selected pollutants are expected to increase by 2050 (Figures 5 and 6). However, the trends differ among regions and pollutants. TDN river exports are projected to increase by more than 20% by 2050 in many sub-basins in North America, Southern Asia, and Russia (Figure 5). Globally, this covers up to 40% of the surface areas (Figure 6b). Conversely, TDN river exports should reduce in several sub-basins, including areas in Europe, China, and Australia (Figure 5). In about 20% of the global land surface, the decreases range between 0-20%, whereas in 40% of the land, the decrease is more than 20% (Figure 6b). The projections of MIP river exports are more pessimistic. Approximately 80% of the global surface area is projected to experience increases in MIP river exports by over 20% from 2010 to 2050 (Figure 6). Increases in MAP and DCL river exports are projected for approximately 40% of the global area, especially in Africa, North America, and Asia (Figures 5 and 6). The differences in future projections among pollutants and across regions are largely associated with population growth, human activities on the land, and socioeconomic developments. For example, the population is expected to increase dramatically in Africa by 2050, increasing the demand for food [101], which in turn may trigger intensification of agricultural production and an increase in nutrient pollution. Urbanization is expected to increase around the world, with over two-thirds of the global population living in cities by the end of the 21st century [102]. This will likely increase sewage connections, discharging pollutants. This may cause more MIP and DCL reaching African rivers, where higher population and sewage connections may not be served by appropriate wastewater treatment. More people will generate more waste, and thus, mismanaged waste will likely contribute to MAP in rivers. Management of waste and treatment depends largely on societal economic developments.

Five GCMs were used as the basis to simulate river hydrology by the VIC model [46, 79, 103]. Hydrological outputs of the VIC model (e.g., river discharges and runoff) were used as input to the MARINA-Multi model to simulate river exports of pollutants for 2010 and 2050 [100]. Generally, GCM simulations show similar spatial patterns of pollutant river exports between 2010 and 2050 (Figures 5 and 6). This indicates the robustness of the future projections by the MARINA-Multi model in terms of climate-induced hydrology. Some discrepancies among simulations are noticeable in some regions, particularly in Africa for TDN (Figures 5 and 6), associated with differences in projected climate forcings to simulate hydrology (more details in [100]).

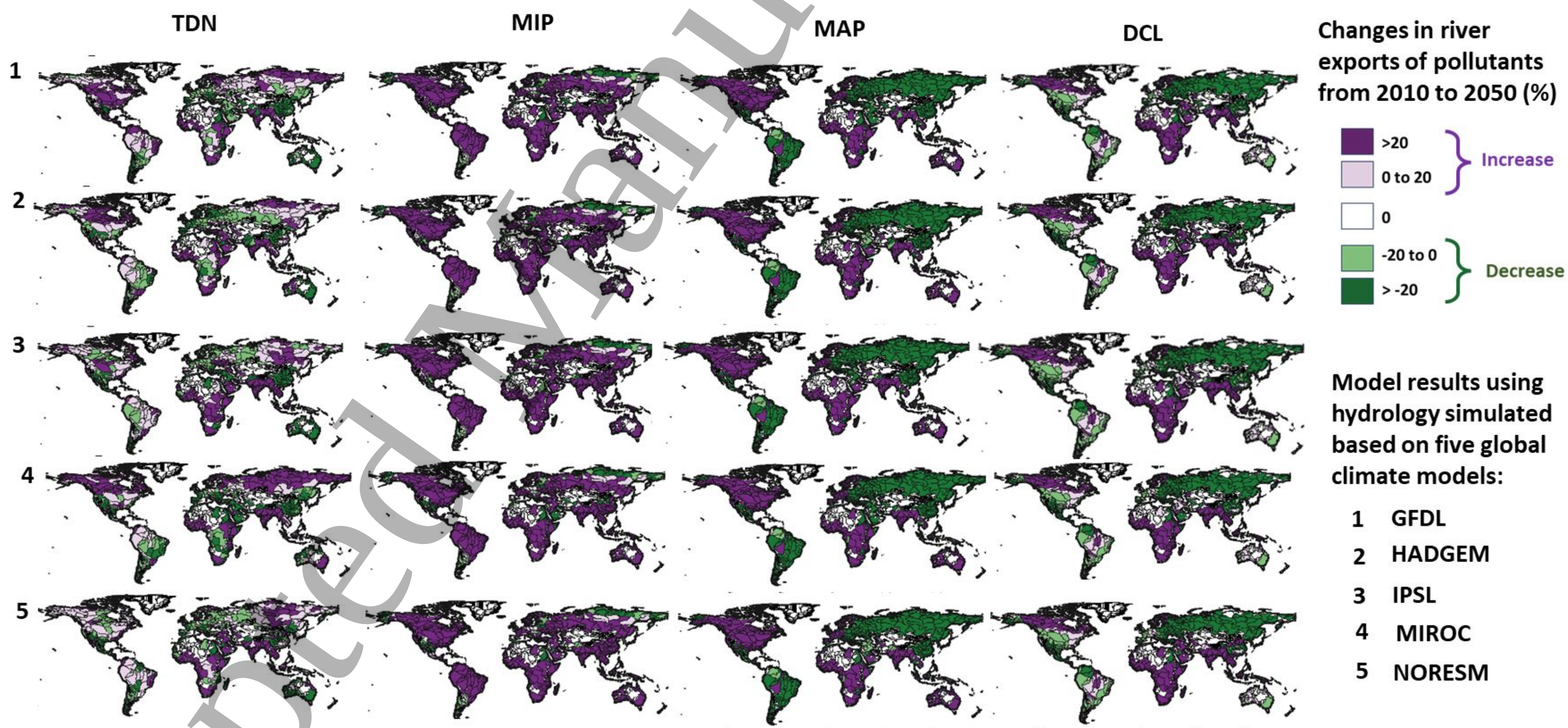

Figure 5. Model intercomparisons of pollutant river load exports from 2010 to 2050 for the combined Shared Socioeconomic Pathway 5 and Representative Concentrative Pathway 8.5 (SSP5-RCP8.5). Model results differ for the hydrology inputs, based on five global climate models, following the ISIMIP protocol, Phase 2b (https://www.isimip.org/). Hydrology was simulated using the VIC model and then used as input into the MARINA-Multi model. Source: the MARINA-Multi model [67, 100].

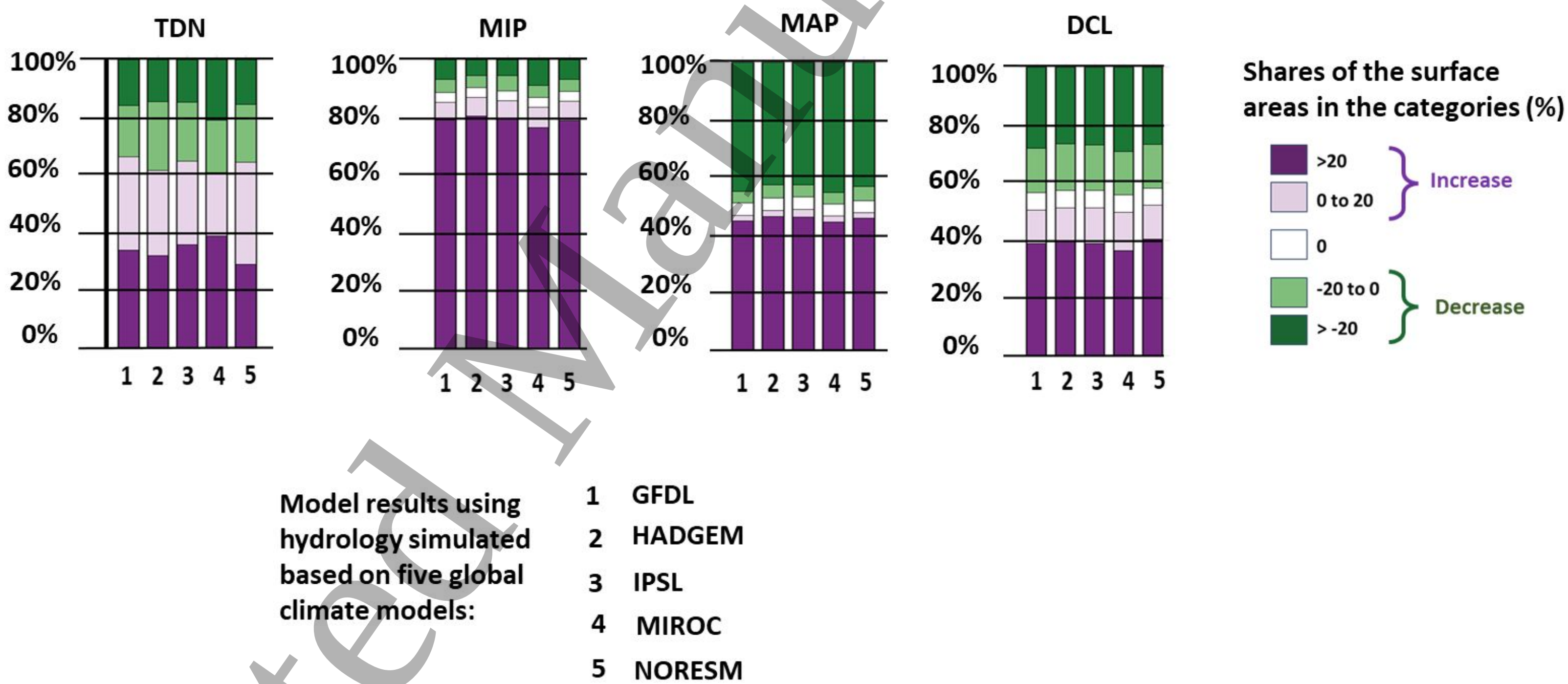

Figure 6. Shares of the surface areas in the categories for changes in river load exports of pollutants from 2010 to 2050 for the combined Shared Socioeconomic Pathway 5 and Representative Concentrative Pathway 8.5 (SSP5-RCP8.5). Model results differ for the hydrology inputs, based on five global climate models, following the ISIMIP protocol, Phase 2b (https://www.isimip.org/). Hydrology was simulated using the VIC model and then used as input into the MARINA-Multi model. Source: the MARINA-Multi model [67, 100].

Example 3: ***Model intercomparisons across sectors – robustness of change and potential impact***

- Purpose: to better understand how climate-driven uncertainties affect water quality trends and their potential impact across sectors;
- Water quality constituents: water temperature, concentrations of total dissolved solids (TDS), biological oxygen demand (BOD), fecal coliforms (FC);
- Models: DynQual v.1.0 model [53] driven by five GCMs;
- Scales: Global;
- Hotspots definition: Robust trends of individual pollutants are defined if at least 3 out of 5 GCMs are in agreement. Trends are defined as changes in pollutant concentrations bigger than 5% between 2010 and 2050 SSP5-RCP8.5;
- Comparisons: among river concentrations using five GCMs but consistent socioeconomic model inputs and structure to identify the robustness of future changes in impact-related water quality parameters.

Following Bak, Micella [100], we set a 5% threshold to determine whether the changes in pollutant concentrations simulated based on five different GCMs exhibited an increasing trend (>5%), a decreasing trend (<5%), or no trend (between -5% and 5%). We then combined the results from different GCMs to assess the robustness in projected changes worldwide, with robust changes identified when there was agreement between at least 3 GCM simulations and non-robust areas when fewer than 3 GCMs agreed (Figure 7a). We relate the results to potential impacts on several sectors (Figure 7b).

Water temperature showed robust increases across 96% of the global land surface, potentially impacting power production from thermoelectric power plants across the globe (Figure 7b: VI)[36]. BOD is often used as an indicator of organic pollution [104]. High concentrations could reduce dissolved oxygen, impacting fish and damaging their natural habitats (Figure 7b: I), as well as changing fish stock for aquaculture (Figure 7b: V). BOD showed robust increases across 50% of the global land surface, mainly in South America, parts of Africa, and Southeast Asia. FC is an indicator of water-related human health impacts [105]. High concentrations in waters could lead to diarrhea in people who swim in it(Figure 7b: III), drink it, or consume fresh produce irrigated with it (Figure 7b: IV) [54, 94]. FC showed robust increases across 43% of the surface area, notably in sub-Saharan Africa, Asia, parts of South America, and northwestern America. Interestingly, the spatial patterns of BOD and FC were similar, suggesting a common underlying trend due to common pollution sources, as also indicated by Jones, Bierkens [39]. TDS is an indicator of salinity [19], with crops sensitive to high salinity levels in irrigated water (Figure 7b: II). The five GCM models generated little agreement in TDP projections (Figure 7). However, TDS projections agreed on an increase of TDS in 25% of the global surface area in parts of South Asia and Central Africa. The spatial variability in TDS increase is more localized than the global trends of water temperature. Apart from water temperature, the other three pollutants exhibit robust decreases along the eastern coast of North America, continental Europe, and the northern part of Asian. On the other hand, Africa generally shows robust increasing trends for all four pollutants.

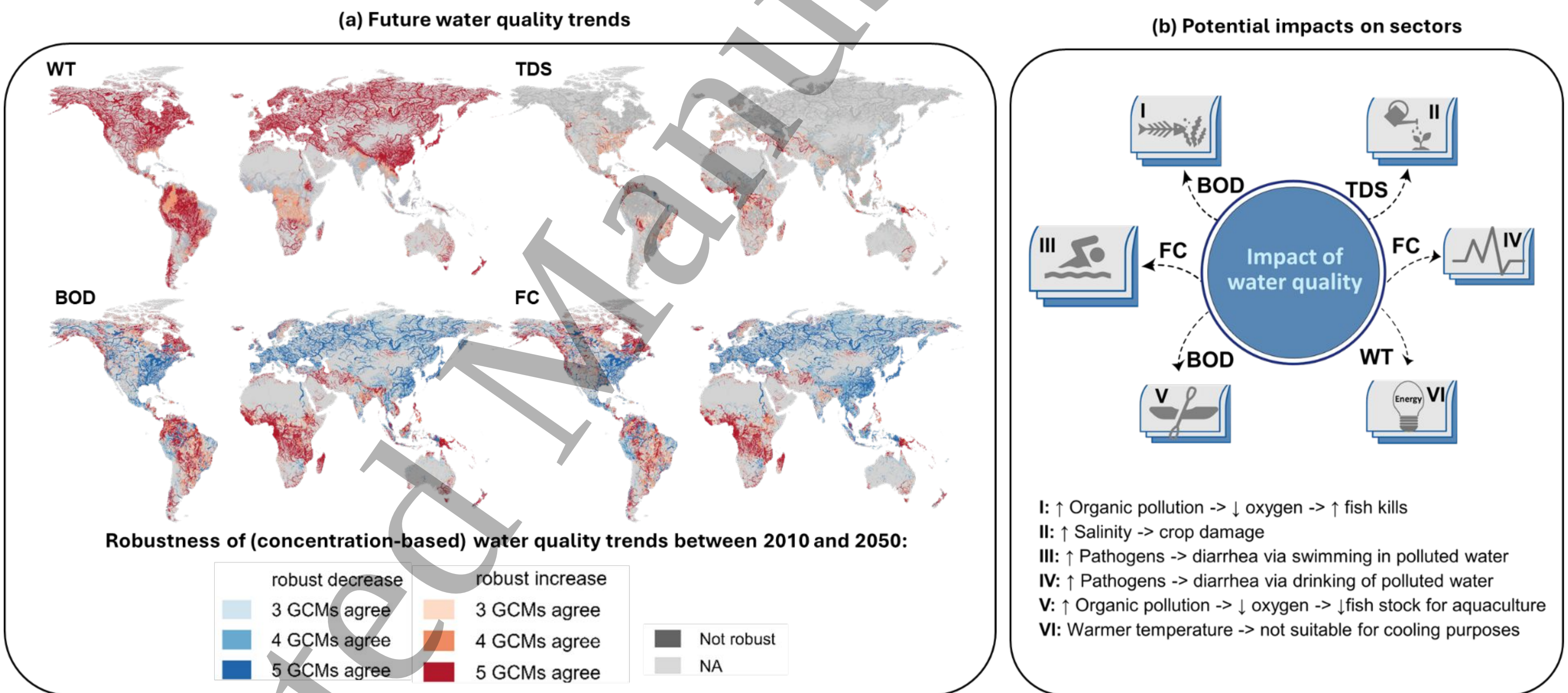

Figure 7. Robustness of changes (a) in water temperature (WT) and concentrations of total dissolved solids (TDS), biological oxygen demand (BOD) and fecal coliforms (FC) between 2010 and 2050 for the combined Shared Socioeconomic Pathway 5 and Representative Concentrative Pathway 8.5 (SSP5-RCP8.5) and potential impacts of these water quality constituents on sectors (b). The robustness is defined as the agreement in trends (decreases of <-5 % or increases of >5%) between three or more out of five Global Climate Model (GCMs)-driven simulations. Source: the DynQual model v1.0 [39, 53] for (a) and Example 3 of Section 3 for references to support (b).

Example 4: ***Model intercomparisons across seas – reduction measures & policies***

- Purpose: to identify robust reduction strategies to mitigate future coastal eutrophication
- Water quality constituents: total nitrogen (TN), total phosphorus (TP), total dissolved nitrogen (TDN), and total dissolved phosphorus (TDP) loadings;
- Models: GREEN [70-71] and MARINA-Nutrients for Europe [83, 106];
- Scales: basin and their European seas;
- Hotspots definition (if applicable): Not applicable
- Comparisons: potential changes in nutrient loadings into the European seas by 2050 under different management scenarios.

GREEN simulated the effects of the full implementation of current and foreseen EU policies (implemented only in the 27 countries of the European Union), whereas MARINA-Nutrients focused on the use of bio-based fertilizers from processed animal manure (for nitrogen) and recovered phosphorus in sludge from treated wastewater. Bio-based fertilizers are the products of processed manure during treatment. The scenario also assumes increased nutrient efficiency (i.e., fewer losses and more recycling).

The comparison shows promising reduction potentials for nutrient loadings in most coastal waters of Europe (Table 2). Both models project reductions in nutrient loadings into the coastal waters of the Baltic, Black, and Mediterranean Seas between 2020 and 2050. However, GREEN suggests a lower reduction in TN and TP loadings than MARINA-Nutrients for TDN and TDP. According to GREEN scenarios, the current EU policies could reduce between 7% and 14% of TN and TP by 2050, which seems promising for the Baltic, Black, and Mediterranean seas. For the other seas, loading changes depend on the intensity of agricultural activities and urbanization. Based on MARINA-Nutrients scenarios, management could potentially reduce between 4% and 19% of future TDN loadings into all European seas except for the Arctic because of its less dominant agricultural land. If recovered phosphorus from treated sewage sludge is used as a bio-based fertilizer, future TDP loadings could be reduced between 3% (Arctic) and 68% (Mediterranean) (Table 2).

The two models are similar in their process-based approaches and simulate N and P exports to coastal waters by rivers and by source. However, they differ in nutrient forms and temporal and spatial resolutions. MARINA-Nutrients focuses on total dissolved N and P, while GREEN focuses on total N and total P. MARINA-Nutrients is uncalibrated for simulating annual nutrient loadings into the EU seas. GREEN is calibrated for simulating annual nutrient loadings into the EU seas. Another difference lies in the baseline scenarios: SSP5-RCP8.5 (MARINA-Nutrients) versus SSP5-RCP4.5 (GREEN). Despite the differences, the two models provide useful insights to identify promising potential reductions in future nutrient loadings into seas, focusing on the effects of European policies (GREEN) and nutrient management strategies (MARINA-Nutrients).

3.3 Reflection on Comparisons

Our four examples

The four examples take different approaches to model intercomparisons of water quality (Table 3) that reflect their purposes. Understanding uncertainties in river pollution levels (Example 1 with nutrients) and trends over time (Example 3 with multiple pollutants) brings new insights and enlarges our scientific knowledge in both space and time. Another purpose is to identify robust multi-pollutant hotspots in the future. Hotspots usually require setting thresholds. Example 1 defined hotspots based on nitrogen levels below which ecosystems are "safe". In Example 2, the load threshold was simple and consistent for all pollutants: a 20% increase between 2010 and 2050. In Example 3, the threshold was set for concentration trends, i.e, change in time. This all highlights a variety of ways to set a threshold.

However, the four examples are part of the ISIMIP exercise and subject to some limitations (Table 3. Examples 1 and 4 focus on one pollution type but suffer inconsistencies in resolution and model input (e.g., Example 1) or assumptions (e.g., in Example 4). Examples 2 and 3 are multi-pollutants but took simple approaches to define the pollution hotspots. For these examples, only one model was used, which increased consistency in model inputs (the same spatial and temporal resolution), and uncertainties focused more on inputs generated by climate projections. Clearly, the insights gained by these examples are very different. They also offer a great opportunity to improve the follow-up WQ-MIPs (e.g., ISIMIP3a and ISIMIP3b runs).

Our four WQ-MIP objectives

Classical MIPs are usually made for one variable among at least two models. This is often the case for impact and hydrological models within the ISIMIP platform. However, this is not always possible in the Water Quality sector because of the many model diversity aspects (see Section 3.1), particularly in the simulated water quality constituents, which results directly from the broad definition of "Water Quality". This model diversity makes intercomparisons challenging across all models, but also brings opportunities for new types of intercomparisons and applications to support water management and decision making at the cross-regional scale. Our four objectives present those opportunities and have advantages and disadvantages.

Objective 1 is the most classical in that it explores simulations of the same variable to better understand uncertainties in pollution levels and their processes. An advantage is the consistency in one variable. A disadvantage is that the large-scale models currently consider only a few common variables: five models for nutrients, three models for pathogen pollution, two models for organic pollution (indicated by BOD), three for salinity, and two for water temperature (see Figure 2). Objectives 2-4 can be achieved by using the same variables, but this is not a requirement. This is where the Water Quality ISIMIP sector is unique and differs from the others. For example, hotspots can be compared across pollutants (Objective 2, Figure 5). The impact of water pollution on societal activities depends on multiple water quality variables (Objective 3, Figure 7) such as salinity levels (irrigation), nitrate pollution (drinking purpose), and pathogen pollution (recreational activities). Uncertainties in pollution reduction effects can be compared across pollutants (Objective 4, Table 2). To achieve the objectives focusing on multi-pollutant aspects, we proposed intercomparisons among GCMs using the same modeling approach (e.g., Figure 5). This is possible for large-scale models that simulate more than one pollutant (Figure 2), thus guaranteeing the consistency in the model approach and resolutions (for inputs and outputs).

We believe that our four objectives are achievable, considering the large-scale models that are already available. We highlight the different types of model intercomparisons that model diversity offers. Modelers should, however, be careful when selecting variables for large-scale model intercomparisons, duly consider inconsistencies, and acknowledge the uncertainties in models.

Static versus dynamic approaches

Some models are dynamic (e.g., DynQual, IMAGE-GNM) while others take a static approach (e.g., MARINA, GREEN, Figure 2). The main advantages of static model simulations are that the models are computationally light. This means that such models can perform a large number of simulations and explore different scenarios. They often have fewer and better-constrained input data (e.g., long-term means of river discharge, nutrient inputs, population, and land management). These models usually produce multi-annual average loads that are well suited for long-term “pressure” assessments (e.g., SDG-6.3 tracking). However, the models do not explicitly consider dynamics and thus legacy effects. The true “static year” may lag drivers by decades and cannot capture year-to-year variability. Such models are usually less suitable for short-term policy evaluation (e.g., seasonal fertilizer bans, real-time forecasting).

The main advantages of dynamic model simulations are that the models resolve year-to-year and intra-annual variability in water quality dynamics (on a monthly to even daily level). This allows for legacy characterization (e.g., in the case of nutrients), intra-annual or seasonal dynamics of variables like water temperature, and analyses of impacts of climate extremes such as droughts, heatwaves, rainstorms, and floods on water quality. Such models can be forced with transient climate and management trajectories, enabling attribution of trends to specific drivers. However, these dynamic model simulations demand high input data and have much higher computation time, allowing for a limited number of scenario runs.

In Example 1 (Figure 4), we compared two dynamic models: SWAT+ and IMAGE-GNM. In Example 2 (Figures 5 and 6), we used the static MARINA model, whereas Example 3 used the dynamic DynQual model. In Example 4 (Table 2), we compared reduction effects for nutrient loadings into European seas between two static models (MARINA and GREEN). Our examples do not mix static and dynamic approaches in model intercomparisons. However, this might be considered and could lead to new insights and model improvements. Thus, we do not disregard such comparisons, but argue for transparency and open discussion on limitations and learned lessons.

On the other hand, the consequences for the development of the Water Quality ISIMIP sector might evolve. For example, to report statically calculated variables versus dynamically calculated variables may require defining two different temporal resolutions for the same output variable. These aspects should be considered when comparing the model outputs from static and dynamic simulations. Harmonizing the protocol for these aspects becomes even more important, which are the next steps in the Water Quality sector (see Section 4, Direction 2).

Roadmaps for overcoming inconsistencies

Roadmaps follow the general ISIMIP protocol that requires the harmonized spatial and temporal level of detail of participating models in the model intercomparisons. This is for all sectors included in the ISIMIP platform (https://www.isimip.org/). In fact, harmonization is needed not only for model inputs but also for model outputs, which is the core of the ISIMIP protocol that requires a resolution of 0.5° grid cell to facilitate cross-sector comparisons. Some models may need aggregation (upscaling, e.g., from 5-arc-min) or disaggregation (downscaling, e.g., from basin) of inputs and outputs.

In the Water Quality sector, several models already operate at the required ISIMIP resolutions, while other models need efforts in harmonizing their inputs and outputs. Models simulating annual means of total nitrogen, total phosphorus, and water temperature operate on the standard 0.5° grid cell. Examples are IMAGE-GNM, mQM, and SWAT+ (Figure 2), which simulations can therefore be combined directly with water availability and water demand data to provide, for example, integrated water-security and water scarcity indicators under current and future climate scenarios (e.g., [2, 26]).

On the other hand, models that work at 5-arc-min resolution (~10 km resolution, e.g., DynQual, WorldQual) require aggregations (upscaling) and on sub-basins (e.g., GREEN, MARINA) disaggregation (downscaling) to the scale of a 0.5° grid cell (~50km) for consistency with the other ISIMIP output. An open-source toolkit (Python or R) can be used to perform automated re-gridding and basin-to-grid translation, so users may choose between detail and ease of integration. Such scripts can be used to route sub-basin nutrient loads into downstream lake polygons (Lake sector in ISIMIP) or marine coastal water bodies (Coastal Systems sector in ISIMIP), enabling, for example, eutrophication-risk studies that couple MARINA river exports to the Marine biogeochemistry ensemble. Section 4 elaborates on four future directions, of which harmonization is one of them.

Table 2. Changes in nutrient loadings into the coastal waters of the European seas between 2020 and 2050 (%). TN and TDN are total nitrogen and total dissolved nitrogen, respectively. TP and TDP are total phosphorus and total dissolved phosphorus, respectively. ReNuRe-NUE and Padv-PUE assume increased nitrogen (NUE) and phosphorus (PUE) use efficiencies and the application of bio-based fertilizers: processed manure (ReNuRe) and sludge (Padv). The study area and definitions of the seas, as well as the scenario descriptions, are provided in SI Figures B.1 and C.1 in Appendix B and C.

Seas in the MARINA model	**TDN**	**TDP**	**Sources and remarks**
Atlantic Ocean	-5	-51	o MARINA-Nutrients model (Figure B.1 and Table B.1) [83, 85] o Strategies: the ReNuRe-NUE scenario for N and Padv-PUE scenario for P assuming the use of ReNuRe fertilizers (N), increased use efficiencies (N and P), recovered P from treated sewage sludge & advanced upgrade of wastewater treatment plants (for P) o 2020: average of 2017-2020 o 2050: SSP5-RCP8.5 o N and P: total dissolved including inorganic & organic
Baltic Sea	-10	-40	
Black Sea	-4	-57	
Mediterranean Sea	-19	-68	
Arctic Ocean	5	-3	
North Sea	-4	-35	
Seas in the GREEN model	**TN**	**TP**	**Sources and remarks**
Atlantic Ocean (Greater North Sea, Bay of Biscay and the Iberian Coast, Celtic Sea)	-5	0	o GREEN model (Figure C.1 and Table C.1) [70-71, 98] o Strategies: combined effects of EU policy measures* and climate change o 2020: average of 2015-2024 o 2050: average of 2015-2024 using SSP5-RCP4.5 o N and P: totals including inorganic, organic, and particulate
Baltic Sea	-14	-14	
Black Sea	-10	-7	
Mediterranean Sea	-13	-13	

**Main EU policies such as the Common Agricultural Policy (CAP), the updated legislation addressing greenhouse gas emissions, and the revision of the Urban Waste Water Treatment Directive*

Table 3. Summary of the four examples of model intercomparisons of water quality, including their general information, strengths, and limitations. Pollutants: TN = total nitrogen; TDN = total dissolved nitrogen; TP = total phosphorus; TDP = total dissolved phosphorus; MIP = microplastics; MAP = macroplastics; WT = water temperature; BOD = biological oxygen demand; TDS = total suspended solids; FC = fecal coliforms. Section 2.1 provides references to the models.

	Example 1 (pollution levels)	**Example 2 (hotspots & trends)**	**Example 3 (hotspots & impact)**	**Example 4 (strategy effects)**
General information				
Link to Figure 3 objectives	Pollution levels	Multi-pollutant hotspots	Multi-pollutant hotspots	Reduction strategies
Example objectives	Uncertainties in pollution levels	Uncertainties in hydrology-related hotspots	Robustness of change and potential impact	Robust reduction effects
Pollutants	TN	TDN, MIP, MAP, DCL	WT, BOD, TDS, FC	TDN & TDP* and TN & TP**
Covered areas	Africa & Europe	Global	Global	Europe
Used models	SWAT+, mQM, IMAGE-GNM (ensembles over 5 GCMs)	MARINA-Multi, 5 GCMs	DynQual v.1.0, 5 GCMs	MARINA-Nutrients, GREEN (averages)
Years	2050	2010 & 2050	2010 & 2050	2020 & 2050 ***
Water resources	Rivers	Rivers & seas	Rivers	Seas
Units	Concentrations	Loadings	Concentrations	Loadings
Comparisons	Between the models & regions	Between the GCMs & pollutants	Between the GCMs & pollutants	Between the models & pollutants
Hotspots based on	Thresholds for levels	Thresholds for trends (>20% increase)	Thresholds for trends & GCMs (>3/5)	-
Strengths & limitations				
Strengths	Easy comparison for one pollutant; >2 models exist for nutrients and their thresholds.	Easy comparison using one model; simple & consistent thresholds for multiple pollutants	Easy comparison using one model; simple & consistent thresholds for multiple pollutants	Simple comparison between seas; >2 models exist for nutrients
Limitations	Inconsistency in inputs between the models (space, time), approaches; Efforts for harmonization	Efforts for harmonization of simulated hydrology to sub-basins; No link to the impacts	Data harmonization efforts; Robustness focuses on 3/5 GCMs; Implicit link to impacts	Inconsistency between the models (basin delineations, years, scenarios)

*TDN and TDP are for MARINA-Nutrients. ** TN and TP are for GREEN.
***Averages centered on the reference year

4. Concluding Remarks and Future Agenda

In our study, we synthesized existing insights and proposed four objectives for model intercomparisons of water quality with four promising and illustrative examples for specific models. All water quality models were developed and evaluated independently. They have similarities (e.g., harmonized storylines of the future scenarios) and differences (e.g., spatial and temporal aggregations). Nevertheless, the examples serve as an inspiration to develop model intercomparisons further, and proceed towards full harmonization of model inputs and outputs. In sketching a water quality ISIMIP community future agenda, we identify four main directions to advance water quality model intercomparisons under global change.

Direction 1: Developing and enhancing existing large-scale datasets for model evaluation

To support the development of more reliable and comprehensive multi-pollutant and multi-sector water quality models, consistent datasets are needed. Datasets comprise model inputs, model outputs, and monitoring data. We call for a greater effort to combine broader data coverage, emerging sensing technologies, and state-of-the-art data-model fusion scheme frameworks. These datasets will enable scientific communities and decision-makers to better project and manage water resources under the pressure of global change.

Model evaluation, including validation against monitoring data, is essential to build trust in model results. Often, monitoring data is available only for certain water quality constituents (e.g., mainly nutrients) and is limited in time and space (https://gemstat.org/), challenging the validation of large-scale water quality models [41].Particularly in the context of global change, large-scale datasets are needed to capture both the breadth (multiple sites and conditions) and depth (long time series in key catchments) for robust projections. Strokal, Wang [107] propose 13 alternative strategies for further development and enhancement of large-scale existing datasets (e.g., model inputs) with the use of innovations (e.g., remote sensing, deep learning). Traditionally, ground-based monitoring records, such as gauge monitoring networks (e.g., https://gemstat.org/), could be integrated with new observations made available by technological innovation and methodological developments [41]. Examples are satellite remote sensing data that could be used to derive near-continuous spatial coverage related to water color, turbidity, and chlorophyll concentrations. However, remote sensing data cannot directly capture many water quality constituents (e.g., emerging contaminants), so other approaches are needed [107]. Text mining (e.g., [108-109]) can help to systematically extract valuable water quality records from the growing body of published and grey literature, further expanding our knowledge base. Citizen science-based initiatives, such as a workstream in the WWQA (https://my.ltb.io/www/#/stack/ABRER) and Ocean CleanUp (https://theoceancleanup.com/) harness widespread public engagement and can expand data coverage, complementing traditional monitoring efforts [110-111]. These data collection efforts would expand global spatial coverage with local-scale detail, producing more accurate and valuable detailed datasets (e.g., water quality records for model validation and model parameterization).

In parallel, advanced data-model fusion techniques, including machine learning (ML) and other forms of artificial intelligence (AI), hold great promise for synthesizing multiple data streams into coherent baseline water quality assessments at regional to global scales [112]. By assimilating information from remote sensors, drone flights, and in situ measurements along with text-mined information, advanced data-based approaches for model inputs can identify novel patterns. These expanded datasets will not only enhance our understanding of existing water quality conditions (allowing reasonable baseline estimates) but also provide a stronger foundation for the parameterization and evaluation of large-scale models.

When drawing on in-situ or other observational datasets, we should adopt a common metadata schema—covering sampling protocols, analytical techniques, constituent names, units, detection limits, and location precision. Where such metadata are incomplete or inconsistent, the associated observations should be flagged with higher uncertainty or, if necessary, omitted from further (modelling or benchmarking) analyses. This precaution allows records from disparate observational datasets to be combined transparently while acknowledging their differing quality. Regional models could provide datasets for large-scale models. We also argue for more connections to those models. They could be used to improve global models in terms of parameters and regional characteristics. Global models are often simplified, and it is not easy to consider region-specific characteristics. Sometimes knowledge is also limited (e.g., African regions where monitoring data is also limited). Regional models could be useful to improve global models in terms of parameterization and regional characteristics, and ultimately build trust in global model simulations.

Direction 2: Harmonization of large-scale datasets for water quality modeling

The harmonization of large-scale datasets of model inputs for modeling water quality across scales, pollutants, and sectors under contemporary and future global change must be strengthened. The ISIMIP platform is useful because it provides sector-specific protocols and offers model-driven datasets (for both model inputs and outputs) that are harmonized in time and space, including scenarios (https://www.isimip.org/). For example, the ISIMIP Agricultural sector focuses on modeling agricultural and terrestrial systems and nutrient cycling with integrated assessment models that can provide nutrient balances for modeling water quality and source attribution. Also, water quality results can be used in other impact models. Socioeconomic [113] and climate [96] projections are often used as inputs to water quality models (e.g., Table 1). We believe that our community efforts, along with flexibility and creativity, will bring harmonization approaches forward. This will facilitate “ensemble modelling” that will be a stepping stone to model intercomparisons of water quality.

Drivers of some water quality constituents – nutrients, BOD, or fecal coliforms – can be derived from the ISIMIP repository (climate, water discharge, land-use, population, fertilizer, wastewater). The next steps could be to perform new simulations using harmonized data following updated climate scenarios (e.g., ISIMIP3). This will enable the two types of ISIMIP interactions: (1) other sectors provide data to the Water Quality sector, and (2) the Water Quality sector provides simulations to other sectors. This will enable cross-sectoral water quality assessments under climate impacts. However, several emerging pollutant classes, such as micro- and macroplastics, pharmaceuticals, and pesticides, depend on inputs that ISIMIP does not yet supply. Yet, model inputs may also differ among the models simulating those pollutants. Water quality assessments have been expanding with more pollutants because of ongoing urbanization. This will bring more challenges in the harmonization of inputs and outputs among water quality models. In this case, the harmonization needs to be pragmatic. The UN-WWQA scenario storylines for water quality models [45] are practical examples of harmonization for multi-model and multi-constituent modeling.

We outline two pragmatic pathways for reducing inconsistencies among models until fully harmonized inventories become available.

Pathway 1: Source information via direct or proxy inventories. For every selected pollutant, we recommend an open, version-controlled template that couples existing ISIMIP drivers to release factors. For example, mismanaged plastic mass is linked to the release fraction of plastic loads from land to rivers, or livestock density plus excretion coefficients for veterinary antibiotics. Where direct observations are sparse, we could draw on agreed proxy information, such as the global mismanaged plastic waste map [37] or the FAO gridded pesticide-use database (https://www.fao.org/home/en/) and scale them to ISIMIP land-use classes.

Pathway 2: Common metadata, grid, and units. Whatever the native dataset resolution, all pollutant inputs are downscaled to the standard 0.5° ISIMIP grid and expressed in uniform units (e.g., kg of nitrogen per year). Datasets must have metadata documenting data origin, scaling assumptions, and emission-factor uncertainty. Here, using the ISIMIP approach of reconstructing input data, we can provide an open-source script library to automate the re-gridding and unit conversion so that every water-quality model reads identical layers and can pass its outputs to other sectors. This would allow considering the uncertainty in underlying databases transparently.

In achieving these pathways, key challenges remain. For example, pesticide or pharmaceutical consumption data are often available only as coarse national totals and over a limited period, and the emission factors for emerging contaminants may be poorly constrained. While any of our adopted approaches to reformat driver data does not solves these issues outright, it will render every assumption transparent, quantify uncertainty, and provide the community with the same set of input data.

Direction 3: Development of comprehensive and consistent water quality scenarios

A key future direction in water quality research lies in developing scenarios that incorporate both disruptive events, such as pandemics (e.g., COVID-19 [114]) or geopolitical conflicts (e.g., the Russia–Ukraine war [115-116]), and positive societal transformations [91, 117-119]. These disruptions can have cascading effects on global supply chains, the cost of fertilizers, agricultural practice changes, and ultimately, pollutant discharges to water bodies. Global Change Analysis Models [120] and existing SSP scenarios could be useful tools. Existing SSPs largely focus on food security or broad economic drivers [113], but they rarely address water resources policies and regulations (e.g., the Clean Water Act in the U.S. or the European Water Framework Directive), often because of their regional coverage [82]. The development of innovative water quality scenarios should consider regional policies [121] as well as disruptive events, and analyze their plausible impacts on water quality constituents. Further, as emphasized in Bouwman, Bärlund [45], the integration of water quality–centric storylines into broader socioeconomic pathways will help identify robust pollution "hotspots" across various scales, pollutants, and sectors—thereby informing strategies that can remain effective under disruptive conditions.

The scenario-building efforts should align with the climate-driven changes in hydrology and biogeochemistry, drawing on the growing field of impact attribution that disentangles climate warming from anthropogenic influences versus natural variability. To this end, ongoing initiatives such as ISIMIP3 provide a framework for systematically incorporating different drivers, like climate alone versus climate plus (human) management changes, into future water quality model intercomparison analysis. By leveraging multimodal ensembles and incorporating diverse scenario elements (implicit vs. explicit human influences or anthropogenic vs. non-anthropogenic climate drivers), we can further understand and disentangle complex driver interactions that shape future water quality trajectories. These activities would support providing guidelines on targeted mitigation actions, inform adaptive management strategies, and support evidence-based policy development to reduce pollution risks under a range of plausible future conditions.

Direction 4: Integrated understanding of the role of water quality in a changing world

There is a need for an integrated and holistic approach to understanding the role of water quality in a changing world. Urbanization and climate change will pose more challenges to water resources, reducing their availability and increasing pollution [27, 122]. Clean water availability is and will be essential for society and nature, but its definition varies and often depends on water use and pollutants (e.g., [2, 19, 123]). Integrating water quantity and quality [124] is needed to develop indicators of clean water scarcity [26] or clean water availability [3]. Not all sectors are affected by pollution in the same way [2, 19, 27]. Thus, the risks posed by polluted waters could also differ among sectors and scales.

Furthermore, changes in water quality due to climate change (e.g., weather extremes) and socioeconomic development are still not well understood [125]. Multi-pollutant assessments of water quality are limited by data availability (Directions 1-2) and scenarios (Direction 3) [25]. Hence, we need advanced and integrated multi-scale, multi-pollutant, multi-sector assessments of water quality [25, 45]. Moreover, we need to learn from the historical trends (Directions 1-2) and improve our future projections (Direction 3).

We recommend strengthening transdisciplinary approaches in which science and society are better connected via knowledge exchange on water quality (e.g., UN-WWQA citizen science workstream). Such approaches will enhance society's awareness of water quality issues across scales, pollutants, and sectors (based on Directions 1-2) and co-create support to policymaking in designing effective strategies to preserve water quality in the future (based on Direction 3).

630 **Data availability statement**

631 The data supporting this study's findings are publicly available in published papers that we refer to in the
632 main text can be downloaded from the ISIMIP repository (https://www.isimip.org/).

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