

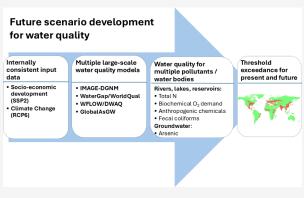
pubs.acs.org/journal/estlcu

Multimodel and Multiconstituent Scenario Construction for Future Water Quality

A. F. Bouwman,* I. Bärlund, A. H. W. Beusen, M. Flörke, M. Gramberger, J. Rivera Cardona,
J. Podgorski, J. van den Roovaart, B. Grizzetti, A.B.G. Janssen, R. Kumar, S. Langan, S. Poikane,
B. M. Spears, M. Strokal, T. Tang, T. A. Troost, O. Vigiak, M. T. H. van Vliet, Y. Vystavna, M. Wang, and N. Hofstra*



one of today's most severe and pervasive threats to the global environment. Comprehensive and spatially explicit scenarios covering a wide range of constituents for freshwater quality are currently scarce. In this Global Perspective paper, we propose a novel model-based approach for five water quality constituents relevant for human and ecosystem health (nitrogen, biochemical oxygen demand, anthropogenic chemicals, fecal coliform, and arsenic). To project the driving forces and consequences for emissions and impacts, a set of common data based on the same assumptions was prepared and used in different large-scale water quality models including all relevant demographic, socioeconomic, and cultural changes, as well as threshold concentrations to determine the risk for human and ecosystem health. The



analysis portrays the strong links among water quality, socio-economic development, and lifestyle. Internal consistency of assumptions and input data is a prerequisite for constructing comparable scenarios using different models to support targeted policy development.

KEYWORDS: Anthropogenic chemicals, Arsenic, Biological oxygen demand, Fecal coliform, Future, Global, Groundwater, Nitrogen, Scenario, Surface water, Water quality

INTRODUCTION

Water is a vital natural resource, but it is not always available in the right place at the right time or of sufficient quality. Water quality is a measure of the physical, chemical, and biological conditions of the water based on the standards that regulate its usage.¹ Today, poor freshwater quality is one of the most severe and pervasive threats to the global environment, because many pollutants occur in water that affect human and ecosystem health through, for example, contamination threatening water and food security.² With the global population projected to grow to between 8.5 and 10 billion by 2050,³ improved understanding of the effects of future climate and socio-economic changes on freshwater quality is urgently needed to evaluate the progress toward the United Nations Sustainable Development Goals (SDGs)⁴ and target 2 of the Global Biodiversity Framework.⁵ Scenarios for river export of individual pollutants to regional or global coastal waters,⁶⁻⁸ and for individual water quality constituents in freshwaters were recently presented.⁹⁻¹³ However, comprehensive and spatially explicit scenarios covering a wide range of constituents for freshwater quality, developed using multiple water quality models, are currently lacking.

This paper presents the results and lessons learned of a working group of researchers from several international universities and institutes, represented by the authors of this paper, that focused on developing approaches to scenario construction for a World Water Quality Assessment, organized by the "Water Quality Modelling" Work Stream of the United Nations Environment Programme (UNEP) coordinated World Water Quality Alliance (WWQA).¹⁴ The working group extended the community consensus Shared Socio-economic Pathways (SSP), developed in recent years to assess future climate changes and impacts,³ with the driving forces of water pollution.

Received:September 23, 2024Revised:November 20, 2024Accepted:November 20, 2024Published:November 22, 2024





© 2024 The Authors. Published by American Chemical Society

WHO standard for drinking water²⁶

Table 1. Selected Water Quality Constituents and Threshold Values below Which Harmful Effects Are Considered Tolerable

Constituent	Threshold and unit	Comment	
Water quality constituent causing a	risks to ecosytem health		
Total nitrogen (TN) in freshwater	2.5 mg-N/L	Based on values from literature which vary from 0.5–4.0 mg TN l^{-1} ²³	
Organic pollution indicated by biochemical oxygen demand (BOD) in freshwater	4 mg/L	UNEP ²	
Anthropogenic chemicals in freshwater	0.05 [-], multispecies Potentially Affected Fraction, (msPAF)	Concentrations of 1785 chemicals related to human activities (varying from country to country) were expressed in terms of the msPAF ranging from 0 (no species affected) to 1 (all species affected); ²⁴ values <0.05 represent a low risk	
Water quality constituent causing risks to human health			
Fecal coliform (FC) in freshwater	200 colony forming units (cfu)/100 mL $$	Reder et al. ²⁵ This threshold was used prior to 1986 by US EPA, ²⁷ and still in China. ²⁸ WHO ¹⁹ uses intestinal enterococci as their primary indicator instead	

Arsenic (As) in drinking water	r 10 μg/L
--------------------------------	-----------

Constructing a scenario of global freshwater quality is complex, as it involves a large number of the following:

- (i) water quality constituents (nutrients, pathogens, anthropogenic chemicals, plastics, etc.)
- (ii) sources in relation to different terrestrial processes and transport pathways (point and diffuse, natural and anthropogenic sources, e.g. weathering processes, sanitation systems, agricultural practices, urban runoff and atmospheric deposition)
- (iii) water body types (streams, rivers, lakes, reservoirs, temporarily flooded areas such as wetlands, floodplains, and groundwater)
- (iv) impacts (human health, ecosystem health, direct and indirect, e.g., oxygen depletion following enhanced primary production in water)
- (v) interactions between the different water quality constituents, pollutant sources, and impacts

Scenarios should consider, therefore, the complex chain of sources and their main driving mechanisms as well as their regional variability, including the following

- (i) growing populations with changing human diets toward more livestock products leading to increasing food demand and consequently increasing use of fertilizers, pesticides, and veterinary drugs
- (ii) the need for improved human health and public wellbeing fostering sewage connection and wastewater treatment and simultaneously increasing consumption of human pharmaceuticals and products
- (iii) the use of chemicals in many consumer products and industrial processes.

We first considered SDG 6 (clean water and sanitation by 2030) target 6.3, which aims to improve ambient water quality. Indicator 6.3.2 (the proportion of water bodies with good ambient water quality) is based on an index that incorporates five core parameter groups, i.e., (i) oxygen and (ii) phosphorus (P), (iii) salinity, (iv) nitrogen (N), and (v) acidification (pH) (i–v refer to surface water and iii–v also in groundwater).^{15,16} As water quality includes many aspects not covered by these five core groups, we also considered water quality constituents that go beyond the SDG 6.3.2 indicator list, in line with the water quality constituents considered in the Water Framework Directive of the European Union.^{17,18}

Five water quality constituents are included in this paper (Table 1), based on diversity in sources and impacts and availability of spatially explicit models covering all water body types. Three of these constituents are relevant to ecosystem health (nitrogen, N; biochemical oxygen demand (BOD);

anthropogenic chemicals), and two are indicators for human health (fecal coliform, FC; arsenic). Excessive loading of the plant nutrients (N together with P) into water bodies enhances aquatic primary production leading to eutrophication and its associated impacts of biodiversity loss and oxygen depletion. This is accounted for by BOD, reflecting the consumption of oxygen associated with organic matter. We note that some inorganic forms of N such as nitrate and ammonia may be directly related to human health.¹⁹

of FC. However, for the scenario model runs data are available for FC only.

Various chemicals used by humans are found in surface waters and affect ecosystem health. They can be grouped based on their application (e.g., nutrients, biocides, pesticides, pharmaceuticals, or cosmetics), effects (e.g., cytostatics, endocrine-disrupting agents), or sources (e.g., synthetic versus naturally occurring hormones). To capture the impact of chemical mixtures on ecosystem health, the mixture toxicity metric "multisubstance potentially affected fraction of species" (msPAF) based on the no-observed-effect concentration (NOEC) is used in this study as a proxy for anthropogenic chemicals.

Fecal coliform in water is, despite controversy, often used as an indicator of recent fecal contamination and the presence of pathogens. The geogenic contaminant Arsenic (As) in groundwater stems from natural weathering processes in subsurface geological materials and mine waste. Climate change can have long-term effects on the geochemical conditions that favor As accumulation.²⁰ Arsenic can threaten human health, especially where groundwater is an important source of drinking water.^{21,22}

In this Global Perspective paper, we describe the construction and assessment of a "middle of the road" water quality scenario with an indifferent attitude toward water quality deterioration. We present a novel approach in which we share common input data to run multiple spatially explicit models for multiple constituents and multiple water bodies. The Methods and Materials section provides the constituents, their thresholds, and the models employed. Using the scenario, we evaluate future trends of water quality, assess if and where SDG targets will be achieved in the middle of the road scenario, and summarize the lessons learned in the scenario development process.

METHODS AND MATERIALS

Threshold concentrations are often used to reflect the levels (e.g., concentrations) above which a particular water quality constituent is likely to pose a significant risk to human health or the aquatic ecosystem. Since threshold values may differ within and between countries, the working group selected

values for their global assessment that reflect commonly used standards related to aquatic ecosystems or human health (Table 1). Although one single global value for thresholds related to ecosystem health may not reflect the local conditions or differences among water body types,²³ such thresholds are helpful to assess the impact of global changes and future socio-economic developments and compare regional water quality effects consistently.

Models are powerful tools to visualize historical, contemporary, and future sources and drivers of contaminants and to define the pathways of contaminant transport and biogeochemical transformation through surface waters from land to sea. Models also allow for gap filling in regions where in situ monitoring data are sparse. Global-scale models, previously verified with monitoring data, were used by the working group to simulate water quality constituents, including total N (TN) and total P (TP),²⁹ dissolved inorganic N (DIN) and P (DIP), plastics and triclosan,³⁰ pathogens,³¹ chlorophyll-a in lakes,³² FC²⁵ and BOD,³³ anthropogenic chemicals,²⁴ and As in groundwater.²¹ The four spatially explicit models that are capable of simulating future changes in concentrations of the five selected water quality constituents are listed in Table 2. The WFLOW-DWAQ model for anthropogenic chemicals describes the impact on water quality of the use of such chemicals. The per country use of chemicals is approximated on the basis of a relationship with the per capita income. The emission to surface water is based on a country-specific pollution control factor, which is also a function of income. The toxic pressure of the mixture of chemicals was calculated on the basis of a correlation between these approximations and the detailed simulation of the multispecies Potentially Affected Fraction (msPAF) derived from the predicted concentrations of 1785 chemicals of various uses (including 105 pharmaceutical products and 332 pesticides) in 10,658 water bodies in Europe.^{34,35} Uncertainties of this first global inventory with the msPAF approach are briefly discussed in the supporting material. Brief descriptions of the four models, their performance, and validation against monitoring data for concentrations of the five water quality constituents are in the supporting material; more details are in various literature reports (see supporting material).

Using a common source of model input data is essential to ensure intermodel consistency and enable comparison of model outcomes across scales and constituents.³⁶ Therefore, the models of this study consistently used the same set of climate data from the Representative Concentration Pathways (RCP) data sets,³⁷ and scenario assumptions and data sets for computing future water quality, based on the SSPs (Table 2).³ The SSPs were developed using a wide spectrum of assumptions based on demographic and economic growth and attitude toward environmental problems and resource depletion. SSP implementation by the integrated assessment model IMAGE-DGNM generates output at the scale of 26 world regions, countries, and 0.5° grids (e.g., land use, crop and livestock production, fertilizer use, manure management, sanitation level). Data exchanged by IMAGE-DGNM used by the various models are at the scale of world regions (industry value added) and country (livestock and sanitation level data).

The working group extended the SSPs to drivers of water pollution. The "middle of the road" SSP2 scenario was selected for this exercise as it matches the most recent population data.³⁸ This scenario is not a simple continuation of the past trends. For example, future food demand and production and

Model	Constituents simulated		Constituent used in this study	Common data among all models ^a	Key scenario driver for 26 from IMAGE-DGNM used	Water body type covered	Spatial resolution	Time step	Key reference
IMAGE-DGNM	TN, TP, Si in surface water, TN in groundwater	NT		RCP 6 climate, population, GDP		Surface water	0.5 degree, base year 2015	Year	29
WaterGAP- WorldQual	Water temperature, TP, BOD, FC BOD, TDS, FC	BOD, FC			Sanitation level, population, GDP, industry value added,	Surface water	Surface water 5 arc minutes, base year 2015	Month	25, 33

Table 2. Water Quality Models Used in This Paper Simulate Global Concentrations of TN, BOD, FC, and Anthropogenic Chemicals in Surface Water and As in Groundwater

24

Year

30 arc seconds, base year 2010

Surface water

Population, GDP

livestock

21

Year

Ground water 1 km, base year 2015	
Population	current situation and the scenario are provided in the supporting material.
As	bles for th
As in groundwater	ie technical details on the input variables for th
GlobalAsGW	^a The technical d

Cumulative impact on ecology for 1785 chemicals of emerging concern, including pharmaceuticals and pesticides

Anthropogenic chemicals in surface water

WFLOW-DWAQ

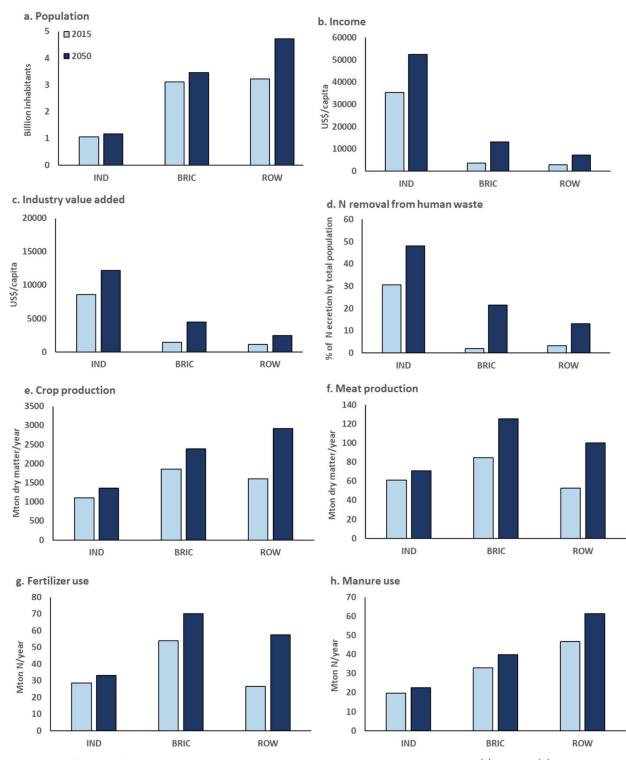


Figure 1. Drivers of water pollution used in the scenarios construction, including direct drivers population (a), income (b), industry value added (c), and intermediary drivers N removal from human waste (d), crop production (e), meat production (f), N fertilizer use (g), and manure use (h) for 2015 and 2050 for industrialized countries (IND, USA, Canada, Europe, Japan and Oceania), the BRIC region (Brazil, Russian Federation, India, China), and the rest of the world (ROW) according to the SSP2 scenario implemented with the IMAGE model.⁹

associated land use are important elements in this study. Important drivers for future food demand are population, economic growth, and consequent changes in food preferences with shifts toward more/less meat depending on the cultural habits and income level, which differentiates the direction of change in terms of overall food intake. In the SSP2 implementation used here, governments of many countries invest in wastewater treatment, but often population increases more rapidly than pollution removal in treatment plants. Future use and emission of anthropogenic chemicals is considered to be dependent on incomes in two ways. With increasing wealth, the overall use of chemicals increases but also the environmental control on emissions. Common input data were implemented by the four models at resolutions from 30 arc seconds to 30 arc minutes using hydrology models and routing schemes as the basis for delivery from different sources and pathways, subsequent transport and processing in surface water, and their subsequent removal in streams, wetlands, lakes, and reservoirs.

RESULTS AND DISCUSSION

Water pollution is strongly related to economic development level and culture, and therefore, large differences exist in water quality conditions between countries and even within countries. Therefore, we present the water quality conditions in terms of exceedance of the thresholds as maps for 2015 and 2050, showing this heterogeneity. The data were aggregated from these maps, as well as the direct and intermediary drivers of water pollution, to the level of three large world regions. These regions include the industrialized countries (IND, including USA, Canada, Europe, Japan, Oceania), the BRIC region (Brazil, Russian Federation, India, China), and the rest of the world (ROW) (a list of countries in each of these regions, as well as more detailed results for the water quality conditions, are presented in the Extended Data (in the SI).

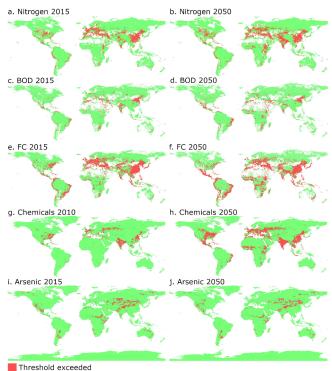
The primary driver of water pollution is the population. Figure 1a presents the SSP2 projections for global population growth from 7.4 billion inhabitants in 2015 to 9.3 billion by 2050, with 76% of this growth projected for the ROW region. Economic development is an important factor because it influences the consumption level and pattern, such as human diets and anthropogenic chemicals use, and thus the required production, mechanization level, inputs of fertilizers and pesticides and emissions of chemicals. The data show a doubling of the world average per capita income with large variation between high- and low-income countries (Figure 1b). Industry value added, an important indicator of industrial production activity, is projected to increase by 40% in IND countries and by a factor of 2 (ROW) to 3 (BRIC) elsewhere (Figure 1c).

With an indifferent attitude toward environmental problems in the SSP2 scenario and resource intensity of medium, human diets, food wastage, degree of environmental management and control, and agricultural efficiencies will continue the trends observed in recent decades.

Quantified data on the connection to sewers, open defecation, and wastewater treatment for SSP2 indicate that by 2050 there will be a reduction in the number of people lacking access to improved sanitation, except for Sub-Sahara Africa,³⁹ where rapid population expansion and urbanization coupled with the underdevelopment of wastewater management infrastructure likely leads to increased pollution discharges.⁴⁰ Although wastewater treatment plant capacity grows in all regions resulting in increasing N removal from human waste, the population grows faster so that increasing amounts of human waste are discharged to surface water, particularly in BRIC and ROW countries (Figure 1d). Emissions of the use of chemicals show massive increases in SSP2, particularly in low-income countries due to rapid economic growth and lagging environmental control.²⁴

The quantifications of the SSP2 production for crops and meat (globally 46% and 49% increase between 2015 and 2050, respectively, see Figure 1e and f) result in a significant global increase of N from animal manure production (24%) and use of N fertilizers (49%). While meat and crop production increase by around 20% in IND countries, the production in BRIC (+47% and +29%, respectively) and ROW countries (+90% and +89%, respectively) accounts for the major part of the global increase (Figure 1g and h). N fertilizer use (+30% in BRIC and +16% in IND) and manure N use (+21% in BRIC and +15% in IND) grow more slowly than the global average, with a dramatic growth in ROW countries by more than 100% for N fertilizer and 31% for manure use. The projected greenhouse gas emissions for SSP2, as calculated by the IMAGE model, result in a global radiative forcing level of 6 W m⁻² in the year 2100, which is equivalent to the RCP 6 climate scenario⁴¹ and a temperature increase of 2.3 °C compared to 1860.⁴²

Exceedances of the threshold concentrations in 2015 and the scenario year 2050 were calculated with the four models following the multimodel approach employed in this paper (Figure 2). For this comparison, the landscape or basin areas



Threshold not exceeded

Figure 2. Exceedance for 2015 (a–e, i) or 2010 (g) (left column) and 2050 according to SSP2-RCP6.0 (right column) of the thresholds for a subset of modeled water quality constituents: (a, b) total nitrogen (TN), (c, d) biochemical oxygen demand (BOD), (e, f) fecal coliform (FC), (g, h) "multisubstance potentially affected fraction of species' (msPAF), and (i, j) As. Threshold values are listed in Table 1.

affected by water quality changes were calculated for the constituents relevant to ecosystem health and the number of inhabitants affected for those constituents relevant to human health.

Comparing the estimated concentrations in the "current" situation with the threshold values revealed a widespread exceedance of the concentrations of N, BOD, FC, and anthropogenic chemicals in surface water and As in groundwater (Figure 1a, c, e, g). Insufficient water quality is not only a severe problem in industrialized countries (IND), where a large landscape area experiences exceedance of thresholds for TN (4.7 million km²), BOD (0.4 million km²), and msPAF (0.3 million km²); in Brazil, the Russian Federation, India, and

China (BRIC), the situation is worse (6.6 million km^2 for N, 1.6 million km^2 for BOD and 0.5 million km^2 for msPAF) (Figure 3).

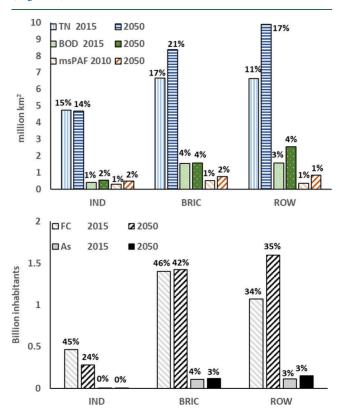


Figure 3. (a) Areas of landscapes within river basins where surface water bodies show exceedance of the thresholds for TN, BOD, and msPAF. (b) Inhabitants residing in regions where surface water (FC) or groundwater (As) as the main source of drinking water exceed the threshold values in IND, BRIC, and ROW countries, indicating a potential health risk. Numbers above each bar indicate the % of the total land area (for TN, BOD, and msPAF) and % or total population (for FC) and % of population in regions where groundwater is the main source of drinking water (for As).

In the rest of the world (ROW), mainly low-income countries, the situation for TN and BOD is comparable to that in the BRIC countries, while the area affected by high msPAF is smaller than in IND and BRIC countries. The global number of inhabitants at risk due to high FC concentrations of ~3 billion people is largely concentrated in BRIC and ROW countries (Figure 3). For the geogenic contaminant As (Figure 2i), the exceedance of the concentration threshold is related to a combination of climate and chemical characteristics of the geological parent material.²¹ Due to local geohydrological settings, the number of people at risk (Figure 3) is concentrated in a limited number of locations in a few BRIC and ROW countries (Figure 2i).

The SSP2-RCP6.0 projections for 2050 show increasing water quality problems associated with N, BOD, and anthropogenic chemicals in nearly all parts of the world (Figure 1b, d, h) compared to 2015 (Figure 1a, c, g). TN pollution stabilizes in industrialized countries but rapidly expands in BRIC (from 7 to 8 million km²) and ROW (from 7 to 10 million km²) countries (Figure 3) and exceedance of the BOD threshold spreads in all parts of the world. SSP2 scenario results portray a small increase of the areas with exceedances of

msPAF values in industrialized countries, and sharp increases in BRIC (i.e., from 0.5 to 0.8 million km^2) and ROW countries (i.e., from 0.4 to 0.9 million km^2). FC indicates an improvement in many industrialized countries (declining from 0.5 to 0.3 billion inhabitants that are potentially at risk), a stabilization in BRIC countries, but a deterioration in ROW countries (a sharp increase from 1.1 to 1.6 billion inhabitants potentially at risk) (Figure 3) due to the lagged projected time lines of increasing connection to sewage systems in the SSP2 scenario (Figure 1).

Finally, groundwater used to produce drinking water changes only slightly in the coming decades (Figure 2j). With population growth, climate change induced increases in drought frequency and intensity and an increased reliance on groundwater as a drinking water source, the number of inhabitants with potential risk of health problems associated with As intake is expected to grow in the same areas where problems occurred in 2015.

From the above, it is clear that water quality in most of the IND and BRIC regions will not improve in this environmentally indifferent middle-of-the-road SSP2 scenario. The areas with risk of aquatic ecosystem degradation (due to exceedance of TN concentrations, BOD) and the populations with human health risks (due to elevated FC and As concentrations) in the ROW region already exceeded those in the IND and BRIC regions in 2015. With the projected dramatic increase in population, income, food and industry production, fertilizer use, and animal manure production, and lagging wastewater treatment and environmental control in the ROW region between 2015 and 2050, risks caused by anthropogenic chemicals will further deteriorate water quality, and problems caused by the other four constituents that already existed in 2015 will aggravate. Within the ROW region, the projected population growth is particularly rapid in Africa, and the maps show rapid expansion of water quality problems for all constituents in North Africa and Sub-Saharan Africa between 2015 and 2050 (Figure 2).

Our first scenario results revealed that the remaining time between now and the target year 2030 in SDG6 is insufficient to implement all the technical, behavioral, and societal changes required-let alone to achieve the aspired effects on water quality. In the "middle of the road" SSP2 scenario considered, even two decades beyond the SDG 6 target year of 2030, the projected coverage of water bodies with exceedance of thresholds for TN and BOD (as a proxy for oxygen) included in indicator 6.3.2 and other water quality constituents (anthropogenic chemicals and FC) will not decline in industrialized countries and are projected to increase in many low-income countries. This points to the urgency for developing strategies to control water quality degradation and the need to develop scenarios for increasing awareness of this problem and to support policy development. Spatially explicit data are indispensable because of the heterogeneity of sources, in-stream processes, and impacts of water quality degradation and its trans-boundary nature in many river basins.

The implementation of SSP2-RCP6.0 for the five water quality parameters selected in this work is a starting point. From the methodological issues that evolved in this scenario construction, the workgroup concludes that

 (i) The novel scenario approach for a wide spectrum of water quality constituents relevant to aquatic ecosystem and human health (expanding from the SDG framework) shows that water quality deterioration is a severe and persistent problem and requires a fundamentally transformative path for human development and lifestyle to ensure truly sustainable development.

- (ii) The SDG framework definition of water quality is incomplete. Global water quality assessment would benefit from clear globally accepted thresholds for all relevant pollutants; this allows a focus on synergetic policy options, because they could help to account for interactions between multiple pollutants, water bodies and SDG targets and indicators, and thus solve not only water pollution issues, but also lead to synergies with other sustainability objectives.
- (iii) Use of internally consistent input data among models is a prerequisite for comprehensive and coherent largescale spatially explicit water quality modeling and scenario analysis. This supports the development and evaluation of targeted policies (constituent, source, water body) to mitigate the transboundary problem of water pollution. Such analyses involve inputs from different models, combined with knowledge and experience of many researchers of diverse disciplines.

We demonstrate, here, the potential of multimodel, multipollutant, and multiwater body large-scale spatially explicit water quality modeling and scenario analysis to improve understanding of current and future water quality. This integrated modeling approach, as envisaged by WWQA, allows for the development of targeted policy interventions across the sustainability landscape. The approach also addresses a recent call for better integration of water quality assessments across all member states, transboundary agreements, and global initiatives as laid out in the United Nations Environment Assembly Resolution UNEP/EA.6/Res.13. The modeling approach and outputs presented here can be used as a tool to support better integration of water quality assessments across a range of actors and global initiatives. These may include the UNESCO-International Initiative on Water Quality,⁴³ the Kunming-Montreal Global Biodiversity Framework Targets (e.g., Target 7 Reduce pollution risks and the negative impact of pollution from all sources, by 2030 ...), and other coordinated actions (e.g., through the Water Action Agenda) across international organizations such as World Health Organization (WHO), the UN Food and Agriculture Organization (FAO), and the United Nations Environment Programme (UNEP). Finally, we demonstrate, here, the potential for governments to interrogate the model outputs to support the development of national water quality monitoring, assessment, and recovery strategies, for example, following the framework of Sustainable Development Goal 6.3.2.

KEY MESSAGES

- This paper proposes a novel model-based approach for constructing spatially explicit future scenarios for five water quality constituents relevant for human and ecosystem health (total nitrogen, TN; biochemical oxygen demand, BOD; anthropogenic chemicals; fecal coliform, FC; and arsenic, As) with different large-scale water quality models.
- Internal consistency is achieved by using common data including all relevant demographic, socio-economic, and

cultural changes, as well as threshold concentrations to determine the risk for human and ecosystem health.

- According to the "middle of the road" scenario that was analyzed as an example, even two decades beyond the SDG 6 target year of 2030, the projected coverage of water bodies with exceedance of thresholds for TN and BOD included in SDG indicator 6.3.2 and other water quality constituents (anthropogenic chemicals and FC) will not decline in industrialized countries and are projected to increase in many low-income countries.
- This points to the urgency for developing strategies to control water quality degradation and the need to develop scenarios for increasing awareness of this problem and to support policy development.
- Spatially explicit data are indispensable because of the heterogeneity of sources, in-stream processes, and impacts of water quality degradation and the transboundary nature in many river basins.

ASSOCIATED CONTENT

Data Availability Statement

All results presented in this paper are available on request from the corresponding authors.

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.estlett.4c00789.

Technical background of water quality scenario development (PDF)

Scenario results: exceedance of threshold for 26 world regions (XLSX)

AUTHOR INFORMATION

Corresponding Authors

- A. F. Bouwman Department of Earth Sciences–Geochemistry, Faculty of Geosciences, Utrecht University, 3508 TA Utrecht, The Netherlands;
 orcid.org/0000-0002-2045-1859; Email: a.f.bouwman@ uu.nl
- N. Hofstra Earth Systems and Global Change Group, Wageningen University & Research, 6700 AA Wageningen, The Netherlands; orcid.org/0000-0002-0409-5145; Email: nynke.hofstra@wur.nl

Authors

- I. Bärlund Research Unit Water Resources and Environment, Helmholtz Centre for Environmental Research-UFZ, D-39114 Magdeburg, Germany; © orcid.org/0000-0003-0777-7130
- A. H. W. Beusen Department of Earth Sciences–Geochemistry, Faculty of Geosciences, Utrecht University, 3508 TA Utrecht, The Netherlands; PBL Netherlands Environmental Assessment Agency, 2500 GH The Hague, The Netherlands; © orcid.org/0000-0003-0104-8615
- M. Flörke Institute of Engineering Hydrology and Water Resources Management, Ruhr University Bochum, 44801 Bochum, Germany
- M. Gramberger Prospex, 10178 Berlin, Germany
- J. Rivera Cardona Institute of Engineering Hydrology and Water Resources Management, Ruhr University Bochum, 44801 Bochum, Germany

- J. Podgorski Department of Water Resources and Drinking Water–Eawag, Swiss Federal Institute of Aquatic Science and Technology, 8600 Dübendorf, Switzerland; © orcid.org/ 0000-0003-2522-1021
- J. van den Roovaart Deltares, 2600 MH, Delft, The Netherlands
- B. Grizzetti European Commission, Joint Research Centre (JRC), I-21027 Ispra, VA, Italy; in orcid.org/0000-0001-5570-8581
- A.B.G. Janssen Earth Systems and Global Change Group, Wageningen University & Research, 6700 AA Wageningen, The Netherlands
- R. Kumar Department Computational Hydrosystems, Helmholtz Centre for Environmental Research-UFZ, 04318 Leipzig, Germany; orcid.org/0000-0002-4396-2037
- S. Langan International Water Management Institute, CGIAR, 2075 Colombo, Sri Lanka; Orcid.org/0000-0003-0742-3658
- S. Poikane European Commission, Joint Research Centre (JRC), I-21027 Ispra, VA, Italy; Occid.org/0000-0002-2253-2097
- **B. M. Spears** UK Centre for Ecology and Hydrology, Edinburgh EH26 0QB, United Kingdom
- M. Strokal Earth Systems and Global Change Group, Wageningen University & Research, 6700 AA Wageningen, The Netherlands
- T. Tang Biological and Environmental Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia; Water Security Research Group, Biodiversity and Natural Resources Program, International Institute for Applied Systems Analysis, Laxenburg A-2361, Austria
- T. A. Troost Deltares, 2600 MH, Delft, The Netherlands; orcid.org/0000-0002-8646-3641
- **O. Vigiak** European Commission, Joint Research Centre (JRC), I-21027 Ispra, VA, Italy
- M. T. H. van Vliet Department of Physical Geography, Faculty of Geosciences, Utrecht University, 3508 TC, Utrecht, The Netherlands; ◎ orcid.org/0000-0002-2597-8422
- Y. Vystavna International Atomic Energy Agency, Isotope Hydrology Section, Vienna International Centre, Vienna 1400, Austria; o orcid.org/0000-0002-1366-0767
- **M. Wang** Earth Systems and Global Change Group, Wageningen University & Research, 6700 AA Wageningen, The Netherlands

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.estlett.4c00789

Author Contributions

Conceptualization and methodology: N.H., A.F.B., I.B., A.H.W.B., M.F., M.G. Data preparation and model runs: A.H.W.B., J.R.C., M.F., A.G.B.J., R.K., J.P., J.v.d.R., M.S., T.T. Writing-original draft: A.F.B, N.H., all authors. Writing-review and editing: A.F.B., N.H., M.F., B.M.S.

Funding

United Nations Environment Programme (UNEP) provided funding for the online workshop (21, 24, 28, and 30 June 2021) and the workshop in Leipzig (14–17 February 2022) during which this paper was developed (Contract No. SSFA/ 2020/4643).

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

The authors are grateful to Melissa Denecke (IAEA) for her comments on an earlier version of this paper and Jos van Gils for his contribution to the Wflow-DWAQ description. The working group contributes to the work stream "Water Quality Modelling" for the global multistakeholder World Water Quality Alliance (WWQA) aiming to provide global water quality assessments for the current and future situations. This Global Perspective paper is output from two workshops organized by the WWQA workstream with seed money provided by the United Nations Environment Programme (UNEP). M.F. and J.R.C.: Research work was performed as part of the project "Erarbeitung, Testung und pilothafte Anwendung einer integrierten und skalenübergreifenden Analyse- und Bewertungsmethodik der Wasserqualität von Oberflächenund Grundwasser für eine globale, internetbasierte Wasserqualitätsplattform", GlobeWQ (02WGR1 527C), carried out with the support of the Federal Ministry of Education and Research (BMBF) within its research initiative "Global Resource Water (GRoW)".

REFERENCES

(1) Johnson, D. L.; Ambrose, S. H.; Bassett, T. J.; Bowen, M. L.; Crummey, D. E.; Isaacson, J. S.; Johnson, D. N.; Lamb, P.; Saul, M.; Winter-Nelson, A. E. Meanings of Environmental Terms. *J. Environ. Qual* **1997**, *26* (3), 581–589.

(2) A Snapshot of the World's Water Quality: Towards a Global Assessment; United Nations Environment Programme: Nairobi, Kenya, 2016.

(3) Riahi, K.; van Vuuren, D. P.; Kriegler, E.; Edmonds, J.; O'Neill, B. C.; Fujimori, S.; Bauer, N.; Calvin, K.; Dellink, R.; Fricko, O.; Lutz, W.; Popp, A.; Cuaresma, J. C.; Kc, S.; Leimbach, M.; Jiang, L.; Kram, T.; Rao, S.; Emmerling, J.; Ebi, K.; Hasegawa, T.; Havlik, P.; Humpenöder, F.; Da Silva, L. A.; Smith, S.; Stehfest, E.; Bosetti, V.; Eom, J.; Gernaat, D.; Masui, T.; Rogelj, J.; Strefler, J.; Drouet, L.; Krey, V.; Luderer, G.; Harmsen, M.; Takahashi, K.; Baumstark, L.; Doelman, J. C.; Kainuma, M.; Klimont, Z.; Marangoni, G.; Lotze-Campen, H.; Obersteiner, M.; Tabeau, A.; Tavoni, M. The Shared Socioeconomic Pathways and Their Energy, Land Use, and Greenhouse Gas Emissions Implications: An Overview. *Global Environmental Change* 2017, *42*, 153–168.

(4) The 17 Goals, 2022. United Nations, Department of Economic and Social Affairs Development. https://sdgs.un.org/goals.

(5) Final Text of Kunming-Montreal Global Biodiversity Framework, 2022. Convention on Biological Diversity (CBD). https://www.cbd.int/article/cop15-final-text-kunming-montreal-gbf-221222.

(6) Bouwman, A. F.; Van Drecht, G.; Knoop, J. M.; Beusen, A. H. W.; Meinardi, C. R. Exploring Changes in River Nitrogen Export the the World's Oceans. *Global Biogeochem Cycles* **2005**, *19*, GB1002.

(7) Seitzinger, S. P.; Mayorga, E.; Bouwman, A. F.; Kroeze, C.; Beusen, A. H. W.; Billen, G.; Van Drecht, G.; Dumont, E.; Fekete, B. M.; Garnier, J.; Harrison, J. A. Global River Nutrient Export: A Scenario Analysis of Past and Future Trends. *Global Biogeochem Cycles* **2010**, *24* (4), GB0A08.

(8) Strokal, M.; Bai, Z.; Franssen, W.; Hofstra, N.; Koelmans, A. A.; Ludwig, F.; Ma, L.; van Puijenbroek, P.; Spanier, J. E.; Vermeulen, L. C.; van Vliet, M. T. H.; van Wijnen, J.; Kroeze, C. Urbanization: An Increasing Source of Multiple Pollutants to Rivers in the 21st Century. *npj Urban Sustainability* **2021**, *1* (1), 24.

(9) Beusen, A. H. W.; Doelman, J. C.; Van Beek, L. P. H.; Van Puijenbroek, P. J. T. M.; Mogollón, J. M.; Van Grinsven, H. J. M.; Stehfest, E.; Van Vuuren, D. P.; Bouwman, A. F. Exploring River Nitrogen and Phosphorus Loading and Export to Global Coastal Waters in the Shared Socio-Economic Pathways. *Global Environmental Change* **2022**, *72*, No. 102426.

(10) Jones, E. R.; Van Vliet, M. T. H.; Qadir, M.; Bierkens, M. F. P. Country-Level and Gridded Estimates of Wastewater Production, Collection, Treatment and Reuse. *Earth Syst. Sci. Data* **2021**, *13* (2), 237–254.

(11) Wang, M.; Bodirsky, B. L.; Rijneveld, R.; Beier, F.; Bak, M. P.; Batool, M.; Droppers, B.; Popp, A.; van Vliet, M. T. H.; Strokal, M. A Triple Increase in Global River Basins with Water Scarcity Due to Future Pollution. *Nat. Commun.* **2024**, *15* (1), 880.

(12) Jones, E. R.; Bierkens, M. F. P.; van Vliet, M. T. H. Current and Future Global Water Scarcity Intensifies When Accounting for Surface Water Quality. *Nat. Clim Chang* **2024**, *14* (6), 629–635.

(13) Jones, E. R.; Bierkens, M. F. P.; van Puijenbroek, P. J. T. M.; van Beek, L. P. H.; Wanders, N.; Sutanudjaja, E. H.; van Vliet, M. T. H. Sub-Saharan Africa Will Increasingly Become the Dominant Hotspot of Surface Water Pollution. *Nature. Water* **2023**, *1* (7), 602–613.

(14) WWQA. https://www.unep.org/explore-topics/water/whatwe-do/improving-and-assessing-world-water-quality-partnershipeffort.

(15) An Introduction to SDG Indicator 6.3.2: Proportion of Water Bodies with Good Ambient Water Quality, 2022. *United Nations*. https://www.unwater.org/our-work/integrated-monitoring-initiativesdg-6/indicator-632-proportion-bodies-water-good-ambient.

(16) Desbureaux, S.; Mortier, F.; Zaveri, E.; van Vliet, M. T. H.; Russ, J.; Rodella, A. S.; Damania, R. Mapping Global Hotspots and Trends of Water Quality (1992–2010): A Data Driven Approach. *Environmental Research Letters* **2022**, *17* (11), 114048.

(17) Water Framework Directive (Directive 2000/60/EC) of the European Parliament and of the Council of 23 October 2000 Establishing a Framework for Community Action in the Field of Water Policy; European Commission: Brussels, 2000.

(18) DIRECTIVE 2013/39/EU of the EUROPEAN PARLIAMENT and of THE COUNCIL of 12 August 2013 Amending Directives 2000/ 60/EC and 2008/105/EC as Regards Priority Substances in the Field of Water Policy (Text with EEA Relevance); European Union, 2013.

(19) *Guidelines for Drinking-Water Quality*, Fourth ed., Incorporating the First and Second Addenda; World Health Organization: Geneva, 2022.

(20) Aribam, B.; Alam, W.; Thokchom, B.. Chapter 8 - Water, Arsenic, and Climate Change. In *Water Conservation in the Era of Global Climate Change*; Thokchom, B.; Qiu, P.; Singh, P.; Iyer, P. K., Eds.; Elsevier, 2021; pp 167–190. DOI: 10.1016/B978-0-12-820200-5.00003-8.

(21) Podgorski, J.; Berg, M. Global Threat of Arsenic in Groundwater. *Science* (1979) **2020**, 368 (6493), 845–850.

(22) Fatoki, J. O.; Badmus, J. A. Arsenic as an Environmental and Human Health Antagonist: A Review of Its Toxicity and Disease Initiation. *Journal of Hazardous Materials Advances* **2022**, *5*, 100052.

(23) Poikane, S.; Kelly, M. G.; Salas Herrero, F.; Pitt, J.-A.; Jarvie, H. P.; Claussen, U.; Leujak, W.; Lyche Solheim, A.; Teixeira, H.; Phillips, G. Nutrient Criteria for Surface Waters under the European Water Framework Directive: Current State-of-the-Art, Challenges and Future Outlook. *Science of The Total Environment* **2019**, *695*, No. 133888.

(24) Van den Roovaart, J. C.; Troost, T.; Van Gils, J.; Bouwman, A. F.; Beusen, A. H. W.; Altena, W.; Boisgontier, H.; Hegnauer, M.; Liguori, C.; Wardani, I.; Bleser, J. Global Scenarios for Ecosystem Health. Deltares Report 11207465-000-ZWS-0004, 2022. https://pub.kennisbank.deltares.nl/Details/FullCatalogue/1000020907.

(25) Reder, K.; Flörke, M.; Alcamo, J. Modeling Historical Fecal Coliform Loadings to Large European Rivers and Resulting In-Stream Concentrations. *Environmental Modelling and Software* **2015**, *63*, 251–263.

(26) Arsenic in Drinking-Water. Background Document for Development of WHO Guidelines for Drinking-Water Quality; Report WHO/ SDE/WSH/03.04/75; World Heath Organization: Geneva, 2003.

(27) Recreational Water Quality Criteria; 820-F-12-058; US Environmental Protection Agency, 2012.

(28) Environmental Quality Standard for Surface Water (GB3838-2002), 2002. Ministry of Environmental Protection (MEP). https://english.mee.gov.cn/Resources/standards/water_environment/ quality_standard/200710/t20071024_111792.shtml (accessed by January 2024).

(29) Beusen, A. H. W.; Bouwman, A. F. Future Projections of River Nutrient Export to the Global Coastal Ocean Show Persisting Nitrogen and Phosphorus Distortion. *Frontiers in Water* **2022**, *4*, na DOI: 10.3389/frwa.2022.893585.

(30) Strokal, M.; Bai, Z.; Franssen, W.; Hofstra, N.; Koelmans, A. A.; Ludwig, F.; Ma, L.; van Puijenbroek, P.; Spanier, J. E.; Vermeulen, L. C.; van Vliet, M. T. H.; van Wijnen, J.; Kroeze, C. Urbanization: An Increasing Source of Multiple Pollutants to Rivers in the 21st Century. *npj Urban Sustainability* **2021**, *1* (1), 24.

(31) Vermeulen, L. C.; van Hengel, M.; Kroeze, C.; Medema, G.; Spanier, J. E.; van Vliet, M. T. H.; Hofstra, N. Cryptosporidium Concentrations in Rivers Worldwide. *Water Res.* **2019**, *149*, 202–214.

(32) Janssen, A. B. G.; Teurlincx, S.; Beusen, A. H. W.; Huijbregts, M. A. J.; Rost, J.; Schipper, A. M.; Seelen, L. M. S.; Mooij, W. M.; Janse, J. H. PCLake+: A Process-Based Ecological Model to Assess the Trophic State of Stratified and Non-Stratified Freshwater Lakes Worldwide. *Ecol Modell* **2019**, *396*, 23–32.

(33) Voß, A.; Alcamo, J.; Bärlund, I.; Voß, F.; Kynast, E.; Williams, R.; Malve, O. Continental Scale Modelling of In-Stream River Water Quality: A Report on Methodology, Test Runs, and Scenario Application. *Hydrol Process* **2012**, *26* (16), 2370–2384.

(34) van Gils, J.; Posthuma, L.; Cousins, I. T.; Brack, W.; Altenburger, R.; Baveco, H.; Focks, A.; Greskowiak, J.; Kühne, R.; Kutsarova, S.; Lindim, C.; Markus, A.; van de Meent, D.; Munthe, J.; Schueder, R.; Schüürmann, G.; Slobodnik, J.; de Zwart, D.; van Wezel, A. Computational Material Flow Analysis for Thousands of Chemicals of Emerging Concern in European Waters. *J. Hazard Mater.* **2020**, 397, 122655.

(35) Posthuma, L.; van Gils, J.; Zijp, M. C.; van de Meent, D.; de Zwart, D. Species Sensitivity Distributions for Use in Environmental Protection, Assessment, and Management of Aquatic Ecosystems for 12 386 Chemicals. *Environ. Toxicol. Chem.* **2019**, 38 (4), 905–917.

(36) van Vliet, M. T. H.; Flörke, M.; Harrison, J. A.; Hofstra, N.; Keller, V.; Ludwig, F.; Spanier, J. E.; Strokal, M.; Wada, Y.; Wen, Y.; Williams, R. J. Model Inter-Comparison Design for Large-Scale Water Quality Models. *Curr. Opin Environ. Sustain* **2019**, *36*, 59–67.

(37) van Vuuren, D. P.; Edmonds, J. A.; Kainuma, M.; Riahi, K.; Weyant, J. A Special Issue on the RCPs. *Clim Change* **2011**, *109* (1), 1.

(38) World Population Prospects 2022; United Nations Department for Economic and Social Affairs, 2016. https://www.un.org/ development/desa/pd/sites/www.un.org.development.desa.pd/files/ wpp2022_summary_of_results.pdf.

(39) van Puijenbroek, P. J. T. M.; Beusen, A. H. W.; Bouwman, A. F.; Ayeri, T.; Strokal, M.; Hofstra, N. Quantifying Future Sanitation Scenarios and Progress towards SDG Targets in the Shared Socioeconomic Pathways. *J. Environ. Manage* **2023**, *346*, 118921.

(40) Van Puijenbroek, P. J. T. M.; Beusen, A. H. W.; Bouwman, A. F. Global Nitrogen and Phosphorus in Urban Waste Water Based on the Shared Socio-Economic Pathways. *J. Environ. Manage* **2019**, *231*, 446–456.

(41) van Vuuren, D. P.; Kriegler, E.; O'Neill, B. C.; Ebi, K. L.; Riahi, K.; Carter, T. R.; Edmonds, J.; Hallegatte, S.; Kram, T.; Mathur, R.; Winkler, H. A New Scenario Framework for Climate Change Research: Scenario Matrix Architecture. *Clim Change* **2014**, *122* (3), 373–386.

(42) Van Vuuren, D. P.; Stehfest, E.; Gernaat, D.et al. *The 2021 SSP Scenarios of the IMAGE 3.2 Model*; PBL-Netherlands Environmental Assessment Agerncy: The Hague, 2021.

(43) UNESCO-IHP IIWQ World Water Quality Portal. https://www.eomap.com/world-water-quality/.