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Global multi-pollutant modelling of water quality: scientific challenges and future directions

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Assessing global water quality issues requires a multi-pollutant modelling approach. We discuss scientific challenges and future directions for such modeling. Multi-pollutant river models need to integrate information on sources of pollutants such as plastic debris, nutrients, chemicals, pathogens, their effects and possible solutions. In this paper, we first explain what we consider multi-pollutant modelling. Second, we discuss scientific challenges in multi-pollutant modelling relating to consistent model inputs, modelling approaches and model evaluation. Next, we illustrate the potential of global multi-pollutant modelling for hotspot analyses. We show hotspots of river pollution with microplastics, nutrients, triclosan and *Cryptosporidium* in many sub-basins of Europe, North America and South Asia. Finally, we reflect on future directions for multi-pollutant modelling, and for linking model results to policy-making.

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Introduction

In many world regions, water quality issues are no longer related to just one type of pollution [1••]. This is because many human activities on land are sources of different river pollutants such as plastic debris, nutrients, chemicals and pathogens. Examples are intensive agriculture, industry and rapid urbanization (see Section 'Multi-pollutant modelling of global water quality'). These are increasing sources of an increasing number of water pollutants over the past decades [2••,3,4]. However, existing, global water quality studies focus often on individual (groups of) pollutants [5•,6,7•,8•]. Thus, water quality assessments are largely incomplete in terms of pollutants for many world regions, which prevents the formulation of effective solutions. This calls for integrated, multi-pollutant modelling for comprehensive water quality assessments at the global scale [1••]. Such assessments should include analyses of hotspots with multiple pollutant (e.g. plastic debris, nutrients, chemicals), their causes and solutions. This information will help to prioritize national monitoring programs and support the Sustainable Development Goal (SDG) 6 for clean water for all [9••]).

Global multi-pollutant modelling is, therefore, needed. In this paper, we synthesize existing knowledge on global multi-pollutant modelling and identify scientific challenges and future directions for global multi-pollutant modelling. First, we explain what we consider multi-pollutant modelling (Section 'Multi-pollutant modelling of global water quality'), Second, we discuss scientific challenges in multi-pollutant modelling (Section 'Scientific challenges for global multi-pollutant modelling'). Next, we illustrate the potential of global multi-pollutant modelling (Section 'Illustrating the potential of global multi-pollutant modelling'). Finally, we reflect on future research directions (Section 'Future directions').

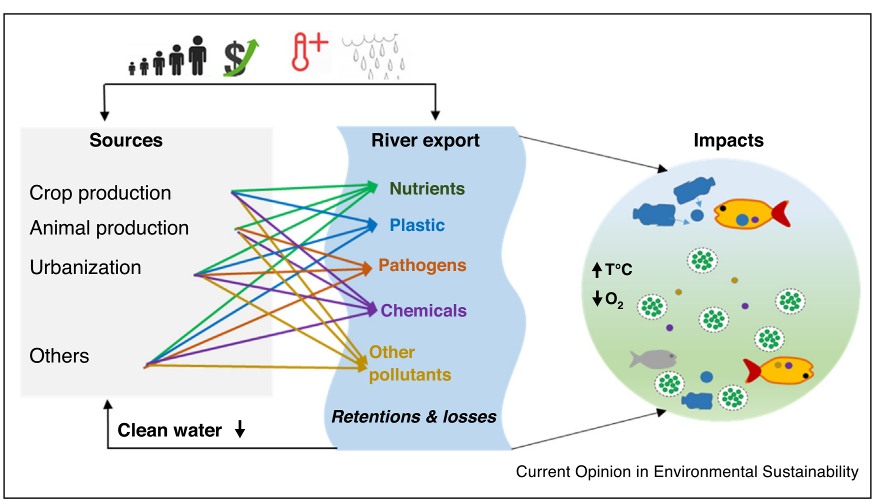
Multi-pollutant modelling of global water quality

In this study, multi-pollutant modelling refers to simultaneous modelling of the river export of a number of pollutants from land to sea. Pollutants include (groups of) substances that do not naturally occur in aquatic systems (e.g. plastic debris or synthetic chemicals) or with concentrations deviating from their optimal range (e.g. nutrients). Multi-pollutant problems typically result in a variety of impacts on aquatic systems and society (Figure 1). For example, nutrient pollution is causing eutrophication problems in many world rivers and seas [10–12,13•,14]. Likewise, plastic pollution is increasing globally [15,16,17•,18]. Plastic debris may contain chemicals (e.g. additives) that can be harmful for aquatic organisms [19–21]. Pathogen contamination of surface water is a cause of diarrhea, particularly in developing countries [5•,22,23]. Organic pollution of rivers can disturb aquatic ecosystems by stimulating microbial growth [24•,25]. There are more groups of pollutants with the potential environmental risk (e.g. pesticides [7•], nanoparticles [26], pharmaceuticals [27,28,29•]). As a result of water pollution, the availability of clean water for nature and human needs (e.g. irrigation) has been declining (Figure 1). Clean water availability is hardly analyzed from a multi-pollutant perspective [24•].

Water pollution results from many different human activities (Figure 1). We may distinguish between point sources of pollution (e.g. pipes draining into rivers) and diffuse sources (e.g. via leaching from soils). For example, crop production can be a diffuse source of nutrients [30] and pesticides [7•] in rivers. Animal production can be a diffuse (via manure use on land) and point (via manure discharges to rivers) source of nutrients [30,31] and pathogens [5•] in rivers. Sewage systems discharge effluents to rivers. Such effluents contain different pollutants such as nutrients [11,30], microplastics [16,17•], pathogens [22,23], pharmaceuticals [27,28,29•], nanoparticles [26] and can contribute to organic pollution [2••,14,32••] in rivers. The sources of pollution may differ among world regions. Recent studies indicate, for example, that open defecation is an important source of nutrients and pathogens in India and Bangladesh [33,34] and that direct manure discharges are major point sources of nutrients in Chinese rivers [31]. The above mentioned existing studies provide useful insights in the sources of individual groups of water quality parameters. Nevertheless, a better understanding of the sources of multiple pollutants in rivers is urgently needed.

Several multi-pollutant models exist for individual watersheds (e.g. [19,35–37]). These are data intensive which makes upscaling to global applications difficult. A multi-pollutant model exists for continental applications (WorldQual [2••] model, Tables S1.1–S1.4, Box S3.1). This model quantifies water pollution from several groups of pollutants (e.g. nutrients, microorganisms) using the consistent and comprehensive modelling framework (Box S3.1). It accounts for point and diffuse sources and for seasonality. However, WorldQual does not quantify pollutants simultaneously. And, the model has not yet been implemented for future scenarios to explore solutions. In contrast, several global or continental scale models have been used for scenario analyses, but mainly for individual groups of water quality parameters (see Tables S1.1–S1.4). These include models for nutrients [11,30,38•], plastics [15,16,17•], chemicals (e.g. triclosan [8•], pesticides [7•]), nanoparticles [26], pathogens [2••,22,23,39•], water temperature [40,41], salinity or biological oxygen demand [2••,14,25,32••,42]. These are not multi-

Figure 1



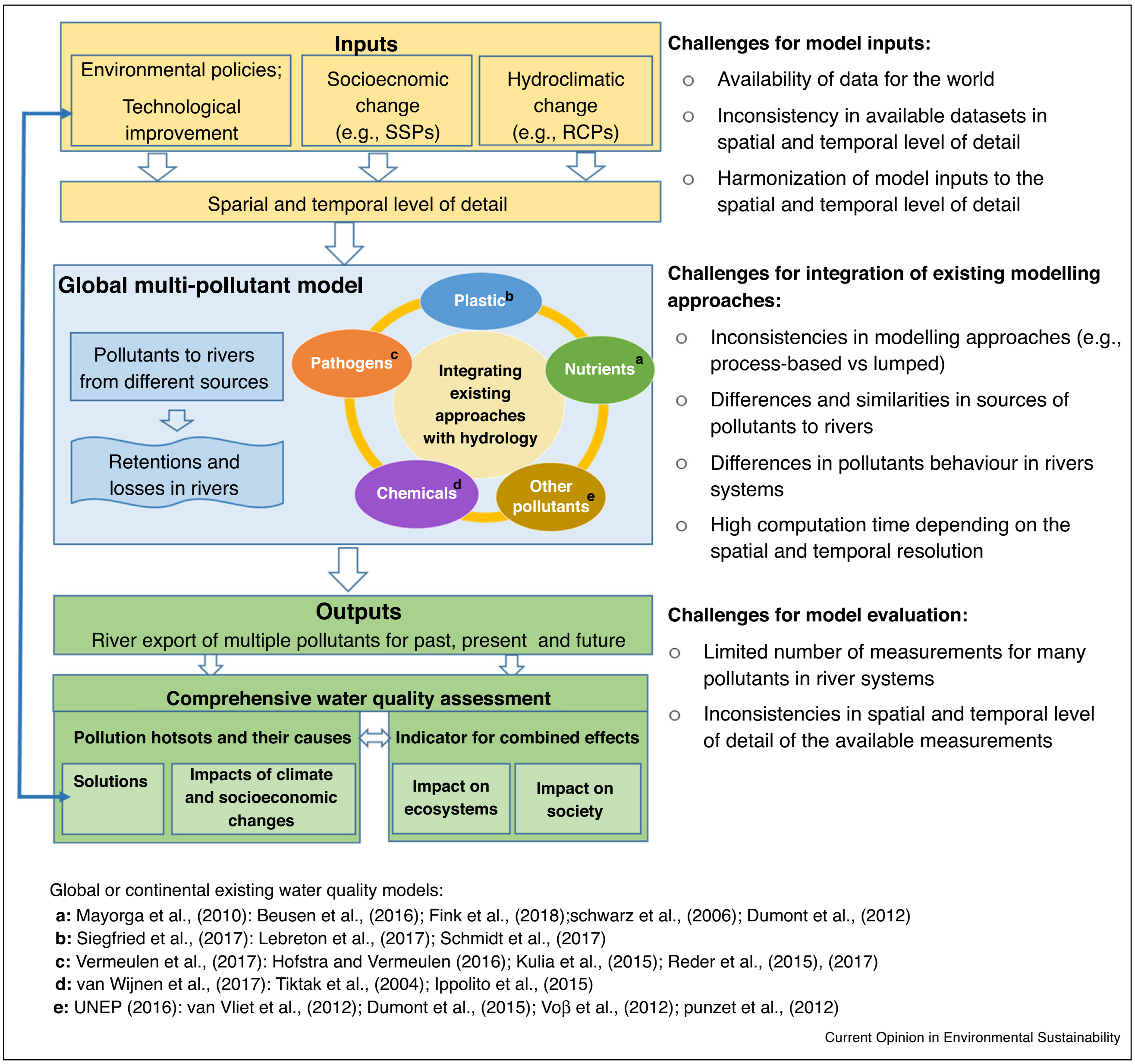
Simplified illustration of the relations between sources of pollutants in rivers and their impacts. Nutrients, plastic, pathogens, chemicals are pollutants when their concentrations deviate from the optimal ranges in aquatic systems. 'Other pollutants' refer to any group of pollutants (e.g. nanoparticles, organic pollution, salt) that are not indicated in the figure. See Kroeze *et al*. [1••] and Text S2 for more information.

pollutant models. Most account for sources of one type of pollutant in aquatic systems, and they differ in several aspects: for example input data sources, modelling approaches, spatial and temporal level of detail (see Section 'Multi-pollutant modelling of global water quality', Tables S1.1–S1.4). These differences make comparisons between model results difficult. To identify hotspots of multiple pollutants, their causes, and solutions requires a consistent and comprehensive multi-pollutant modelling approach.

Scientific challenges for global multi-pollutant modelling

Global multi-pollutant modelling can follow from integration of existing single pollutant models (Figure 2, Box S3.1). Such integration requires consistency in datasets for model inputs in terms of spatial and temporal level of

Figure 2



An illustrative example of a conceptual model for river export of multiple pollutants from land to sea, and the main scientific modelling challenges. Box S3.1 summarizes this conceptual modelling approach, its temporal and spatial level of detail. This example combines pollutants for which global or continental modelling approaches exist. The potential of a multi-pollutant model based on this scheme is given in Section 'Illustrating the potential of global multi-pollutant modelling' and in Figure 3. Figure 3 presents an implementation of part of the conceptual model described in Figure 2.

detail. Figure 2 presents an example of a multi-pollutant model to quantify inputs of multiple pollutants to rivers and their exports to sea. Socioeconomic development, land use change and hydrology are drivers of river export of pollutants in the past, present and future. The calculated pollution loads can be used in different types of analysis, such as hotspot analyses, scenario analyses searching for solutions, or the development of indicators that combine multiple pollutants to assess their impacts on ecosystems and society (Figure 2).

Below, we discuss the main challenges that are associated with model inputs, integration of the existing modelling approaches and model evaluation (Figure 2).

Challenges associated with model inputs

We identified three main challenges (Figure 2): first, availability of data covering the world, second, inconsistencies in available global datasets in spatial and temporal level of detail and third, harmonization of model inputs between the global datasets for spatial and temporal level of details [see also Ref. 32••]. An integrated global multi-pollutant model needs information on socioeconomic development such as trends in economy, population, urbanization, sanitation, food production (e.g. number of animals, application of fertilizers to crops), and land use. We also need information on climate and meteorological forcing, and on hydrology to account for retentions of pollutants in river systems and to calculate concentrations of pollutants in rivers. In addition, information is needed on environmental policies and technological development, to explore solutions. These inputs can be user-defined (e.g. by stakeholders and policy-makers).

Several global databases exist for main socioeconomic drivers (e.g. population, economy). Some databases provide information by country, and others on a grid cell level. They differ with respect to the years that are covered, and scenario assumptions. Examples of global databases with country-specific information are FAOSTAT for agricultural information (e.g. fertilizer use; http://www.fao.org/faostat/en/#home) and the WHO/UNICEF Joint Monitoring Program for sanitation types (e.g. number of people with sewage connections; https://washdata.org/data) for different historical years. Sometimes, the data or time series are not complete for all countries. Global Shared Socio-economic Pathway (SSPs) databases [43] provide future projections for countries for the main socioeconomic drivers such as the gross domestic product [44–46], total population [47] and urban population for the period 2000–2100 with 10-year time steps [48]. Examples of global databases with grid-specific information are datasets from the IMAGE model (e.g. for nutrient soil balances) at 0.5° cell for the period 1900–2050 based on the Millennium Ecosystem Assessment scenarios [49], and the NCAR database for total, urban and rural population at 0.125° cell for the period 2000–2100 based on the SSP scenarios [50,51]. Another example are the gridded databases for global livestock distribution at finer resolutions of 1 km at the equator [52]. These examples clearly indicate the spatial and temporal inconsistencies.

Hydrological variables such as river discharges are typically modelled at a grid (e.g. 0.5° cells) for longer periods (e.g. up to 2100) with inter-annual variability (e.g. daily, monthly). The Representative Concentration Pathways [53] are often used as the basis to project future trends in hydrology under a changing climate. Several global hydrological models exist (see Tables S1.1–S1.4 for model descriptions). Many simulate water flows at a resolution of 0.5°: for example VIC [54,55], the Water Balance Model [56], and H08 [57,58]. Some hydrological models perform at a finer resolution such as 5' (approximately 0.08°). These are, for example, PCR-GLOBWB [59] and WaterGAP3 [60] (for details see Tables S1.1–S1.4). The existing global models for river pollution use hydrology from different models. For instance, the Water Balance Model is used for nutrients (Global *NEWS*-2), triclosan [8•] and microplastics [17•], the PCR-GLOBWB model for nutrients [11] and the Variable Infiltration Capacity (VIC) for water temperature [61] and pathogens [5•].

Harmonizing model inputs between and within socioeconomic and hydrological databases is an essential step towards a consistent global multi-pollutant model (Figure 2). Existing studies did this for individual water quality parameters (Tables S1.1–S1.4). These provide an opportunity to learn for global multi-pollutant modelling.

Challenges associated with integration of the existing modelling approaches

We identified four main challenges (Figure 2): first, inconsistencies in modelling approaches, second, differences in sources of river pollution, third, differences in pollutant behavior in river systems and fourth, computational (IT) barriers depending on the spatial and temporal resolution.

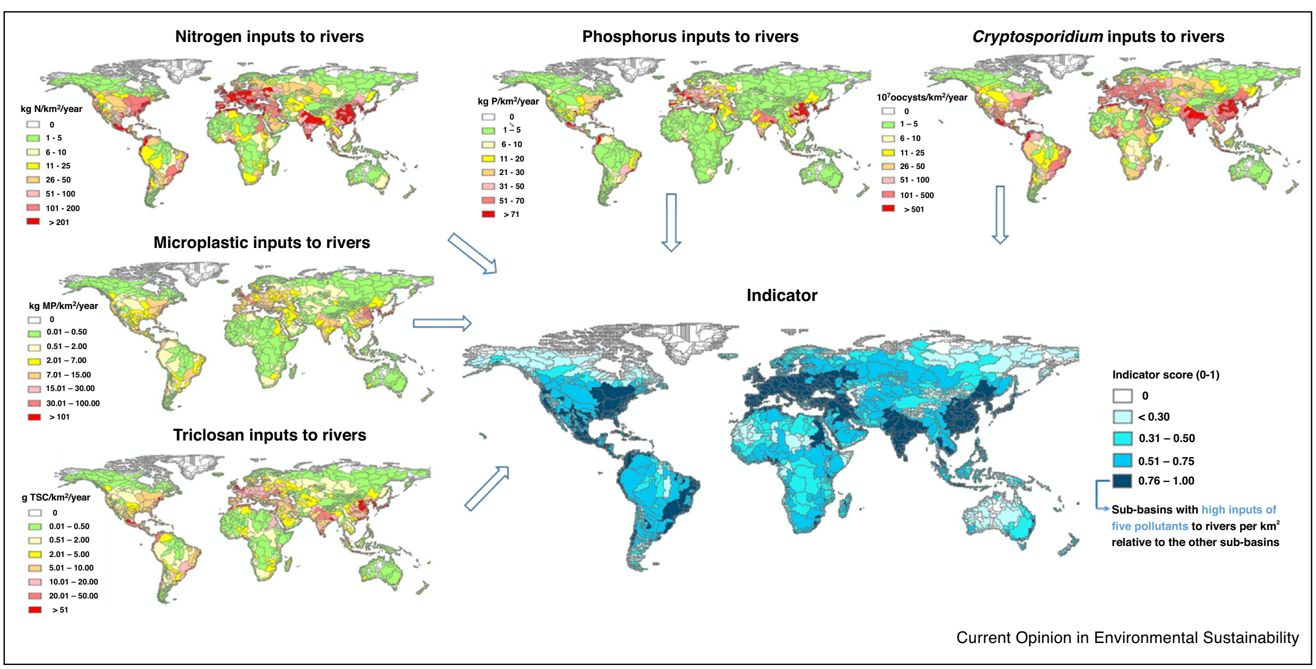
Existing modelling approaches differ in how the processes controlling export of pollutants to rivers and sea are modelled. Some models lump processes, while other are more detailed. Lumped models use rather simple parameter-based approaches to quantify retentions and losses of pollutants in river systems, and often focus on the integration of sources of pollution and possible solutions. They are typically on an annual temporal basis, ignore heterogeneity within a river basin, however, can be easily used for scenario analyses to explore solutions. Examples are the integrated global or continental models for nutrients (Global *NEWS*-2 [30], MARINA [62]), triclosan [8•] and microplastics [17•]. Another type are the distributed, process-based models. Such models more explicitly account for the terrestrial water cycle and substance flows within a river basin. Modelling of processes controlling retentions and losses of pollutants in soils and rivers is typically more complex in distributed than in lumped models, and often account for inter-annual dynamics. Distributed models often run at grid scale (e.g. 0.5° cell). However, data needs and computation time are generally higher. Examples are gridded models for nutrients (IMAGE-GNM [11], WorldQual [2••,38•]), microorganisms (WorldQual [2••,39•] and for pathogens GLoWPa [5•,23]), water temperature (RBM [63,64], WorldQual [65]), biological oxygen demand and salinity (WorldQual [2••,39•]).

For a global, integrated multi-pollutant model, we may start with a rather pragmatic way of integrating existing modelling approaches. This requires changes in existing modelling approaches (e.g. adding new or re-calibration of existing parameters). We argue for a first multi-pollutant model to be in-between lumped and process-based, and to include important sources of different pollutants and their behavior in river systems for scenario analyses.

Existing global models differ in the sources of pollutants that are accounted for (see Section 'Introduction', Figure 1). But there are also similarities. This relates to the fact that some pollutants have common sources. For example, pollutants from personal care products (e.g. triclosan [8•] and microplastics [17•]) are discharged in rivers through sewage systems (point source), that also transport pathogens and nutrients from households. Meanwhile, manure use on land is also a source of pathogens and nutrients (diffuse source). The existing modelling differ in how they approach point and diffuse sources, making integration possible, but also a challenge (see example in Section 'Scientific challenges for global multi-pollutant modelling' and Figure 3).

In addition, it is challenging to integrate modelling approaches to represent behaviors of different pollutants in river systems. Reasons are different modelling approaches (e.g. lumped versus process-based) and the complex interactions between pollutants and the environment variables (see Kroeze *et al.* [1••] and Text S2). For example, water temperature has an important impact on other water quality indicators/variables by affecting the rate of several biochemical processes and the solubility of many chemical compounds (e.g. [66]). An increased

Figure 3



Illustrative example of how global multi-pollutant models can be used to identify hotspot areas, where rivers receive high inputs of more than one pollutant from point sources in 2010. We integrate existing modelling approaches for annual point source inputs of nitrogen, phosphorus [30,62], *Cryptosporidium* [23,73], microplastics [17•] and triclosan [8•] to rivers. Annual inputs of the pollutants to rivers are quantified for 2010. The year 2010 was selected for this example to show the hotspots of the current river pollution in the world. This is the baseline for analyses to explore effective solutions. Maps with green–red colors show annual inputs of the pollutants to rivers from point sources (kg or g or 10^7 oocysts/km^2 of sub-basin/year). Point sources include sewage systems and open defecation. The map with blueish colors shows an indicator that combines annual inputs of five pollutants to rivers into a standardized score of 0–1. The indicator is based on the approach of Vörösmarty *et al.* [79] (see the Supplementary materials for the summary on the methodology).

temperature would lead to increased growth of pathogens, as long as the water temperature (e.g. in lakes) does not reach above the 37 °C [67,68]. Water temperature influences salinity also indirectly via increased evapotranspiration that gives rise to salt accumulation (see Text S2). A strong link between cycles of carbon, nitrogen, phosphorus and silica is reported [69]. However, a better understanding is still needed how different pollutants can affect each other (e.g. nutrient-induced eutrophication and micro-pollutants [19]) and what their combined impacts are on ecosystems.

Challenges associated with model evaluation

Evaluation of model performance is essential to understand and reduce model uncertainties. One way to evaluate is to compare model results against observations. We identified two main challenges: first, limited number of measurements for many pollutants in river systems and second, inconsistencies in spatial and temporal level of detail of the available measurements. Global database of observations exist: GEMS/GLORI (http://web.unep.org/gemswater/), but for a limited number of pollutants and areas (e.g. data from developing countries is scarce). Possible reasons are that national monitoring programs often consider limited range of water quality parameters. Furthermore, sampling locations do not often match with locations of modelled results especially for lumped water quality models.

Existing models for global applications were evaluated for individual water quality parameters, but with limited observations. Therefore, other options were used to build trust in model performance [e.g. 70,71]. One option is a sensitivity analysis to test the sensitivity of model outputs for changes in model parameters [72]. Another option is to compare model inputs with independent datasets: for example river discharges from different hydrological models, GDP from different projections (see above). And multi-model comparison is important for robust hotspot assessments. Expert knowledge may reveal uncertainties in model parameters.

Illustrating the potential of global multi-pollutant modelling

To illustrate the potential of global multi-pollutant modeling we present an implementation of part of the conceptual model described above (Figure 2). We focus on river quality in 10 226 sub-basins in the world. We aggregated 10 226 sub-basins based on the VIC flow direction [54,55]. Drainage areas of large rivers (e.g. Amazon, Danube, Mississippi, Yangtze, Yellow, Pearl) were divided into smaller sub-basins following [62]. We focus on point sources of a number of pollutants in rivers: sewage systems and open defecation (Table 1). Our analysis focuses on annual values for 2010 to illustrate the potential of global multi-pollutant modelling. This implies that monthly or seasonal variations in river pollution are not within the scope of our analysis (Figure 3).

We integrate existing modelling approaches for annual point source inputs of nitrogen, phosphorus [30,62], *Cryptosporidium* [23,73], microplastics [17•] and triclosan [8•] to rivers for 2010. For example, Global *NEWS-2* [30] quantifies nitrogen and phosphorus export by world rivers. We use the modelling approach of Global *NEWS-2* to quantify inputs of nitrogen and phosphorus to rivers. Validation results of Global *NEWS-2* indicate a good performance at the global scale (R^2 ranges from 0.51 to 0.90 depending on nutrient form Ref. [30]). Global *NEWS-2* was also validated at regional scales [34,74–78]. We use the approach of the GLoWPa model [73] for *Cryptosporidium* that was evaluated through a sensitivity analysis. The modelling approaches of microplastics [17•] and triclosan [8•] were also evaluated by comparing modeled values with measurements available for a few rivers [details are in Refs. 8•,17•]. All this builds trust in using these existing modelling approaches in our illustrative example for global multi-pollutant modelling. Table 1 summarizes model inputs that we used from existing studies. We also compared our results with other studies (Table S3.8). Table 1 summarizes how inputs of the pollutants to rivers are quantified.

We integrate model results for five pollutants into a simple indicator to show how multi-pollutant models can be used for hotspot analyses. The indicator is based on the approach of Vörösmarty *et al.* [79] (Figure 3). Details on the methodology are in the Supplementary materials.

We focus on hotspot areas where rivers are considerably polluted (Figure 3). Such hotspots can be found worldwide for 2010. For example, river inputs of more than 100 kg of nitrogen per km^2 and more than 50 kg of phosphorus per km^2 are found in Europe, North America and South Asia. Many rivers in Europe and South Asia received >15 kg of microplastics and >10 g of triclosan per km^2, respectively. High river inputs of *Cryptosporidium* (>100 10^7oocysts per km^2) are quantified for many sub-basins (Figure 3). Over two-thirds of the pollutant loadings were from urban sewage systems. Open defecation in urban areas contributed to river pollution (especially with *Cryptosporidium*) in some sub-basins in developing countries like India and Indonesia.

We use an indicator for hotspots of multi-pollutant problems (Figure 3). These hotspots are sub-basins with high river inputs of all five pollutants (i.e. when the indicator score is higher than 0.75). Multi-pollutant hotspots are found in Europe, North America and South Asia (Figure 3). These are the areas with relatively high population densities and relatively intensive human developments [e.g. 48,80••]. The hotspot sub-basins (score >0.75 in

Table 1

Summary of method to quantify annual inputs of the selected pollutants to rivers from point sources as shown in Figure 3. First, we quantified annual inputs to rivers by grid of 0.5° cell for 2010. Then, we aggregated results to 10 226 sub-basins based on the VIC flow direction [54,55]. Drainage areas of large rivers (e.g. Amazon, Danube, Mississippi, Yangtze, Yellow, Pearl) were divided into smaller sub-basins following [62]. Details on the methodology are in the Supplementary materials

Group of pollutants	Representatives	Point sources
Nutrients	Nitrogen, phosphorus[a]	Sewage systems and open defecation (human waste)
Pathogens	*Cryptosporidium*	Sewage systems and open defecation (human waste)
Plastic	Microplastics	Sewage systems (e.g. personal care products)
Chemicals	Triclosan	Sewage systems (e.g. personal care products)

Inputs of pollutants to rivers from sewage systems and open defecation are calculated as a function of
◦ urban and rural population [48], open defecation rates [23,73] [b], connection rates to sewage systems [23,73] [b], removal efficiencies [8•,17•,73,83], excretion (for nitrogen [83] [c], phosphorus [83] [c], *Cryptosporidium* [73]) or consumption (for products containing microplastics [17•] and triclosan [8•]) rates

[a] We account for detergents based on Ref. [83].
[b] Country-specific. For missing values we used regional averages.
[c] Nitrogen and phosphorus excretion is estimated as a function of the gross domestic products [details in Ref. 83]. We adjusted the approach for units of 2005 US$/capita/year.

Figure 3) cover 20% of the global land area, but accommodate over two-thirds of the total population in the world, of which half urban [48]. For many of these hotspot areas water scarcity issues have been reported [80••,81,82]. We can contribute to the existing studies by providing water quality information to improve water scarcity assessments [24•,32••].

In our illustrative example, we focused on five pollutants from point sources. However, more pollutants exist that may enter rivers from point and diffuse sources. For example, the WorldQual model shows that around one-third of all river stretches were affected by severe pathogen pollution in Latin America, Africa, and Asia, while around one-seventh are affected by severe organic pollution and one-tenth by high salinity levels in 2010 [2••] (Box S3.1). Integrating the approaches of the WorldQual model (and also other global models, see Figure 2) with our global multi-pollutant model will allow to have water quality information on more pollutants and for more sources. This will facilitate comprehensive water quality assessments and help to identify robust hotspot areas in the world. Such information is essential when exploring effective solutions.

Future directions

We highlight three main directions for future research.

First, there is a need to further develop multi-pollutant models at the global scale. The associated scientific challenges include harmonizing model inputs, integrating the existing modelling approaches and evaluating model uncertainties (see Section 'Scientific challenges for global multi-pollutant modelling'). We need to better use existing knowledge and do more research. Examples exist of how to harmonize model inputs into consistent datasets, but only for individual pollutants (see Sections 'Multi-pollutant modelling of global water quality' and 'Scientific challenges for global multi-pollutant modelling'). We can use these examples for multi-pollutant modelling. An example is the GLoWPa model [23] in which country data on sanitation were combined with gridded data on population to quantify pathogen inputs to rivers by grid. Another example is the Global *NEWS-2* model of McCrackin *et al.* [83] for which a method was developed to downscale annual model inputs into a consistent, seasonal dataset for nutrient management. For integrating existing modelling approaches, expert knowledge is important. It can help to better understand the dominant processes that control river export of multiple pollutants from land to sea. However, our understanding of interactions of pollutants in rivers at the larger scale is limited. Thus, more research is needed to better understand how pollutants interact with each other biogeochemically in rivers. This knowledge will help to improve the modelling approaches and will allow us to include more pollutants to assess their combined effects. Uncertainty analysis is essential to build trust in the results of multi-pollutant models [72]. This is challenging, but possible. For example, it is possible to combine validation results of the existing global models for individual pollutants with other options to build trust in multi-pollutant models. These options are, for example, sensitivity analysis, multi-model comparison, and use of expert knowledge (see Section 'Scientific challenges for global multi-pollutant modelling'). This will facilitate comprehensive assessment of the impacts of global change on water quality and facilitate the development of effective policies.

Second, we need to better link the results of multi-pollutant river modelling with other research fields. Various research fields can benefit from this. Examples are water scarcity studies [24•] and risk assessments. Furthermore, we can contribute to a better understanding of interactions between surface and ground water quality. Ground water is an important source of freshwater for irrigation and drinking water in many parts of the world [84] and should also be part of water quality assessments. Sharing data through international platforms (e.g. ISIMIP, https://www.isimip.org/) can enhance the collaboration between research groups in the world.

Third, science needs to be better linked with policy through participatory modeling and scenario analysis. For instance, hotspot analyses as presented in this paper can be used as a basis for policy making and to prioritize monitoring programs. Platforms such as the 'Water Futures and Solutions' Initiative of the International Institute for Applied Systems Analysis (IIASA; http://www.iiasa.ac.at/web/home/research/wfas/water-futures.html) can facilitate dialogues between scientists and stakeholders. This is needed to ensure that modelling exercises are policy relevant. Participatory scenario analysis can thus help to explore effective solutions. Multi-pollutant modelling may also support the process to realize SDG 6 for 2030: clean water for all. This can be done through, for example, scenario analysis (how to reach the targets), optimization analysis (what is the optimal solution) and/or back-casting exercises (how to get to the desired water quality level). Thus, developing multi-pollutant models will help to better understand water pollution and assist the search for effective solutions.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.cosust.2018.11.004.

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- • of special interest
- •• of outstanding interest

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