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How to model algal blooms in any lake on earth☆

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Algal blooms increasingly threaten lake and reservoir water quality at the global scale, caused by ongoing climate change and nutrient loading. To anticipate these algal blooms, models to project future algal blooms worldwide are required. Here we present the state-of-the-art in algal projection modelling and explore the requirements of an ideal algal projection model. Based on this, we identify current challenges and opportunities for such model development. Since most building blocks are present, we foresee that algal projection models for any lake on earth can be developed in the near future. Finally, we think that algal bloom projection models at a global scale will provide a valuable contribution to global policymaking, in particular with respect to SDG 6 (clean water and sanitation).

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Introduction

Lakes and reservoirs provide essential ecosystem services such as water for drinking and irrigation [1], food supply for many people around the world [2–4] and sites for recreation and tourism [3]. Severe algal blooms threaten these ecosystems for example by producing toxins, odors and by causing oxygen depletion [5]. Worldwide, the occurrence and severity of algal blooms are expected to increase in response to ongoing human-driven nutrient loading and climate change [6–8].

Algal blooms are triggered by excess nutrient loads of particularly phosphorus and nitrogen from the catchment [9] and further promoted by relative high water temperatures [10]. In the natural pristine state, excess nutrients loads from the catchment were rather an exception than a rule, since nutrient availability was limited by slow processes such as weathering of rocks [6]. At present, global anthropogenic nutrient sources double natural sources caused by human activities such as phosphorus mining, industrial nitrogen fixation and fossil fuel combustion [6,11]. Similarly, human activities contribute to global warming which is expected to further aggravate the growth of algal blooms in lakes [7]. To which degree algal blooms respond to excess nutrient loadings and climate change differs among individual lakes. First, this response depends on hydraulic residence time and nutri ent loads to the lake which is determined by the location of a lake within a hydrological network. Additionally, lake-specific

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geomorphological and ecosystem characteristics, such as lake depth, size, light climate and water temperature, determine the sensitivity of a given lake's algal bloom dynamics to nutrient loading and climate change [10,12]. For more details on the effect of different kind of geomorphological and ecosystem characteristics on algal blooms formation please refer to supplementary material 1.

Anticipating how algal blooms will respond to future nutrient loading and climate change can help to prioritize regions for attention and mitigation, evaluate alternative mitigation strategies, and adapt to future ecological changes [13,14•]. Mathematical models can be used to project future global developments based on socio-economic scenarios, as found in, for example, climate research [15] and global nutrient assessments [16]. Such projections have put the potential impacts of global changes at the top of political, societal and economic agendas and helped to formulate the UN Sustainable Development Goals (SDG) [17]. With respect to SDG 6 (clean water and sanitation), projections are especially important to anticipate threats of algal blooms to clean water provision by lakes. The idea to develop models to project future algal blooms is widely supported by initiatives such as ISIMIP (https://www.isimip.org), GLEON (http://gleon.org/) and IPBES (https://www.ipbes.net/).

Here, we provide a roadmap for the development of models to simulate global scale scenarios for algal blooms in freshwater lakes and reservoirs, hereafter referred to as algal projection models. We define algal blooms as locations with a high phytoplankton biomass, including algal scums, reaching a critical level (e.g. chlorophyll-a, dry weight) at which they are expected to threaten ecosystem services (see Poikanen *et al.* [18] for critical chlorophyll-a levels). First, we present the state-of-the-art in algal projection modelling for lakes and reservoirs. Next, we explore the requirements of an ideal algal projection model. Based on these requirements we discuss the challenges and opportunities for future algal projection model development. We conclude that the time is ripe to develop algal projection models for global assessments of lake water quality, which are urgently needed to meet SDG 6.

State-of-the-art in algal projection modelling

Algal projection modelling for freshwater lakes and reservoirs started with the seminal work of Vollenweider, Rast and Lee [19,20]. Using a simple regression model based on hydraulic residence time and nutrient load data, chlorophyll-a concentrations for multiple lakes were estimated. By then, Rast *et al.* [19] noticed: "*Despite tens of millions of dollars spent on water quality management, adequate load and response data are available for less than a dozen water bodies*". Despite Rast's critical note, nowadays, nutrient load data to model lake water quality are still scarce, especially in developing regions [21]. This data scarcity is, to a large extent, caused by the costs and complexity of monitoring nutrient loads. Today, this data scarcity can be addressed by using nutrient load models to estimate nutrient loads to lakes based on different land uses in the lake's catchment [16,22•]. Similarly, data on water temperature at different depths, residence times and local light climate are scarce. This data scarcity can be covered by improved simulations by models such as GLM [23,24] and FLAKE [25]. In contrast, data on key ecological variables for lakes (e.g. lake morphology, phosphorus, nitrogen, and chlorophyll-a concentrations) have become increasingly available at high temporal and spatial scales caused by technological innovations. These innovations constitute, for example, high frequency devices to quantify for example nutrient concentrations, algal biomass and pH [26•], eDNA techniques to identify organisms present in the lake [27], and remote sensing techniques to measure lake morphology [28••] and various water quality parameters (for a full overview see Gholizadeh *et al.* [29]). Increased data availability allowed for modelling, and validation thereof, of an increased number of lakes than has previously been possible (Table 1).

Each model listed in Table 1 has advantages and limitations. The majority of these models are statistical and in most cases based on regression techniques (e.g. GLOBIO-aquatic in combination with Håkanson [30] and the model by Kosten *et al.* [31]). As an advantage, statistical approaches are generally simple and may point to causal relationships [32]. However, statistical techniques do not necessarily reveal an understanding of the true underlying biological processes [33]. For example, a statistical model between fish biomass and dissolved nutrients in the water may show high correlations, however, it fails to acknowledge that fish do not feed directly on dissolved nutrients. A further drawback is that often linear regression is applied in statistical models, which is not capable of capturing sudden threshold shifts or other non-linear relationships. As an example, the growth of an organism may linearly increase with temperature. However, at some point a temperature threshold is reached, leading to a sudden drop in growth rate, which is not covered by the linear regression. Applying a hierarchical 'hurdle' model [34] in which regression analysis is based on a data set that is split into two parts, solves the threshold issue to a certain degree. Another approach is the generalised additive model (GAM) [35] where the relationship between the response and the explanatory variables is allowed to be a smooth function instead of linear. Nonetheless, all statistical approaches are based on data from past conditions which are not necessarily the same in the future [33]. Therefore, care should be taken when statistical models are applied beyond the calibration domain. Consequently, using statistical models for projections of algal blooms is generally not recommended.

Conversely, process-based models like VEMALA v3, PCLake, Delft3D-WAQ/ECO, NiRReLa (Nitrogen

Table 1

A list of models simulating water quality variables in freshwater lakes and reservoirs and that are used to simulate at least 100 lakes on Earth. These models have at least output on in-lake nutrients or a state variable for phytoplankton: chlorophyll-a, biovolume or biomass

Name of model	Application area	Water type	# of lakes or reservoirs	Minimum lake size (km^2)	Output variable[a]	Model type	Data on nutrient load to lake or reservoir	Advantages (+) and limitations (−) of the model
(OECD)-Vollenweider-Rast-Lee and Jones model [19,20][b]	USA, Europe, Asia	Lakes and reservoirs	~200	Unknown	Chl-a	Statistical model	Measured	+ Widely used for many lakes + simple model to calculate chlorophyll-a + Requires little input data − Only applied using measured input data − Cannot be used outside the calibration domain
NiRReLa [37]	World	Lakes and reservoirs	243893	>0.1	N retention	Process-based model	Large lakes: modelled [62] Small lakes: estimated	+ Simulates a high number of lakes around the world + Accounts for smaller lakes and reservoirs − Is not able to provide output on algal blooms − In-lake processes are based on simplified equations
Delft3D-WAQ/ECO (BLOOM) [41] and case-specific reports	World	Lakes and reservoirs	>100	>0.01	Algal biomass, Chl-a, P, N, SS, zooplankton, shellfish	Process-based model	Case-dependent (Measured or modelled)	+ The model accounts for detailed in-lake processes + Output may have high spatial detail − Run-time is relatively long − Requires relatively much input data
NA [35]	UK	Lakes	134	>0.01	Cyanobacterial biomass	Statistical model	Not used	+ simple model to calculate cyanobacterial biomass + Uses a smooth function instead of a linear regression + Requires little input data − Calculations not based on drivers of change climate change and nutrient load) − Is only used for lakes in the UK − Cannot be used outside the calibration domain
NA [63]	Germany	Lakes	102	NA	Cyanobacterial biovolume	Statistical model	Not used	+ simple model to calculate cyanobacterial biovolume + Requires little input data − Calculations not based on drivers of change (climate change and nutrient load) − Is only used for lakes in Germany − Cannot be used outside the calibration domain
NA [31]	World	Lakes and reservoirs	143	>0.006	Chl-a, algal biovolume	Statistical model	Not used	+ Has a global coverage + simple model to calculate cyanobacterial biovolume + Requires little input data − Calculations not based on drivers of change (climate change and nutrient load) − Cannot be used outside the calibration domain

Table 1 (*Continued*)

Name of model	Application area	Water type	# of lakes or reservoirs	Minimum lake size (km^2)	Output variable[a]	Model type	Data on nutrient load to lake or reservoir	Advantages (+) and limitations (−) of the model
NA [64]	North-America	Lakes and reservoirs	1148	>0.04	Chl-a, cyanobacterial biomass	Statistical model	Not used	+ simple model to calculate cyanobacterial biovolume and chlorophyll-a + Requires little input data − Calculations not based on drivers of change (climate change and nutrient load) − Is only used for lakes in North-America − Cannot be used outside the calibration domain
SiRReLa [36,38]	World	Lakes and reservoirs	243893	>0.1	Si retention	Process-based model	Large lakes: modelled with IMAGE-GNM [65] Small lakes: estimated	+ Simulates a high number of lakes around the world + Accounts for smaller lakes and reservoirs − Is not able to provide output on algal blooms − in-lake processes are based on simplified equations
PCLake [39,44,66]	World	Lakes and reservoirs	>125	>0.01	N, P, SS, phytoplankton, zooplankton, fish	Process-based model	Measured	+ Process-based model that is broadly applicable + The model accounts for detailed in-lake processes − Model is not linked to other models that are able to estimate the drivers of change (climate change and nutrient load) − Model requires more input data than statistical models
Hierarchical “hurdle” model [34]	USA	Lakes and reservoirs	1127	>0.001	Microcystin concentrations	Statistical model	Not used	+ Simple model to calculate microcystin concentrations + Splits data in two parts, thereby solving the threshold issue to a certain degree + Requires little input data − Calculations not based on drivers of change (climate change and nutrient load) − Cannot be used outside the calibration domain
GLOBIO-aquatic in combination with Håkanson [30,67]	World	Lakes and reservoirs	3607	>50	Chl-a, MSA	Statistical model	Modelled with IMAGE-GNM [65]	+ The drivers of change (climate change and nutrient load) are simulated + Relatively simple model to calculate chlorophyll-a − Is only used for larger lakes and reservoirs − Cannot be used outside the calibration domain
VEMALA v.3 [40,42]	Finland	Lakes	58000	>0.01	N, P, SS, TOC and phytoplankton	Process-based model	Modelled using a build-in process-based model [42]	+ Simulates a high number of lakes + The model accounts for in-lake processes − Needs much input data − Is limited to the Finnish watersheds

[a] Explanations of abbreviations: Chl-a: chlorophyll-a, N: Nitrogen, P: Phosphorus, Si: Silicates, SS: suspended solids, TOC: Total Organic Carbon, MSA: Mean Species Abundance.
[b] A number of variants or extensions of the Vollenweider statistical model exists, which are not included in this table.

Retention in Reservoirs and Lakes) and SiRReLa (Silicate Retention in Reservoirs and Lakes) have the advantage that they include a theoretical understanding of relevant ecological processes. On the other hand, process-based models are more complex than statistical approaches and need calibration using empirical data. NiRReLa and SiRReLa are simple process-based models used for nutrient retention simulations of a large number of lakes worldwide [36–38]. However, neither models have been used to estimate algal blooms, in contrast to VEMALA v3, PCLake and Delft3D-WAQ/ECO [39–41]. VEMALA v3 is used to model phytoplankton concentrations under simulated nutrient loading, however, it is currently only applied to Finnish watersheds [42]. Delft3D-WAQ/ECO has been applied to many places around the world, typically using spatial simulations that are highly detailed, which applications are suitable for simulations of individual lakes but are less suitable for large runs that include many lakes on earth [41]. PCLake has been applied to many cases around the world as well [43–45] but is limited to shallow lakes. A stratifying version of PCLake has recently been developed [46] but this model has not yet been applied to existing lakes.

Both the statistical and process-based modelling approaches listed in Table 1 still exclude the majority of lakes on Earth. There are over 117 million lakes larger than 0.0002 km^2 on earth [47••]. NiRReLa and SiRReLa simulate 0.2% of these lakes, which is the most compared to the other models listed in Table 1. This gap in model application to lakes could lead to underestimation as well as overestimation by models because the missing lakes could be responsible for a large share of processes, including nutrient retention and algal bloom formation. For example, underestimation would occur for total worldwide nutrient retention when small lakes are discarded since nitrogen removal in all small lakes ($<50\ km^2$) together is double of that in all large lakes [37]. In contrast, exclusion of small lakes would lead to overestimation of global turbidity, since small lakes appear to have a higher chance to be in a vegetated clear water state [12].

Requirements of ideal algal projection models for global scale scenarios

In order to project algal blooms worldwide over coming decades, one must, at a minimum, represent the major drivers of algal blooms: nutrient loading and climate change (*environmental component*) [10]. Moreover, a lake's position within the hydrological network (*network component*) and lake-specific characteristics (*lake ecosystem component*) should be considered since they affect the sensitivity of individual lakes to nutrient loading and climate change (see introduction) [12]. Therefore, we consider an ideal algal projection model as a model that at least consist of three components: firstly environmental, secondly network and thirdly lake ecosystem component (Figure 1 and Table 2). As noted in the previous section, statistical models perform poor beyond their calibration domain which is less of an issue for process-based models. Therefore, we recommend using process-based models to project algal blooms under changing climate and nutrient loading.

Environmental component

The environmental component quantifies the various natural and anthropogenic nutrient sources to the network component (Figure 1 and Table 2). First, natural nutrient sources stem from biogeochemical processes including conversion (e.g. denitrification), mineralization (e.g. organic matter decomposition), fixation (e.g. N_2-fixation) and release (e.g. weathering) [48]. Second, anthropogenic nutrient sources stem from human activities such as industrial production of goods, fertilizer use and energy generation by fossil fuel combustion [48,49]. These anthropogenic activities are affected by developments in socio-economic factors such as population density, economy, policies, technology, lifestyle and resources [49]. The effect of future climate and socio-economic developments on natural and anthropogenic nutrient sources should be simulated using scenarios such as the Representative Concentration Pathways (RCPs) for climate objectives [50], and the Shared Socioeconomic Pathways (SSPs) for socio-economic development [51].

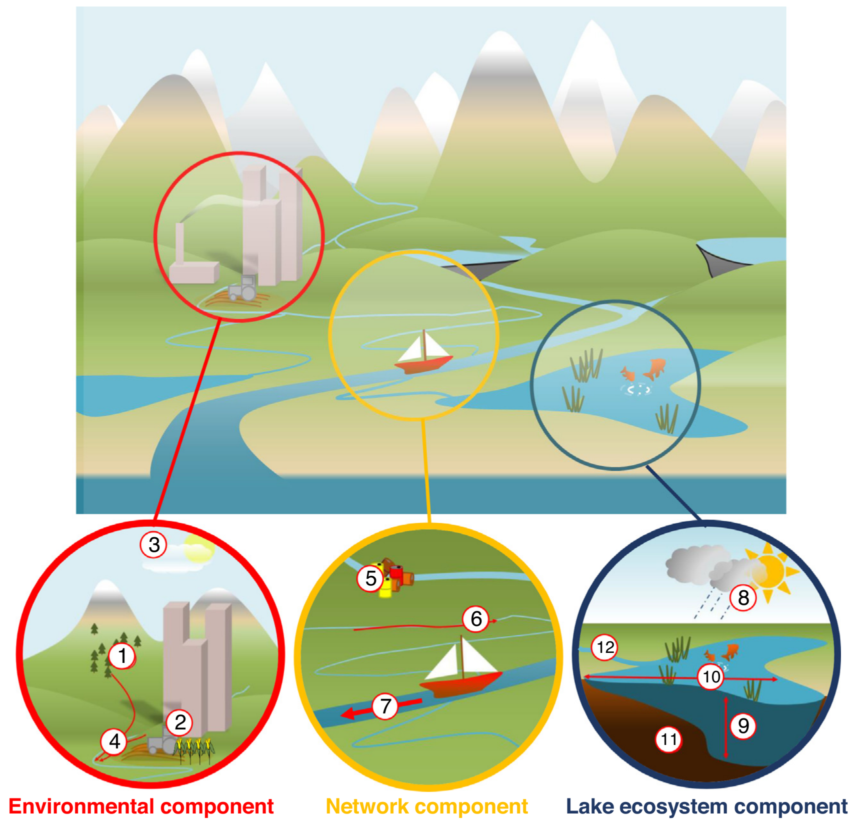
Network component

The network component quantifies transport of both water and nutrients into lakes. Therefore, this component connects lakes and reservoirs with the environmental component through a hydrological network consisting of small and large rivers and streams, groundwater and the atmosphere (Figure 1 and Table 2). First, the transport of water into lakes follows from water balances based on global climate data. The amount of water to lakes should be estimated because it, together with lake volume, determines hydraulic residence times of lakes. A long residence time in lakes allows biogeochemical processes to dominate lake ecosystem dynamics, while short residence times result in efficient flushing of solutes and suspended materials including algae [44,52]. Second, nutrient loads to lakes should be simulated based on quantified nutrient release from the environmental component. The calculation of nutrient loads to lakes is important as they support lake primary producers, including algae, which in-turn support all other lake organisms. Phosphorus and nitrogen are generally seen as the most important nutrients for algal growth [53], though silicates are important for diatom growth [36]. Additionally, carbon regulates the pH and is a substrate for microbial life [54]. Therefore, we consider phosphorus and nitrogen essential, and silicates and carbon supplementary to include in the ideal algal projection model.

Lake ecosystem component

The lake ecosystem component simulates the response of algal blooms to climate change and nutrient load (Figure 1

Figure 1



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Three essential components of the ideal algal projection model: **(a)** an *environmental component* accounting for major anthropogenic and natural pressures, **(b)** a *network component* connecting the lakes within the network, and **(c)** a generic *lake ecosystem component* with lake-specific characteristics. Essential elements of the *environmental component* are 1) nutrient emissions from the natural sources, 2) nutrient sources from human activities, 3) climate conditions and 4) nutrient release to the network component. Elements of the *network component* are 5) nutrient type (e.g. nitrogen, phosphorus, silica or carbon), 6) hydrological network and 7) amount of water and nutrients transported by the network. Elements of the *lake ecosystem component* are: 8) local climate conditions, 9) water depth 10) surface area, 11) sediment type and 12) inputs of water and nutrients to lakes and reservoirs.

and Table 2). For this, the major processes in aquatic ecosystems determining algal blooms in lakes, such as algal growth, grazing, competition and stratification, should be included. Because of slow nutrient uptake and release processes by sediments, and the possibility of alternative stable states, a response of algae to a change in nutrient load can take many years to occur, or might even be hampered from occurring at all [55]. Accounting for this legacy-effect of lakes would be ideal to prevent deviations of model results from field data. Using these major processes in aquatic ecosystems, including the legacy-effect, the lake ecosystem component translates lake-specific characteristics to lake-specific algal bloom responses [24]. Lake-specific characteristics are for example local climate conditions, lake depth, lake surface area, sediment type and input of water and nutrients. Water and nutrient inputs are quantified by the network component, whereas the other lake characteristics can be obtained from high-frequency monitoring [26•], global maps, global databases, satellite images [28••,29], or, if necessary, estimated using geomorphometric scaling relationships as done by Messager *et al.* [28••].

Coupling of the three components

The ideal algal projection model connects the environmental component via the network component to the lake ecosystem component. Furthermore, lakes influence each other through the hydrological network by, for example, nutrient retention in lakes upstream that lowers nutrient concentrations in lakes downstream [37]. Therefore, also such influences of the lake ecosystem component on the network component should be included (Table 2).

Challenges and opportunities in algal bloom projection model development

To the best of our knowledge, there are currently no algal projection models that meet the requirements for such model as described in the previous section (Figure 1 and

Table 2

Requirements of the ideal algal projection model that includes three components: environmental component, network component and lake ecosystem component. Text in bold show required links to other components, text in *italic* show potential links to other components

Component	Requirements	Input	Output
Environmental component	-Simulation of natural nutrient sources -Simulation of anthropogenic nutrient sources -Uses scenarios to simulate the effect of future climate and socio-economic developments	-Climate scenarios -Socio-economic scenarios	Quantification of the various nutrient sources to the **network component**
Network component	-Includes a hydrological network including rivers and streams, groundwater and the atmosphere -Quantification of water inflow to lakes is based on global climate data -Quantification of nutrient input to lakes is based on quantified nutrient release from the **environmental component**	-Global climate data -Hydrological network **-Nutrient release from the environment to the network** *(– nutrient retention by lakes in the lake ecosystem component)*	Quantifies transport of both water and nutrients into **lake ecosystem component**
Lake ecosystem component	-Quantifies algal blooms based on water and nutrient load from the **network component** and lake-specific characteristics (e.g. depth, area, sediment type and local climate) -Includes major processes in aquatic ecosystems determining algal blooms (e.g. growth, grazing, competition, stratification) -Includes the legacy-effect	-Lake-specific water input and nutrient load from the network component -Lake-specific characteristics	Simulates the response of algal blooms to climate change and nutrient load

Table 2). Many lake ecosystem models listed in Table 1 have not been linked to any kind of network component. Additionally, most models in Table 1 are either much simpler than the ideal algal projection model described in Table 2 or are far more limited in their application domain. Below we describe four major challenges and opportunities that will be faced when developing algal projection models.

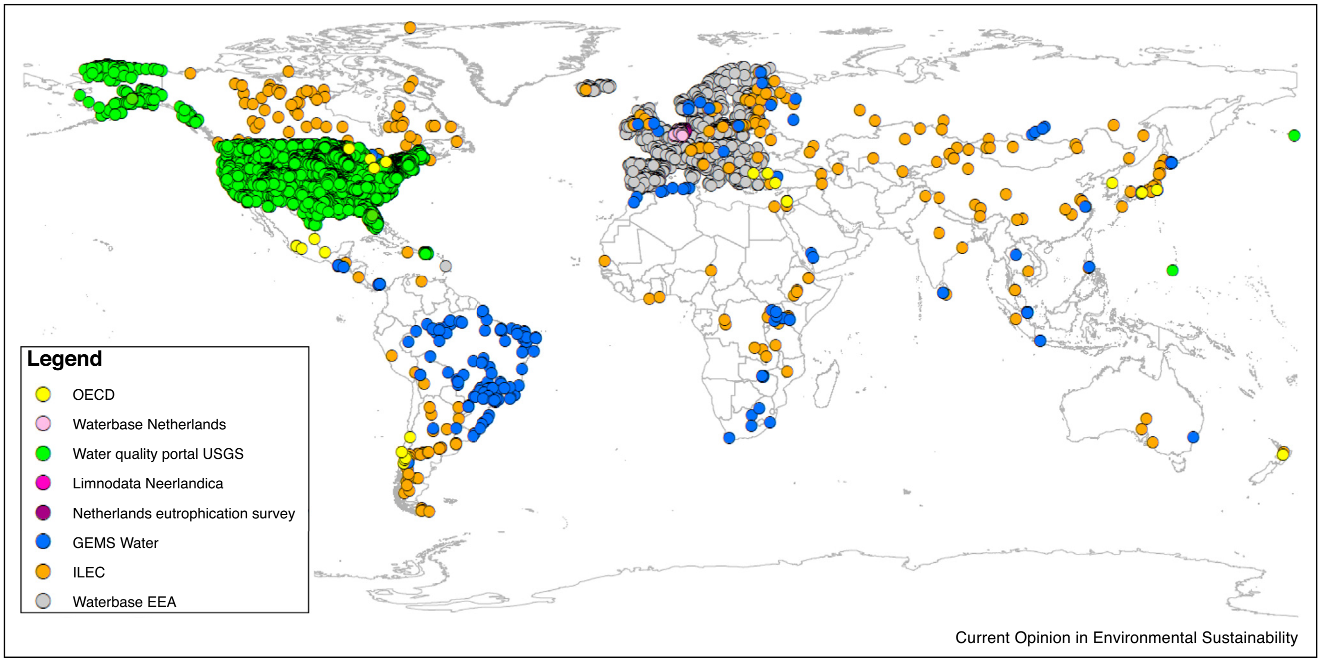
(1) The ideal model should be complex enough to be credible, yet simple enough to be applied at the global scale. The whole suite of statistical models seems unsuitable to perform this task since they are too simple and have the risk to perform poorly beyond the calibration domain. Process-based models are not limited to their calibration domain and therefore more promising. In addition, process-based models are more complex then statistical models and include a theoretical understanding of relevant ecological processes. However, since processed-based models are simplifications of nature, it will still be a challenge to include all major processes in aquatic ecosystems determining algal blooms including the lakes' legacy-effect.

(2) Uncertainties propagate through the modelling framework, from the environmental component through the network component to the lake ecosystem component. The quality of algal bloom projections, therefore, depends on the output of other components. There are several technical opportunities available to deal with this issue, including ensemble modelling, sensitivity analysis, and validation of both the input and output data [56•]. First, ensemble modelling is a common technique to communicate uncertainty in weather forecasts and requires simulations from multiple models [14•,56•]. Second, sensitivity analysis helps to understand the impact of uncertainty originating from the network component to the output of the lake ecosystem component [39,57]. Third, validation based on historical data builds confidence in the output (for example Kong *et al.* [45]).

(3) There is a mismatch in spatial scales. Most nutrient flow models are grid-based and have a spatial resolution not finer than 0.5 degrees ($\sim$50 km) [16], whereas the vast majority of lakes are smaller than 50 km [28••]. The NiRReLa model found a workaround for this issue [37]. By assuming that the spatial distribution of the smallest lakes scales with the distribution of the larger lakes, the NiRReLa model includes lakes down to 0.1 km^2 in size. Other options are using 'representative lakes' as an average of all lakes in a grid cell (ISIMIP2b, https://www.isimip.org/protocol/) or using a delineation approach to account for different spatial scales [58]. Ideally, however, the network component would be described in detail, such as has been done for VEMALA v3 [42]. Recent hydrological simulations at a resolution of 1 km^2 at a global scale are promising in this respect [59••].

(4) Validation data on key ecological variables for freshwater lakes (e.g. chlorophyll-a, nitrogen and phosphorus) on a global scale are still mostly originating from Europe and America (Figure 2). Data from other parts of the world are partly locked within institutions or simply not there [56•]. Multi-lake observations by remote sensing could fill this spatial data gap since this technique is less restricted by the location on earth [29]. Fortunately, data on general lake characteristics, such as lake surface area and lake depth,

Figure 2



Global distribution of lakes for which water quality data on key ecological variables for freshwater lakes (e.g. chlorophyll-a, nitrogen and phosphorus) is available per dataset.

recently reached global coverage; using geomorphometric scaling relationships, a new, freely available global dataset was obtained containing 1.43 million individual lakes larger than 0.1 km^2 [28••].

Although there are currently no models available to simulate global scale scenarios for algal blooms in freshwater lakes and reservoirs, the building blocks are there. First, multiple models exist that connect an environmental and a network component (see for a list Kroeze *et al.* [16]). Additionally, ample models are available to simulate the lake ecosystem component (see for a list Table 1). Moreover, models combining the three components (environmental, network and lake ecosystem component) have been developed and used at the national scale (e.g. VEMALA v3 [40,42]). First steps to upscale such models towards a global scale have already been taken by the models NiRReLa and SiRReLa for nutrient cycling [36,37] and a next step is to include simulations of algae. Since the development of the building blocks for this last step are progressing [46], we think that an algal projection model can be developed in the near future. This development will be supported further by an increased data accessibility [56•,60•], increased computational power, and advanced modelling techniques [24,56•,61]. Considering these developments, we envision that calculations from first-cut attempts will already provide insights to anticipate future algal blooms and, not to mention, to spur improvements on this first-cut attempt.

Conclusion

To reach the UN Sustainable Development Goals (here particularly focussing on SDG 6), there is an urgent need for global models capable of simulating algal blooms under scenarios for future climate change and nutrient loading. However, no such model currently exists. Here we have provided a roadmap for developing algal bloom projection models, arguing that it should include the following coupled components: environmental component, network component and lake ecosystem component. In the near future, we foresee that the development of such models is feasible because most challenges have been solved and the building blocks are there. We envision that algal projection models will increasingly gain interest and provide a valuable contribution to global policymaking, in particular, with respect to SDG 6 (clean water and sanitation).

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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.2018.09.001.

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- • of special interest
- •• of outstanding interest

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