

Individual-based modelling of cyanobacteria blooms: Physical and physiological processes
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Abstract

Lakes and reservoirs throughout the world are increasingly adversely affected by cyanobacterial harmful algal blooms (CyanoHABs). The development and spatiotemporal distributions of blooms are governed by complex physical mixing and transport processes that interact with physiological processes affecting the growth and loss of bloom-forming species. Individual-based models (IBMs) can provide a valuable tool for exploring and integrating some of these processes. Here we contend that the advantages of IBMs have not been fully exploited. The main reasons for the lack of progress in mainstreaming IBMs in numerical modelling are their complexity and high computational demand. In this review, we identify gaps and challenges in the use of IBMs for modelling CyanoHABs and provide an overview of the processes that should be considered for simulating the spatial and temporal distributions of cyanobacteria. Notably, important processes affecting cyanobacteria distributions, in particular their vertical passive movement, have not been considered in many existing lake ecosystem models. We identify the following research gaps that should be addressed in future studies that use IBMs: 1) effects of vertical movement and physiological processes relevant to cyanobacteria growth and accumulations, 2) effects and feedbacks of CyanoHABs on their environment; 3) inter and intra-specific competition of cyanobacteria species for nutrients and light; 4) use of high resolved temporal-spatial data for calibration and verification targets for IBMs; and 5) climate change impacts on the frequency, intensity and duration of CyanoHABs. IBMs are well adapted to incorporate these processes and should be considered as the next generation of models for simulating CyanoHABs.

Keywords: Agent-based modelling; Cyanobacteria; Climate change; Individual-based modelling; Physical processes; Physiological processes

1. Introduction

Cyanobacteria, sometimes also known as blue-green algae, are the Earth's oldest phytoplankton. Their survival through periods of changing environments reflects their array of ecophysiological adaptations and strategies (Paerl and Paul, 2012). Cyanobacteria strongly influence water quality, with toxin-producing species affecting human health, and cyanobacterial harmful algal blooms (CyanoHABs) also impacting ecosystem services and the economy (Codd et al., 1999; Paerl et al., 2001; Hamilton et al., 2014). CyanoHABs are likely to increase in the future due to factors associated with climate change such as global warming, altered precipitation patterns (Reichwaldt and Ghadouani, 2012; Burford et al., 2020; Paerl and Barnard, 2020) and land use change (Hamilton et al., 2016).

Mechanistic models or process-oriented aquatic models (Vincon-Leite and Casenave, 2019), based on knowledge of how target species respond to various ecosystem drivers, can be used to predict changes in biological communities with simulation output used to inform and guide management actions (Franks, 2018). The main advantage of mechanistic models is that they can capture the interactions between the different mechanisms that shape ecosystem state (Hipsey et al., 2020) and may therefore be more appropriate than statistically based models for future predictions (Ralston and Moore, 2020). The ecosystem drivers that can be considered in mechanistic models include physiological adaptations of biota, nutrient availability, inter and intraspecific competition, vertical and horizontal transport, mixing and flushing rates, thermal stratification, and life cycle characteristics of species (Rousso et al., 2020). Mechanistic modelling can be challenging because of incomplete knowledge of the complex interactions of individual organisms with each other and with their environment. In addition, multiple complex processes contributing to the development and distribution of

CyanoHABs need to be incorporated into mechanistic models to simulate blooms. These processes are usually derived from laboratory studies of isolated strains. As a result, the processes can remain poorly defined in model formulations (Ralston and Moore, 2020), leading to uncertainties and errors in model outputs. Furthermore, many processes have several parameters that need to be calibrated, leading to potential for equifinality and uncertainty in model output under a different set of forcing conditions (Rousso et al., 2020). Results of mechanistic ecosystem models are often strongly dependent on parameter calibration, which may be obtained from the literature, experimental studies or field observations. Advances in sensor technology have opened up new opportunities for better modelling procedures through improving the spatial and/or temporal resolution of model initialization and boundary condition specifications, as well as for rigorous calibration and validation of model output against intensive measurements. In situ sensors, often using chlorophyll fluorescence or phycocyanin as a proxy for phytoplankton and cyanobacteria biomass, respectively, can provide the required data for calibrating mechanistic phytoplankton models at high temporal resolution (McBride and Rose, 2018). These sensors only provide a proxy for biomass; however, they do not resolve phytoplankton at a species or strain-level (Bertone et al., 2018). Remotely sensed aerial or satellite images provide an opportunity for detailed model calibration based on snapshots of optical properties of surface waters over large spatial scales (e.g., Allan and McBride, 2018) but they do not resolve at species level and cannot capture vertical distributions of populations (Odermatt et al., 2012a), which can lead to high variability of chlorophyll in remotely sensed images (Kutser, 2004). While great advances have been made in sensor technology, they are still not able to provide the detailed species- and individual-based resolution that would be useful to help advance species or succession-based phytoplankton models (Harris, 1997).

Variability of individual organisms within populations or communities in the aquatic

environment is governed by complex nonlinear interactions between physiological and physical processes. Two modelling methods are commonly used to simulate the dynamics of a population of organisms: Eulerian and Lagrangian. Eulerian models simulate time-dependent variables at specific fixed locations, whereas Lagrangian models follow moving particles through space and time (Curchitser et al., 2013).

Eulerian models have been used since the 1970s to simulate eutrophication, water quality, and biogeochemical processes (e.g., Chapra, 2008; Hellweger et al., 2016b; Vincon-Leite and Casenave, 2019). They are composed of ordinary differential and partial differential equations which simulate community dynamics in spatially homogeneous and spatially structured spaces, respectively (Hellweger et al., 2016a). Eulerian models have three main advantages. First, they are relatively simple in form and, in turn, have lower knowledge and data requirements (Hellweger et al., 2016a). Second, these models provide a convenient description of the mass and momentum governing equations that are fundamental for describing mixing and transport in aquatic systems (Soontiens et al., 2019). Third, they can be easily coupled to hydrodynamic models; indeed most of these models are underpinned by Eulerian formulations (Soontiens et al., 2019). In Eulerian methods, however, species are usually allocated into a small number of state variables or may even be lumped into a single state variable (e.g., Oliver et al., 2012; Hellweger et al., 2016a; Kreft et al., 2017). Therefore, Eulerian ecological models are often termed lumped-system models (Feng et al., 2018) or population-level models (PLMs) (Hellweger and Kianirad, 2007). Aquatic ecosystems are characterised by high levels of heterogeneity and physiological differences that exist at an intraspecific isolate level (e.g., Cai et al., 2012; Guedes et al., 2019). Furthermore, strains of species isolated from a single waterbody can have quite different growth parameters (Xiao et al., 2020b). For example, there is considerable intraspecific variation in the growth responses to light and temperature of freshwater CyanoHAB species, particularly *Microcystis*

aeruginosa and *Rhaphidiopsis raciborskii* (Xiao et al., 2020b). Willis et al. (2016) found substantial differences in physiological variables in 24 *C. raciborskii* strains from a single sample of lake water. Traditional PLMs have difficulty in capturing this strain-level diversity. This shortcoming may need to be addressed as metagenomics research reveals the increasing numbers of CyanoHAB species and strains (Hellweger et al., 2016b).

Lagrangian models, by contrast, allow for different classes of particles to have individualised properties (Zhu et al., 2018; Soontiens et al., 2019) that can vary from physical to physiological components. However, conducting Lagrangian simulations in which a large number (order of billions) of particles are simulated is challenging (Van Sebille et al., 2018). This is because the computational time of Lagrangian models is proportional to the number of particles in the simulation. Lagrangian models can be divided into two main groups: individual-based models (IBMs) – sometimes referred to as agent-based models – and particle tracking models (PTMs). According to the definition of Grimm (1999), IBMs refer to “simulation models that treat individuals as unique and discrete entities, which have at least one property in addition to an age that changes during the life cycle.” PTMs are identical to IBMs but without the additional attributes included.

IBMs are gaining popularity in ecological modelling because they can address questions that are beyond the scope of traditional models like PLMs (Xue et al., 2018). They often seek to capture interspecific adaptive behaviour (Grimm et al., 2006; DeAngelis and Grimm, 2014) but can equally be used to capture the aspects of intra-specific variability discussed above (Hellweger and Bucci, 2009). They can also simulate the interactions of individuals with each other and with their biotic or abiotic environment (DeAngelis and Grimm, 2014), as well as the life cycles of individuals (Grimm et al., 2006; Hellweger et al., 2008; Hense and Beckmann, 2010).

One important difference between IBMs and both PLMs and PTMs is that particles in IBMs

carry a memory (e.g., of light history, nutrient status, etc.). In conventional PLMs/PTMs, a population state variable or Lagrangian element responds directly to exogenous variables only within the current time step. By contrast, particles with a ‘memory’ allows for adaptive biological traits can be included (Feng et al., 2018). It also means that photosynthetic responses and vertical migration of cyanobacteria resulting from light exposure history, can be considered. The ability to transfer information on physiological properties of cells through successive time steps is one of the reasons why IBMs are likely to be an increasingly valuable tool to study the development and spatiotemporal distribution of CyanoHABs.

The main disadvantages of IBMs are their complexity and high computational demand, especially in modelling large systems where there are a large number of species. To overcome these limitations, super individual-based modelling is suggested (Scheffer et al., 1995; Hellweger and Bucci, 2009; Hellweger et al., 2016a). In this method, similar individuals are lumped into a single representative individual which has a common set of physiological and anatomical characteristics. This lumping procedure can reduce the computational simulation time. However, it also decreases the heterogeneity in populations, which is at the heart of the justification for IBMs. Alternately, representative spaces may be used in larger systems. In this method, a smaller statistically representative volume or area of a large-scale system is simulated, and the heterogeneity in the representative space is considered to be similar to that of the larger system (Hellweger et al., 2016a).

IBMs are usually forced by water elevation, currents, turbulent diffusivity, and temperature field from Eulerian hydrodynamic models driven by external boundary conditions (e.g., atmospheric and inflow conditions) and nutrient concentrations from ecological models (Fig. 1). In IBMs, each organism has a set of attributes and behaviours and is simulated as an individual entity (DeAngelis and Grimm, 2014). As discussed earlier, a memory of past events also dictates how these individuals respond in IBMs (Fig. 1). These models are one of

the few that can capture the complex nonlinear interactions between physiological and physical processes that govern transport and variability of autonomous individual organisms (Feng et al., 2018). Therefore, IBMs are theoretically the most realistic and effective way of modelling the life cycle of individual organisms (Hense, 2010).

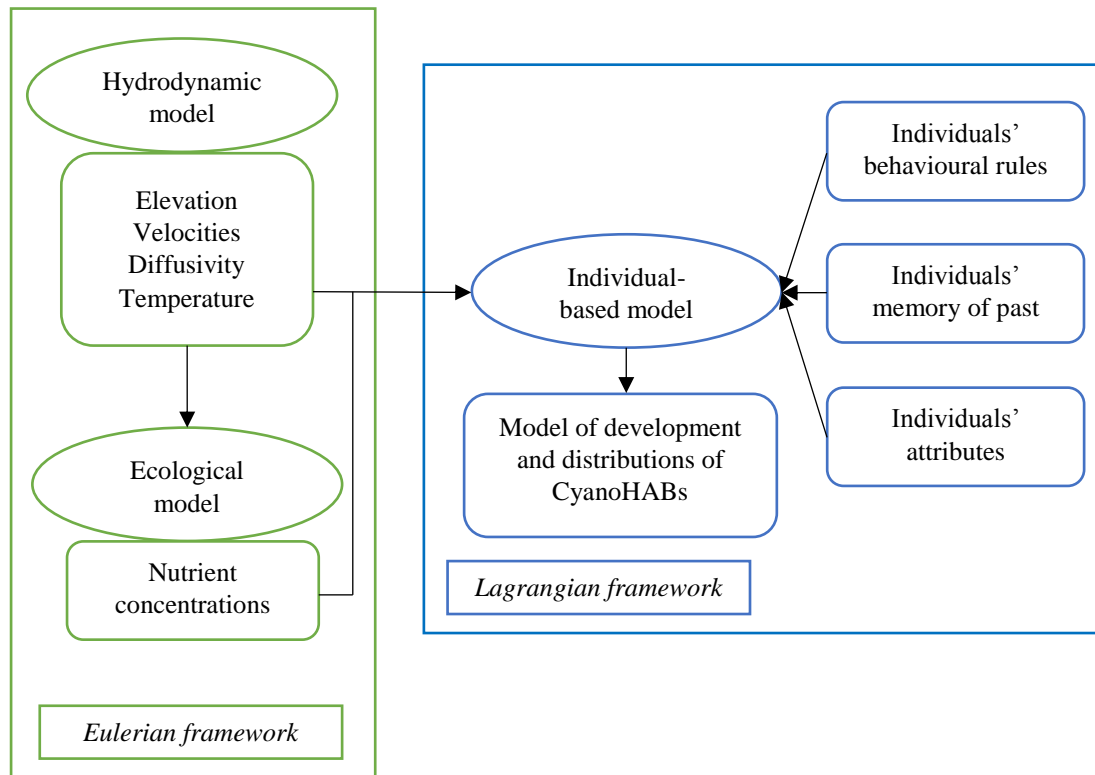


Fig. 1. Conceptual approach for modelling of CyanoHABs using IBMs.

Compared with IBMs, PTMs have a lower level of complexity at the cost of ignoring physiological processes contributing to CyanoHABs. In PTMs, particles are usually advected through the modelling domain according to current fields (e.g., Pinto et al., 2016; Silva et al., 2016). PTMs can be used to simulate short-term CyanoHAB transport (e.g., Wynne et al., 2011; Wynne et al., 2013; Soontiens et al., 2019). The premise of CyanoHAB PTMs is that growth and loss processes are generally insignificant compared with the effects of dispersion and transport of cyanobacteria at the short time scales (~days) used for model simulations (Feng et al., 2018; Soontiens et al., 2019). In these cases, cyanobacteria can be considered to

act like passive particles that are transported by physical processes, and their growth and loss can be neglected (Dippner et al., 2011; Wynne et al., 2011; Wynne et al., 2013; Rowe et al., 2016). This assumption of conservative behaviour over short time scales is reasonable for slow-growing cyanobacteria species whose in situ growth rates are generally less than 0.1 day⁻¹ (Fahnenstiel et al., 2008; Wynne et al., 2010).

Only two studies have compared the performance of different modelling methods for the transport of bloom-forming *Microcystis* species. Soontiens et al. (2019) showed that an Eulerian tracer method simulated the algal bloom transport better than a Lagrangian one. In their study, phytoplankton was represented as a passive Eulerian tracer with an assigned buoyant velocity. Different horizontal mixing schemes employed in each of the *in silico* tracing experiments undertaken by Soontiens et al. (2019) might have affected the ability to make direct comparisons between each modelling technique. Additionally, the comparison of Eulerian and Lagrangian schemes is likely to be affected by the vertical mixing assigned to the Eulerian tracers. Wang et al. (2017) simulated the transport behaviour of colony-forming *Microcystis* with both IBM and Eulerian models. Based on a comparison of model results with measurements of chlorophyll a, as a proxy for the abundance of *Microcystis*, they showed that results of the IBM were more accurate than those of the Eulerian model. Vertical migration simulated by the IBM was mostly upward, while vertical migration simulated by the Eulerian model was mostly downward. This resulted in different horizontal distributions of *Microcystis* between the models.

With the growing attention on IBMs in ecological modelling, there has been a number of reviews in the last few years (e.g., Grimm, 1999; Grimm et al., 2006; Hellweger and Kianirad, 2007; Hellweger and Bucci, 2009; Grimm et al., 2010; DeAngelis and Grimm, 2014; Hellweger et al., 2016a). However, none of these studies have focused exclusively on CyanoHAB IBMs and processes that should be incorporated into these models. Better

understanding of how CyanoHABs develop and are transported is critical to formulating mitigation strategies for CyanoHABs. Therefore, this paper reviews both physical and physiological processes driving CyanoHABs and discusses CyanoHAB IBMs related to these processes. In addition to providing a state-of-the-art understanding of the key physical drivers and physiological processes controlling CyanoHAB transport and development and discussing the potential for IBMs to be the next generation of CyanoHAB models, objectives of the review are to: discuss the objectives of previous studies that have used IBMs or PTMs to simulate CyanoHABs; describe different approaches to couple IBMs to Eulerian models, including their advantages and disadvantages; outline dimensionality, domain discretization and grid resolution required for Lagrangian CyanoHAB modelling; and describe innovations in measurements that can enhance data input and model comparisons.

2. Current trends in IBMs and PTMs of CyanoHABs

An overview of the objectives of previous studies that have used IBMs or PTMs to simulate CyanoHABs is given in Table 1. In addition, to outline the methodology used to achieve the objective of each study, the model, simulation duration, coupling approach, and dimension of the movement of Lagrangian particles in the model domain in the previous studies are summarized in Table 1. For most IBM studies, the objective has been to hindcast CyanoHAB events to better understand the environmental drivers of blooms and the physical (e.g., wind-driven turbulent mixing) and physiological (e.g., buoyancy regulation) processes affecting their transport. For example, Feng et al. (2018) examined the effects of both physiological and physical processes on the development and transport of CyanoHABs using an IBM. They concluded that surface accumulation and extension of early summer blooms (April–June) were mainly affected by physical forcing, namely horizontal transport and vertical mixing; while for blooms later in the summer season (July–October), physiological processes (i.e., buoyancy control) had an increased importance. PTMs have been used in some studies to

forecast CyanoHAB transport (Table 1) (e.g., Wynne et al., 2011; Wynne et al., 2013; Soontiens et al., 2019). The main focus of these studies was on the physical drivers influencing the passive movement of particles, ignoring physiological processes controlling CyanoHABs. As will be discussed below, a large number of physical and physiological processes may influence the development and spatiotemporal distributions of CyanoHABs. It is difficult to include all of these different processes into cyanobacteria models. Therefore, the previous studies have made some transport-related assumptions that are summarized in Table 1 and discussed in section 4.1.

Table 1. Summary of studies that have used IBMs or PTMs to simulate CyanoHABs.

Objective	Reference	Study site	Model	Simulation duration	Coupling approach	Dimension of individuals' movement	Data used for assessing model performance	Horizontal transport assumptions	Vertical transport assumptions
Short-term forecasts of CyanoHAB transport	Soontiens et al. (2019)	Lake Erie, USA-CAN	PTM (NEMO)	Short-term	Online	2D	Sentinel-3 derived spatial distribution of chlorophyll <i>a</i> concentration	Neglecting effects of wind drift Neglecting effects of Stokes drift	No vertical movement
Investigation of the factors affecting surface blooms	Feng et al. (2018)	Lake Taihu, CHN	IBM (FVCOM + SWAN + GEM)	Long-term	Online	3D	Water temperature DIN and DIP concentration Cyanobacterial biomass MODIS derived	No specific stated assumptions	Neglecting effects of Langmuir circulation Disaggregation of colonies not

							extent of blooms		considered
Understanding the transport behaviour of colony-forming <i>Microcystis</i>	Wang et al. (2017)	Lake Taihu, CHN	IBM (ND)	Short-term	Online	3D	Water levels Surface current speed Vertical and horizontal distributions of <i>Microcystis</i> MODIS derived extent of blooms	Neglecting effects of Stokes drift	Neglecting effects of Langmuir circulation Neglecting effects of changes in cell diameter Neglecting effects of temperature and nutrients on density changes Aggregation between colonies not considered Disaggregation of colonies not considered
Short-term forecast of CyanoHAB abundance	Rowe et al. (2016)	Lake Erie, USA-CAN	PTM (FVCOM)	Short-term	Offline	3D	Vertical profiles of temperature and cyanobacterial	Neglecting effects of wind drift Neglect	Neglecting effects of Langmuir circulation

ce and distribut ion							chloroph yll concentr ation MERIS derived spatial distributi on of cyanoba cterial chloroph yll concentr ation	ting effects of Stokes drift	on Neglecti ng effects of changes in cell diameter Neglecti ng effects of changes in cell density Aggrega tion between colonies not consider ed Disaggre gation of colonies not consider ed
Short- term forecasts of CyanoH AB transport	Wynn e et al. (2013)	Lake Erie, USA- CAN	PTM (GLC FS + GNO ME)	Short- term	Offli ne	2D	MERIS derived spatial distributi on of cyanoba cterial index	Neglec ting effects of wind drift Neglec ting effects of Stokes drift	No vertical moveme nt
Short- term forecasts of CyanoH AB transport	Wynn e et al. (2011)	Lake Erie, USA- CAN	PTM (GLC FS + GNO ME)	Short- term	Offli ne	2D	MERIS derived spatial distributi on of cyanoba cterial index	Neglec ting effects of wind drift Neglec ting effects of	No vertical moveme nt

								Stokes drift	
IBM development for the formation and behaviour of resting stage cells	Hellweger et al. (2008)	Bugach Reservoir, RUS	IBM (iAlgae)	Long-term	Online	1D	Water temperature Secchi disk transparency DIP and chlorophyll <i>a</i> concentration <i>Anabaena</i> cell counts	No horizontal movement	Constant vertical migration velocity
Examining relationship between buoyancy regulation and diurnal stratification	Wallace et al. (2000)	Thomson Lake, AUS	IBM (Buoyancy regulation model + DYRESM)	Short-term	Online	1D	Vertical profiles of temperature chlorophyll <i>a</i> concentration	No horizontal movement	Neglecting effects of Langmuir circulation Neglecting effects of changes in cell diameter Aggregation between colonies not considered Disaggregation of colonies not considered

2.1. Coupling Lagrangian models to Eulerian hydrodynamic-ecological models

Two approaches have been used in IBMs to couple hydrodynamics and biogeochemical variables: online and offline (Table 1). Online, or direct coupling mode, refers to a fully coupled hydrodynamic-ecological IBM which runs concurrently with, though not necessarily at an identical time step to, the hydrodynamic-ecological model. This method has a high computational burden because a large array of variables undergoes the advection-dispersion computations. An alternative method is to launch IBMs in an offline mode, with the hydrodynamic-ecological model outputs first saved and then used to force the IBM (Kim and Khangaonkar, 2012). The offline mode helps to reduce the computational burden (Gillibrand et al., 2016), but it does not capture the two-way interaction between species and their environment. Surface blooms of cyanobacteria, for instance, absorb heat and, therefore, increase light attenuation and surface water temperatures. These effects strengthen thermal stratification and provide a more favourable environment for cyanobacterial blooms (Kumagai et al., 2000; Ibelings et al., 2003; Jones et al., 2005; Rinke et al., 2010) particularly when nutrients are replete or are at elevated concentrations (Paerl and Huisman, 2008; Xu et al., 2015). In addition to strengthening thermal stratification, surface cyanobacterial blooms or scums can influence their physical environment by increasing the viscosity and reducing the momentum transfer from wind to water at low wind speeds (Wu et al., 2019). These changes again provide conditions that are favourable for the development of CyanoHABs. Another example where online models capture dynamic feedbacks of physical and biological processes is in the field of sediment transport. Chen et al. (2007b) examined how seagrasses reduce sediment transport through reductions in shear stress and increases in drag forces and wave attenuation. The feedbacks of cyanobacteria or seagrasses on the physical structure of the water column can only be captured by interactive online modelling in which each model is run simultaneously in a fully coupled mode.

2.2. Dimensionality, domain discretization and grid resolution

Phytoplankton may be transported and mixed in all dimensions and many species, including cyanobacteria, have adaptations that allow them to move or migrate through the water column. Some studies that have used PTMs to simulate CyanoHABs (Table 1) invoked two-dimensional (2-D) transport models, focused on the horizontal plane (Wynne et al., 2011; Wynne et al., 2013; Soontiens et al., 2019). In this approach, the water column is assumed to be fully mixed and vertical heterogeneity or movements of species is ignored (Soontiens et al., 2019). Rowe et al. (2016) compared the results of a three-dimensional (3-D) PTM with those of a 2-D PTM for simulations of CyanoHABs in Lake Erie, USA. As a result of capturing the vertical distribution of the cyanobacteria, the 3-D model simulated the CyanoHAB distribution with higher accuracy, particularly under conditions of increased wind stress when the 2-D model did not adequately disperse the bloom.

One-dimensional (1-D) models that capture only the vertical water column have also been used to simulate CyanoHABs. Wallace et al. (2000) examined the vertical distribution of *Microcystis aeruginosa* in a shallow eutrophic lake using an empirical buoyancy regulation model which was coupled with a 1-D hydrodynamic numerical model. Hellweger et al. (2008) developed an individual-based model for the formation and behaviour of resting stage cells in a cyanobacterium (*Anabaena*) in a shallow reservoir. Their model segmented the reservoir into vertically resolved water column and sediment bed (aerobic and anaerobic) compartments. Hellweger et al. (2008) stated that future work may include adding a horizontal dimension to the model in order to resolve horizontal gradients or differences between shallow- and deep-water sediments. The sediment compartment is required as a repository and specifically to provide a process representation of recruitment from the bottom sediments to the water column (Karlsson-Elfgren and Brunberg, 2004).

Eulerian-based models generally require sufficient resolution to accurately represent the scales of horizontal and vertical heterogeneities of physical and chemical properties that

affect the dynamics of phytoplankton. Domain discretization and grid resolution, therefore, influence the level of success with which IBMs or PTMs simulate observed data. In terms of horizontal discretization, computational meshes of models can be divided into structured (rectangular grids) and unstructured (triangular grids) meshes. Structured meshes usually consist of a uniform grid dimensions (Piggott et al., 2008), while unstructured meshes allow variable resolution in areas of interest such as bays. In addition, structured meshes have a limited ability to reproduce complicated coastlines, whereas unstructured meshes of the same level of resolution can be accurately configured to them (Piggott et al., 2008). Compared to structured meshes, unstructured fine grids can allow finer resolution and flexibility to represent regions with complex coastlines or bathymetry, including smaller waterbodies (Aleynik et al., 2016).

Structured-grid models often use finite difference methods and unstructured-grid models use finite volume or finite element methods (Willis, 2011). The finite difference method has the advantage of simplicity and computational efficiency, while the major advantage of the finite element method is its geometrical flexibility (Weisberg and Zheng, 2006; Chen et al., 2007a). Models based on the finite volume methods like the Finite-Volume Community Ocean Model (FVCOM) can combine the advantages of both finite element and finite difference methods (Chen et al., 2007a). Compared with results obtained from a finite-difference model, Chen et al. (2003) found that FVCOM better resolved the detailed thermal structure and flows in regions with complex topography. The number of CyanoHAB PTMs or IBMs using unstructured grids has increased recently (Rowe et al., 2016; Wang et al., 2017; Feng et al., 2018) in line with the increase of computational speed, although it is still common to use PTMs for CyanoHAB simulations in open waters where grid resolution may be about 2 km or more (Wynne et al., 2011; Wynne et al., 2013; Soontiens et al., 2019).

2.3. Measurements for data input and model comparison

The data required for (i) model initialisation, (ii) boundary conditions and (iii) calibration and validation can be obtained in different ways. Commonly, point or grab samples are used which involve manually collecting water samples at specific locations within a lake. It is then followed by laboratory analyses of relevant analytes. Grab samples are usually taken at low frequency and often with a limited spatial resolution (Hamilton et al., 2015). Recent advances in sensor and information technologies are increasing the spatial and temporal resolution at which water quality parameters can be autonomously measured in situ (McBride and Rose, 2018) and remotely from the air or space (Allan and McBride, 2018). *In situ* high-frequency monitoring creates an opportunity to deepen our understanding of changes taking place over short periods of time relevant to derivation of fluxes (Hamilton et al., 2015). It also enables robust validation of dynamic models (Fringer et al., 2019) and better alignment of the measurements with the high frequency output from dynamic models (Hamilton et al., 2015). Examples of such in situ high frequency sensors include chlorophyll fluorescence or phycocyanin as proxies for phytoplankton and cyanobacteria biomass, respectively (McBride and Rose, 2018). Automated high-frequency monitoring has also been undertaken at cellular level using microscopic imagery and flow cytometry to provide high-frequency phytoplankton composition profiles through the water column (Pomati et al., 2011). This method captured the rapid changes occurring over the duration of a CyanoHAB event, while routine monitoring at two-week intervals did not. High-frequency echosounders have also been used for rapid quantification of *Microcystis* biomass during CyanoHAB events, allowing scanning of the entire water column and reliant up backscatter from gas vesicles in *Microcystis* (Ostrovsky et al., 2020). Many high frequency sensors require careful calibration. However, as they provide proxy measurements for biomass, these sensors are often associated with compensation for interferences associated with changes in temperature, light and phytoplankton community composition and physiology (Bertone et al., 2018).

Comprehensive data for spatial initialisation and validation can improve confidence in the predictive capabilities of all CyanoHAB PLMs, PTMs, and IBMs. To characterize the spatial variability of key variables, several point-based measurements with grab samples or high-frequency monitoring are usually required. Remote sensing with satellites offers an alternative method to detect and quantify distributions of CyanoHABs (Kutser, 2004; Wynne et al., 2008; Isenstein et al., 2020). Remotely sensed imagery can provide information for the entire surface of water bodies and also enable acquisition of information about inaccessible areas or historical datasets (Hadjimitsis and Clayton, 2009). However, remote sensing of chlorophyll *a* cannot resolve its vertical distribution (Odermatt et al., 2012b). Recent satellite Ocean and Land Colour Instruments (e.g., Sentinel 3; Schaeffer et al., 2018) have targeted reflectance wavebands corresponding to specific cyanobacteria pigments such as phycocyanin, but they do not provide information on species composition. Therefore, a combination of remotely sensed data, high-frequency monitoring of the water column using sensors, and conventional cell counts is ideally required to create a 3-D distribution of the species composition and biomass of CyanoHABs that can be used for initialisation, calibration, and validation of all CyanoHAB models.

Remote sensing of phytoplankton distributions, often related to the heterogeneity of CyanoHABs, has been used to initialise and evaluate the performance of IBMs (Wang et al., 2017; Feng et al., 2018) and PTMs (Wynne et al., 2011; Wynne et al., 2013; Rowe et al., 2016; Soontiens et al., 2019). Studies have used high temporal resolution imagery from the Medium Resolution Imaging Spectrometer (MERIS) (Wynne et al., 2011; Wynne et al., 2013; Rowe et al., 2016), Moderate Resolution Imaging Spectroradiometer (MODIS) (Wang et al., 2017; Feng et al., 2018), and Sentinel-3 Ocean and Land Colour Instrument (OLCI) sensor (Soontiens et al., 2019). Although these sensors may provide data several times per week (weather permitting), the data is generally limited to waterbodies with areas larger than

100 ha, because of coarse spatial resolution. MERIS, MODIS, and Sentinel-3 have spatial resolutions of 300 m, 250-1000 m, and 300 m, respectively (Allan and McBride, 2018). For small lakes, the next generation of optical sensors on board Sentinel-2 and Landsat 8 can provide capability to monitor CyanoHABs in waterbodies with a minimum area of 0.5 ha and 1.5 ha, respectively, using multispectral data at 10 m and 30 m resolution (Allan and McBride, 2018). The finer spatial resolutions imply lower revisit times, around 5–16 days, compared with those of MERIS, MODIS, and Sentinel-3 OLCI sensors (Dörnhöfer et al., 2018). To improve the temporal resolution of the fine spatial resolution data, multi-sensor data fusion methods that blend observations from different sensors with different spatial and temporal resolutions can be used, providing high spatiotemporal resolution suitable for dynamic events such as CyanoHABs (Hilker et al., 2009; Dörnhöfer et al., 2018).

Some issues should be considered in the use of satellite images. For example, cyanobacteria populations can be highly vertically heterogeneous and concentrations at the surface can therefore also vary horizontally at small scale, of the order of tens of metres and similar to pixel sizes in satellite images (Kutser, 2004). Moreover, cyanobacteria can be rapidly distributed through the water column or sometimes form dense aggregates of a few millimetres at the water surface (Puddick et al., 2016), dependent on levels of turbulence, vertical migration and buoyancy (Oliver et al., 2012). Clouds and fog are also intermittent obstacles to the continuous use of remote sensing data (Ibelings et al., 2003; Odermatt et al., 2010). Therefore, it is recommended to use satellite images when species are distributed through the surface mixed layer, and the sky is clear (Wynne et al., 2011).

The use of extensive data sets for model calibration and validation requires a more advanced statistical approach (i.e., skill levels) for model calibration and validation. Visual assessments are no longer satisfactory as the sole basis for model assessments, and interrogation of model performance should be made with complementary statistical tests (e.g., Moriasi et al., 2007;

Bennett et al., 2013). These tests also reveal quite different performances among state variables, with decreasing performance from physical to chemical and biological variables (Arhonditsis and Brett, 2004). Wherever possible, performance assessments should consider both state variables (state validation) and key fluxes (process validation), after aligning units of flux measurements to those used in model. For example, phytoplankton productivity is often expressed as a gross volumetric value ($\text{mg C m}^{-3} \text{ d}^{-1}$) but can be divided by phytoplankton biomass (mg C m^{-3}) derived from biovolumes (e.g., using calculations from microscopic enumeration) (Hillebrand et al., 1999) to obtain the rate (d^{-1}) suitable for model flux comparisons. These types of comparisons are valuable because they may help to resolve the issue related to equifinality, where a similar model outcome arises from different combinations of free parameters, i.e., parameter values may misrepresent the ‘actual values’ and lead to poor outcomes when the model is applied to a different condition. In other words, IBMs, like other process-based models that have multiple complex processes, may produce the “right answer for the wrong reason”. By conducting process validation, we can obtain “good results for the right reasons” to correctly capture interactions among variables in the ecosystem and provide greater confidence in forecasts (Hipsey et al., 2020). Fluxes that form the basis for process validation are infrequently used for calibration, partly because they are not routine model outputs.

3. Physical drivers and physiological processes controlling CyanoHABs

3.1. Horizontal and vertical transport of cyanobacteria

As can be seen from Table 1, previous studies that have used IBMs or PTMs to simulate CyanoHABs have made several assumptions about the processes involved in the horizontal and vertical transport of cyanobacteria cells. Some of these assumptions may adversely affect the accuracy of the models. In order to increase the predictive ability of all types of CyanoHAB models to forecast the spatiotemporal distributions of CyanoHABs, it is crucial

to improve the representation of key physical and physiological processes that control CyanoHAB development and distribution. This section gives an overview of the processes that can govern the dynamics of cyanobacteria cells and should be considered in any modelling approach of cyanobacteria dynamics.

The transport of cyanobacteria depends on their physical and biological characteristics (e.g., density, size, and morphology) and environmental forcing (e.g., currents, wind, and waves) (Fig. 2). These constituents vary considerably, and some are stochastic in nature, making the simulation of cyanobacteria transport very challenging.

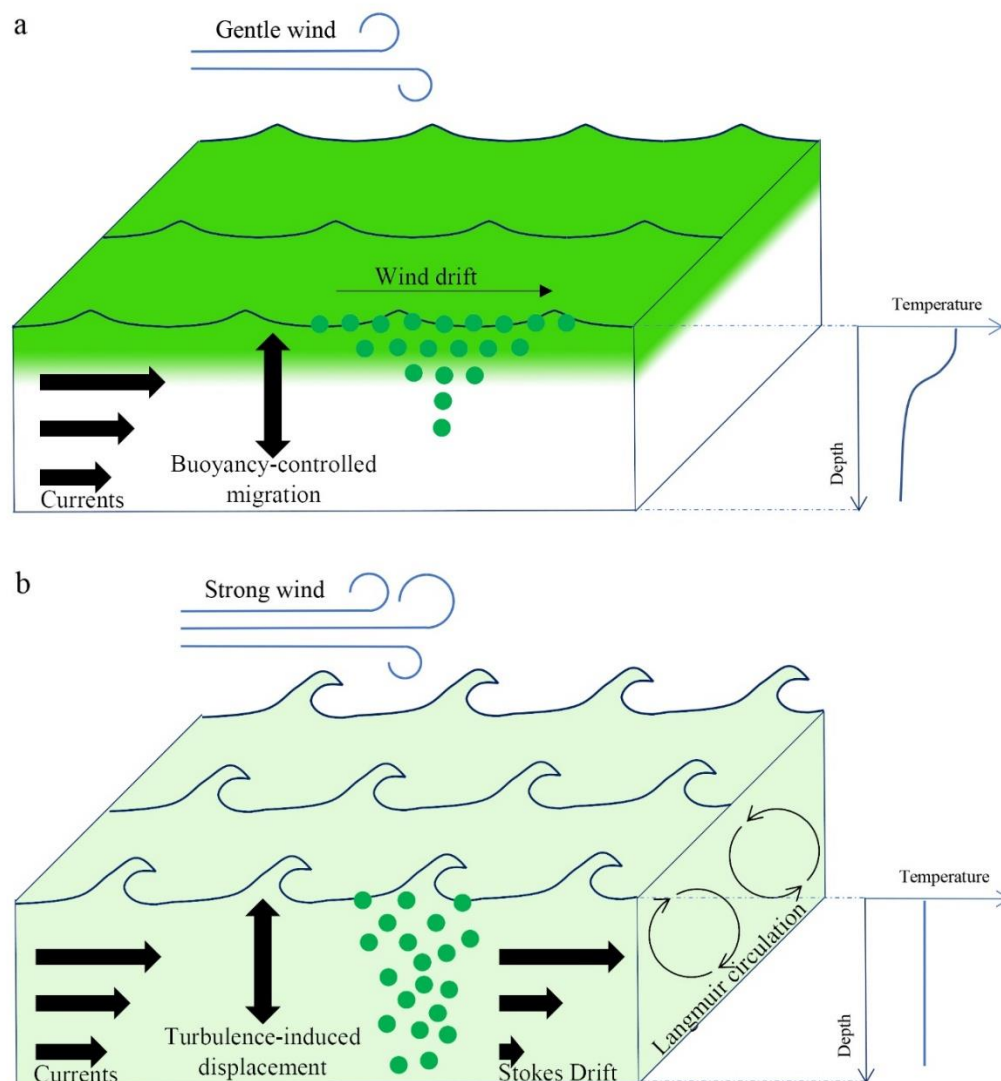


Fig. 2. The primary processes involved in the transport of cyanobacteria species under gentle

(upper) and strong (lower) wind conditions in the surface mixed layer. The background colour represents chlorophyll *a*.

The horizontal trajectory and speed movement of cyanobacteria are mainly controlled by currents, winds, and waves. Currents are the major forcing for the transport of cyanobacteria but wind drift can also generate additional velocity and be important under gentle wind conditions when cyanobacteria colonies accumulate at the water surface (Wynne et al., 2011) (Fig. 2a). Cao et al. (2006) found that surface cyanobacteria blooms develop on the water surface in Taihu Lake, China, when wind speeds are less than 3.1 m s^{-1} . Webster and Hutchinson (1994) reported that wind speeds greater than $2\text{--}3 \text{ m s}^{-1}$ can mix floating phytoplankton cells (or colonies) into deeper water layers while at lower wind speed, surface blooms are expected to remain on the surface. Above a critical wind speed, cells are vertically redistributed (Fig. 2b) and transported by wave-driven Stokes drift (Wang et al., 2016). The horizontal positions of particles are governed by the following equations (Wang et al., 2017; Feng et al., 2018):

$$X(i, t + \Delta t) = X(i, t) + Udt + U_{\text{additional}}dt + \zeta_t \sqrt{2D_H(i, t)\Delta t} \quad (1)$$

$$Y(i, t + \Delta t) = Y(i, t) + Vdt + V_{\text{additional}}dt + \zeta_t \sqrt{2D_H(i, t)\Delta t} \quad (2)$$

where t is time; X and Y are the cyanobacteria cell locations; U and V are the current-induced horizontal velocity components; D_H is the horizontal dispersion coefficient (considered to be identical in X and Y directions). ζ_t is an independent normally distributed random variable with a zero mean value and unit variance. The fourth term on the right-hand side of Eqns. 1 and 2 accounts for lateral mixing of cells (Soontiens et al., 2019), which may be considered relatively small. $U_{\text{additional}}$ and $V_{\text{additional}}$ that represent the surface wind drift and wave-induced Stokes drift (Wang et al., 2016; Feng et al., 2018) are estimated as:

$$U_{additional} = \begin{cases} C_w U_w \sin(W_{winddirection} - \pi) (1 + \gamma_t) & \text{for } U_w \leq U_{critical} \\ \frac{\pi^2 H^2}{L^2} c \frac{\cosh(kh)}{\sinh^2(kh)} \sin(W_{wavedirection} - \pi) & \text{for } U_w > U_{critical} \end{cases} \quad (3)$$

$$V_{additional} = \begin{cases} C_w U_w \cos(W_{winddirection} - \pi) (1 + \gamma_t) & \text{for } U_w \leq U_{critical} \\ \frac{\pi^2 H^2}{L^2} c \frac{\cosh(kh)}{\sinh^2(kh)} \cos(W_{wavedirection} - \pi) & \text{for } U_w > U_{critical} \end{cases} \quad (4)$$

where U_w and $W_{winddirection}$ are the wind speed and direction, respectively. C_w is the wind drift coefficient, γ_t is a random number uniformly distributed between zero and unity, h is the average water depth, H is the wave height, L is the wavelength, k is the wave number ($2\pi/L$) and $c = \frac{gT}{2\pi} \tanh(\frac{2\pi H}{L})$ is wave velocity, where T is the wave period.

Dippner et al. (2011) who used a PTM set a wind drift coefficient (C_w in Eqns. 3 and 4) of 0.015 for modelling of CyanoHABs in coastal waters. Wang et al. (2017) and Feng et al. (2018) calibrated the wind drift coefficient and used a value of 0.016, together with a prescribed wind direction, in Lagrangian modelling horizontal trajectory and speed of cyanobacteria movement. It should be note that the wind drift coefficient that is used in IBMs and PTMs differs from the wind drag coefficient that connects wind velocity to surface water velocity in Eulerian hydrodynamic models.

The vertical position of cyanobacteria species is mainly controlled by the interplay of the buoyancy of the cyanobacteria and water turbulence (Wallace et al., 2000; Hozumi et al., 2019) (Fig. 2). Vertical movement changes environmental conditions that cells encounter and directly influences horizontal transport as horizontal water velocities change vertically. For example, cyanobacteria can be subject to different levels of subsurface currents and wave-driven Stokes drift depending on their vertical position. Therefore, accurate simulation of the vertical transport of cyanobacteria is necessary to represent their spatiotemporal distributions. In addition, knowledge of the vertical position of cyanobacteria populations has an important implementation for water supply from reservoirs. Drinking water supplies can be adversely affected when dense layers of cyanobacteria form under low levels of turbulence and align

with the depth of the water intake (Rowe et al., 2016; Ndong et al., 2017). In some cases, these events have had major impacts on water supplies (Steffen et al., 2017) and have stimulated additional modelling to investigate causal factors (Manning et al., 2019).

3.1.1. Buoyancy control and vertical migration of cyanobacteria

In stratified lakes where light and nutrients are vertically separated, several bloom-forming cyanobacteria genera, such as *Dolichospermum* (basionym *Anabaena*), *Microcystis*, *Aphanizomenon* and *Oscillatoria* (Visser et al., 2016a and references therein), can vertically migrate to position themselves for optimal growth in the water column (Reynolds and Walsby, 1975; Walsby, 1978; Ganf and Oliver, 1982). In natural populations of cyanobacteria, vertical migration mainly occurs through changes in carbohydrate ballast (Kromkamp and Mur, 1984; Ibelings et al., 1991; Wallace et al., 2000) that are complemented by longer-term adjustments in buoyancy from gas vesicles. Gas-vacuolate cyanobacteria may become positively buoyant at night when carbohydrate consumption is not compensated by production from photosynthesis (Villareal and Carpenter, 2003). Consequently, when there is little wind mixing, cells float upwards and form dense surface scums (Huisman et al., 2018). After having access to light, cells become negatively buoyant from the production of carbohydrates, and gas vesicles no longer offset the carbohydrate ballast, enabling cells to exploit nutrients in deeper waters (Visser et al., 1995; Villareal and Carpenter, 2003). Therefore, at low irradiance, the buoyancy of gas-vacuolate cyanobacteria increases while under high irradiance the buoyancy decreases (Kromkamp et al., 1988; Visser et al., 2005).

In addition to light, temperature and nutrient availability influence carbohydrate ballast accumulation and density changes (Spencer and King, 1987; Kromkamp et al., 1988). Nitrogen and phosphorus limitation can lead to a decrease in gas vesicle volume per cell and may, in turn, lead to a loss of buoyancy, whereas under nitrogen and phosphorus replete

conditions, cells may become buoyant (Konopka et al., 1987; Klemer et al., 1996; Brookes and Ganf, 2001; Chu et al., 2007). Chu et al. (2007) showed that nitrogen limitation has a more significant effect on gas vesicle content of *M. flos-aquae* than phosphorus limitation. Brookes and Ganf (2001) showed that *M. aeruginosa* varies its buoyancy as a function of previous nutrient and light history of the cells. In addition, at reduced temperatures, an increase in carbohydrate ballast can lead to a loss of buoyancy although the gas-vesicle volume stays the same (Visser et al., 1995). This can result in the observed autumnal sedimentation of the *Microcystis* population (Visser et al., 1995). Stokes' law can be used to provide insights about the speed of buoyancy-controlled vertical migration (W_s) in quiescent waters with little wind mixing:

$$W_s = \frac{gd_c^2(\rho_w - \rho_{col})}{18\varphi\nu} \quad (5)$$

where g is the acceleration of gravity, d_c is the equivalent diameter of the cell (assumed to be spherical for certain genera such as *Microcystis*), ρ_w is the density of water, ρ_{col} is the density of a cell, φ is a shape coefficient and ν is the viscosity of water.

The effect of variable cell or colony morphology is represented in Stokes' law by the shape coefficient (Eq. 5). In previous IBM studies, colonies of *Microcystis* have been assumed to be spherical (i.e. $\varphi=1$) (Wallace et al., 2000; Wang et al., 2017; Feng et al., 2018). However, *Microcystis* colonies can have irregular shapes (Zhang et al., 2007; Li et al., 2016; Li et al., 2018). It has been shown that any non-spherical particles (except teardrop-shape particles) settle more slowly than spherical particles (McNown and Malaika, 1950; Reynolds, 1997). Therefore, the assumption of spherical particles can lead to overestimation of settling velocity. Additionally, cell or colony size can influence vertical velocities according to Stokes' Law. Many gas-vacuolate cyanobacteria form multicellular trichomes (e.g., *Dolichospermum*) or colonies (e.g., *Microcystis*) that effectively increase ascent and descent velocities as a result of increases in cell diameter (Wu and Kong, 2009). Larger colonies that

migrate more rapidly can access deeper, nutrient-rich layers (Rabouille and Salençon, 2005; Aparicio Medrano et al., 2013). Stokes' law is valid for determining the vertical velocities of particles at low Reynolds numbers (Re), i.e., under quiescent conditions (Reynolds, 1997) but may overpredict floating and sinking speeds for large colonies (Aparicio Medrano et al., 2013), at $Re > \sim 0.1$ (Re increases because colonies are large). Using Stokes' law, Re can be estimated as (Feng et al., 2018):

$$Re = \frac{\rho_{col} d_c}{\mu} \frac{g d_c^2 (\rho_w - \rho_{col})}{18 \phi v} \quad (6)$$

To avoid overprediction of colony velocities at high Reynolds numbers, a non-linear drag term can be added to Stokes' law (Aparicio Medrano et al., 2013; Feng et al., 2018). For example, Aparicio Medrano et al. (2013) showed that considering the non-linear drag can lead to a reduction in the terminal velocity of a colony by 15% at a Reynolds number of 3. On the other hand, it has been found that turbulence can cause disaggregation of cyanobacteria colonies. The disaggregation may increase with increasing intensity and duration of mixing (O'Brien et al., 2004; Li et al., 2018). Li et al. (2018) demonstrated that colonies of *M. ichthyoblabe* may be more susceptible to disaggregation driven by turbulence than colonies of *M. aeruginosa* and *M. wesenbergii*. Therefore, turbulence has an important influence in the selection of different morphospecies of *Microcystis*.

As discussed, Stokes drift generated by waves can cause net advection in the direction of wave propagation. Drift is also important for the transport of cyanobacteria cells under strong wind conditions (Wang et al., 2016) when wave-current interactions are strong. In addition to Stokes drift, dissipation of waves approaching coastlines can lead to the movement of particles parallel and perpendicular to the coastline (see Van Sebille et al., 2020 for a review). In spite of the importance of waves, there is limited literature on their effects on the spatial and temporal distributions of cyanobacteria. In the modelling context, coupling a wave model (e.g., Simulating Waves Nearshore (SWAN) model (Booij et al., 1999)) to an IBM, that has

been already forced by the outputs of a Eulerian hydrodynamic-ecological model, could advance our understanding of the wave impacts.

3.1.2. Vertical turbulence-induced displacement

If a mild horizontal force (e.g., light wind) is applied to the surface layer of the water column, laminar flow can be generated where layers of molecules slide smoothly over one another and fluid flow is dominated by viscous forces. In laminar flow, all layers move parallel to the bed although surface layers move faster than the lower layers (Reynolds, 1997). If the magnitude of wind forcing increase, turbulent motion can be generated where the molecular structure can no longer accommodate the energy of the forcing (Reynolds, 1997), and random velocity fluctuations dominate fluid flow (Reynolds, 2004). According to the Kolmogorov spectrum, turbulent energy cascades from large-scale eddies (metres) adjacent to the source of forcing to small scale eddies (millimetres), until the smallest turbulent eddies (Kolmogorov length scales) are overcome by viscosity (Reynolds, 1997).

The water column in lakes may stratify during several hours to years depending on the balance on stabilizing forces (e.g., solar radiation and convective heating) to destabilizing forces (e.g., wind and convective cooling) and the lake morphology (Imberger and Patterson, 1989). When stabilization persists for more than a few days, a layer of buoyant surface water (epilimnion) forms over cooler, darker waters (hypolimnion) (Howard, 2001; Howard and Easthope, 2002). These two zones are separated by a transitional zone (metalimnion) with a central thermocline (Rodi, 1987). The epilimnion – the layer directly influenced by wind shear and penetrative convection – is considered to be a mixed layer where the temperature is relatively constant (Imberger, 1985; Rodi, 1987). The thickness of the mixed surface layer can vary on a diurnal timescale as a result of wind energy and the amount of heating or cooling during the course of the day. Severe wind events and surface cooling can deepen the surface layer (Imberger, 1985; Rodi, 1987). On a typical summer day, a fairly calm and hot

morning can lead to heating of the surface layer and development of strong stratification that resists mixing (Imberger, 1985; Spigel et al., 1986; MacIntyre and Melack, 1995). However, the combination of strong wind and heat loss (largely due to evaporation) in the afternoon erodes the stratification (MacIntyre et al., 2002). Therefore, stratification can develop and be eroded on a daily basis. Woolway et al. (2015) showed that diel variability in epilimnetic temperature is highly connected with the lake area. Larger lakes are more exposed to wind, which results in a greater surface mixed layer depth. This, in turn, reduces the difference between the maximum and minimum daily epilimnetic temperatures (Woolway et al., 2015). The degree of entrainment of phytoplankton embedded in the turbulent motion can be quantified using ψ proposed by Humphries and Imberger (1982):

$$\psi = W_s[15(\pm w'^2)^{1/2}]^{-1} \quad (7)$$

where w' is the vertical turbulent velocity fluctuation. If $\psi < 1$ sinking phytoplankton are entrained because turbulence dominates their vertical distribution, while if $\psi > 1$ sinking phytoplankton are dis-entrained since their vertical velocity outcompete turbulent eddies. In other words, if turbulent velocity is more than 15 times larger than the sinking velocity of phytoplankton, this can lead to their entrainment. In the case of cyanobacteria with positive buoyancy, ψ is frequently much larger than unity (Spigel and Imberger, 1987). It means that the vertical distribution of positively buoyant cyanobacteria is more affected by their buoyancy than by turbulence (Spigel and Imberger, 1987). Therefore, it has been shown that larger colonies with greater buoyancy and vertical velocity are better able to resist the turbulent entrainment velocity and maintain their position in the water column (Wallace et al., 2000; Rabouille and Salençon, 2005; Aparicio Medrano et al., 2013).

The degree of entrainment can influence intra-specific competition among cyanobacteria species for nutrients and light that may exert a significant effect on the community structure of cyanobacteria (Huisman et al., 2004; Zhou et al., 2015). For example, during weak mixing,

the phytoplankton community will likely be dominated by the species, such as buoyant cyanobacteria, with positive buoyancy that can escape from the turbulent flow entrainment and position themselves at depths of favourable light intensity (Huisman et al., 2004). As a result, they have access to light, while sinking species are shaded by them. When turbulent mixing is strong enough to dominate the sinking or flotation velocity of cells, both buoyant and sinking species are vertically mixed throughout the water column. Sinking species are generally better able to withstand fluctuating light conditions and are therefore likely to outcompete buoyant species in well-mixed environments (Reynolds et al., 1983; Visser et al., 1996; Huisman et al., 2004; Visser et al., 2016a). In lakes, buoyant species, such as the cyanobacterium *Microcystis*, dominate under conditions of low turbulent diffusivity; while sinking species, such as diatoms and green algae, become dominant during periods of high turbulent diffusivity (Huisman et al., 2004; Zhou et al., 2015).

A numerical technique called random walk is widely used to capture the effects of sub-grid scale turbulent diffusion on particle trajectories in Lagrangian models (e.g., Rowe et al., 2016; Wang et al., 2017; Feng et al., 2018). This technique helps to account for the effects of sub-grid scale turbulent transport processes that cannot be resolved by flow fields (Xue et al., 2008). The random walk technique is based on the diffusivity which is represented in Eulerian hydrodynamic models (Fig. 1). Visser (1997) proposed the following random walk formula that can be used in CyanoHAB IBMs and PTMs:

$$\Delta z = \dot{D}_V(Z(i, t))dt + \xi_t \sqrt{2D_V(Z(i, t) + 0.5\dot{D}_V(Z(i, t)))\Delta t} \quad (8)$$

where Z is the location of cyanobacteria cells in the water column; D_V is vertical diffusivity and \dot{D}_V is the derivative of D_V (Hellweger and Bucci, 2009; Feng et al., 2018). The vertical positions of particles are governed by the following equation (Wang et al., 2017; Feng et al., 2018):

$$Z(i, t + \Delta t) = Z(i, t) + W_s dt + \dot{D}_V(Z(i, t))dt + \xi_t \sqrt{2D_V(Z(i, t) + 0.5\dot{D}_V(Z(i, t)))\Delta t} \quad (9)$$

The second term on the right-hand side of Eq. 9 accounts for buoyancy-controlled vertical migration, and the third and fourth terms represent vertical turbulence-induced displacement. Previous Lagrangian modelling studies have provided valuable insights into the processes governing the transport of cyanobacteria populations. As Table 1 shows, some of the key processes mentioned above are often not included in IBMs or PTMs of cyanobacteria, affecting predictive ability of the model. In some studies, buoyancy or buoyancy regulation has not been considered or has been assigned as a constant value rather than being affected by light or nutrient limitation or other environmental factors (Table 1). Many studies have neglected the effects of turbulent mixing on the vertical movement of cells (Table 1). Researchers are recommended to use more advanced models (e.g., FVCOM) that can consider a larger array of these key processes.

3.1.3. Langmuir circulation

Under sustained wind forcing, the interaction between wind shear and surface waves can generate Langmuir cells, a turbulent circulation process with quasi-organized large-eddy structures in the upper layers of lakes (Langmuir, 1938; Thorpe, 2004; Neale et al., 2012; Smyth et al., 2017) (Fig. 2). Phytoplankton species can be transported vertically by this circulation (Neale et al., 2012). Under wind speeds greater than $2\text{--}3 \text{ m s}^{-1}$, large water bodies can experience Langmuir circulation (Wetzel, 2001). For example, in Lake George, NY, USA, with an area of 117.4 km^2 and an average depth of about 19.5 m, the velocity of downward currents was 0.016 m s^{-1} at a wind speed of 6 m s^{-1} (Wetzel, 2001). The effects of Langmuir circulation on phytoplankton species differ considerably from those of turbulence. Langmuir circulation causes entrained phytoplankton to experience organized periodic light fluctuations (Langmuir, 1938), but turbulence causes disorganized random light fluctuations (Wallace and Hamilton, 1999). Langmuir circulation may also indirectly affect phytoplankton

by influencing their physical environment. For example, Langmuir circulation destroys the near-surface stratification (Huang et al., 2014). Turbulence resolving large eddy simulation (LES) models are capable of representing Langmuir circulation (Kukulka et al., 2009). LES models solve the Craik-Leibovich equation using spatially averaging over a subgrid scale. The Craik-Leibovich momentum equations capture Langmuir circulation dynamics by a vortex force (McWilliams et al., 1997; Kukulka et al., 2009).

3.2. *Physiological processes relevant to CyanoHABs*

Developers of CyanoHAB IBMs are faced with a myriad of physiological processes that may be included in these models, aside from formulations that describe growth responses to temperature, light and nutrients, and losses from grazing, viruses and natural attrition (see Oliver et al., 2012). Our intention in this section is not to provide an exhaustive list of physiological processes but to identify some of the processes that are strongly relevant or specific to cyanobacteria. We have focused on the colony formation, overwintering, carbon concentrating mechanism, nitrogen fixation, and luxury phosphorus uptake. These processes are discussed briefly below.

3.2.1. *Colony formation*

The cyanobacterium *Microcystis* has high phenotypic plasticity and can exist as solitary cells or form scums consisting of large colonies (100–2000 μm) under natural conditions (Li et al., 2018; Xiao et al., 2018). Colony formation by *Microcystis* can positively impact its vertical velocities (maximum recorded for a single colony, $\sim 10.08 \text{ m h}^{-1}$ (Xiao et al., 2018)), resulting in resistance to high levels of turbulence (dis-entraining from turbulent mixing or escaping from entrainment in the turbulent flow) and having access to optimal light and nutrient environments. Vertical position may affect grazing pressure by zooplankton and exposure to chemical stressors (Xiao et al., 2018). Therefore, the ability to form large colonies is a key trait of *Microcystis* (Duan et al., 2018) but colony formation can lead to

decreased specific growth rates compared with the solitary (unicellular) habit (Xiao et al., 2018).

Various abiotic and biotic factors can affect colony formation. Flagellate grazing can induce *M. aeruginosa* to actively form colonies but larger colonies may also be resistant to grazing (Yang et al., 2008). There is a positive correlation between colony size of *Microcystis* and the content of extracellular polymeric substance (EPS) surround the cells and colonies (Xiao et al., 2017; Xiao et al., 2019). As a result, EPS can be considered as a precursor to colony formation (Xiao, et al., 2019). The EPS comprises three humic acid-like components (C1 – C3) and a protein-like component (C4). Humic acid-like component C1 is involved in colony formation and colony size growth of *Microcystis* (Xiao et al., 2019).

There is contradictory literature on whether higher nutrient concentrations affect *Microcystis* colony formation. For example, Wang et al. (2010) reported that nutrient enrichment coupled with predation of zooplankton can promote surface *Microcystis* blooms. Duan et al. (2018) also showed that higher phosphorus availability may enhance *Microcystis* scums while nitrogen enrichment may have negligible effect. However, Ma et al. (2014) indicated that increased nutrient concentrations can result in the formation of single cells. It has also been shown that warmer temperatures can elevate colony size (Duan et al., 2018).

3.2.2. Overwintering

Although some cyanobacteria, including *Planktothrix agardhii* and *Planktothrix rubescens*, can develop blooms in the water column of temperate lakes in winter, many others overwinter successfully as akinetes (*Dolichospermum*, *Aphanizomenon*, and *Gloeotrichia*) or as vegetative cells (*Microcystis* sp.) (Visser et al., 2016b). In autumn, *Microcystis* can sink into the sediment and survive in bottom sediments of lakes (Reynolds et al., 1981; Tsujimura et al., 2000). As a result of poor light conditions at the bottom of lakes, their photosynthetic activity can be restricted. Therefore, the overwintering can be considered as a physiological

‘rest’ (Brunberg and Blomqvist, 2002). When environmental conditions become favourable, the benthic population can be recruited from surface sediments to the water column (Zou et al., 2018) and the benthic *Microcystis* population surviving winter can serve as an inoculum for pelagic blooms in spring and summer (Preston et al., 1980; Brunberg and Blomqvist, 2003). Model simulations have shown that the absence of recruitment from the sediment can result in a reduction of 50% in *Microcystis* sp. blooms in summer (Verspagen et al., 2005). Despite its importance, most models do not simulate benthic stages (Cottingham et al., 2021). Hense and Beckmann (2006) developed a mathematical model to investigate the dynamics of cyanobacteria life cycles. The model separates the life cycle into vegetative cells, vegetative cells with heterocysts, akinetes, and recruiting cells (including germinates) and assumes that the transition between each stage depends on the internal energy and nitrogen quotas of the cells. Vegetative cells have high internal energy and high nitrogen quotas without nitrogen fixation. Once nitrogen quotas are low, vegetative cells fix nitrogen. The common characteristic of vegetative cells with and without nitrogen fixation is their positive buoyancy. Low energy and nitrogen quotas of planktonic cells lead to the development of akinetes that sink to the bottom where they take up nitrogen. After the internal nitrogen quota is sufficiently filled, the cells with low energy are recruited to surface waters in vegetative form and are able to replenish their energy reservoir. A simplified version of this cyanobacterial life cycle model that considers two-life cycle stages instead of the four-life cycle stages described above was used by Hense and Beckmann (2010). The simplified model showed good skill in representing the timing and the duration of the blooms, the annual mean nitrogen fixation rates, and the magnitude of year-to-year fluctuations and decadal variability. The model was deemed suitable to be a sub-component of a 3-D ecosystem model.

3.2.3. *CO₂ concentrating mechanism*

Cyanobacteria can take up atmospheric carbon dioxide (CO_2) and bicarbonate (HCO_3^-) from the environment for carbon fixation using the CO_2 fixing enzyme Ribulose biphosphate Carboxylase Oxygenase (RuBisCO) (Visser et al., 2016b; Ma et al., 2019). Since RuBisCO has a low affinity for CO_2 , cyanobacteria possess an active CO_2 concentrating mechanism (CCM) (Giordano et al., 2005; Burford et al., 2016; Ma and Wang, 2020). The CCM involves transport of dissolved inorganic carbon (DIC) into cells to allow accumulation of CO_2 with RuBisCO (Giordano et al., 2005; Burford et al., 2016), resulting in improved photosynthetic performance (Wang et al., 2015). Badger and Price (2003) and Badger et al. (2006) showed that when CO_2 levels are low, CCMs in cyanobacteria are more efficient in comparison with other algae. Therefore, CCMs provide cyanobacteria with a competitive advantage under low CO_2 conditions (Price et al., 2008; Meyer and Griffiths, 2013). However, when inorganic carbon is adequate, the cyanobacteria CCM remains in a constitutive state (Price et al., 2008). Morales-Williams et al. (2017) have suggested that the CCM in cyanobacteria becomes active when at a threshold partial pressure of CO_2 of 393 ppm.

In nutrient-enriched lakes, the high concentration of cells in blooms enhances CO_2 consumption to support photosynthetic activity. This reduces the availability of free CO_2 and increases the pH of affected waters, causing extreme carbon limitation (Paerl and Ustach, 1982; Ibelings and Maberly, 1998). If the water is stratified, in response to CO_2 depletion, cyanobacteria form scums (Paerl and Ustach, 1982). Surface-dwelling blooms can directly intercept the CO_2 influx at the air–water interface, thereby alleviating the limitation of photosynthetic growth by dissolved inorganic carbon (Paerl and Ustach, 1982; Ibelings and Maberly, 1998). Scum formation can therefore promote cyanobacterial dominance under CO_2 -limiting conditions by enabling dense cyanobacteria biomasses to avoid low CO_2 availability in deeper areas and shade sub-surface phytoplankton populations.

3.2.4. Nitrogen-fixation

Several bloom-forming cyanobacteria genera are diazotrophic, such as *Anabaena*, *C. raciborskii*, *Aphanizomenon*, *Nodularia*, *Lyngbya* and *Nostoc*, fixing atmospheric nitrogen (N_2) to complement cellular nutritional requirements (O’Neil et al., 2012; Beversdorf et al., 2013; Visser et al., 2016b). N_2 fixation can enable diazotrophic cyanobacteria to grow rapidly and outcompete non-nitrogen fixing cyanobacteria and eukaryotic phytoplankton, particularly when there are low rates of DIN supply (O’Neil et al., 2012; Huisman et al., 2018; Ma and Wang, 2020). However, N_2 fixation is an energetically costly process (Gobler et al., 2016) and requires absence of oxygen that would otherwise inactivate the nitrogenase enzyme complex (Gallon, 1992; Zehr et al., 2000; Huisman et al., 2018). To protect the nitrogenase, freshwater diazotrophic cyanobacteria form differentiated specialized cells known as heterocysts (Muro-Pastor and Hess, 2012). Heterocysts have a thick cell wall that limits oxygen diffusion (Muro-Pastor and Hess, 2012).

Hellweger et al. (2016b) developed a mechanistic, molecular-level model of *Anabaena*–nitrogen interactions that represent several genes involved in nitrogen uptake and assimilation (e.g., GlnA). In the model, when fixed nitrogen is depleted and the cells become nitrogen-stressed, cells metabolize various forms of nitrogen, grow and divide, and differentiate into heterocysts. They took advantage of individual-based modelling because each individual readily responds to its intracellular state and environmental conditions by changing gene expression, enzyme velocity and photosynthesis, among other physiological features. The model was used to simulate a scenario of reduction of N loading in a hypothetical lake, showing its potential to become part of a comprehensive ecosystem models.

3.2.5. *Luxury phosphorus uptake*

When the concentration of phosphorus (P) is high, cyanobacteria can accumulate P in excess of immediate cellular demand to ameliorate the effects of P deficiency. This phenomenon is known as luxury P uptake (reviewed by Healey, 1982) and it can increase cellular P

concentrations from ~0.3% to ≥ 3 % ash-free dry mass (Reynolds, 2006). When P becomes depleted, this storage can be used as a P source, giving a competitive advantage to cyanobacteria over other phytoplankton that mostly have limited P storage capacity. Luxury P storage capacity varies amongst cyanobacteria genera (Carey et al., 2012). For example, *R. raciborskii* has a high luxury storage capacity (Xiao et al., 2020a), while *Anacystis* has a capacity (Carey et al., 2012).

Two approaches can be used to represent the effect of nutrient availability on phytoplankton growth. The first formulates growth based on ambient concentrations of nutrients (e.g., Monod growth), and the second formulates growth based on the intracellular nutrient content or cell quota that is more mechanistically correct (Cерco et al., 2004; Hellweger and Kianirad, 2007; Cerucci et al., 2010). Growth as a function of the internal nutrients is commonly simulated using the Droop model (Droop, 1973; Hellweger and Kianirad, 2007). By contrast, the Monod method (Monod, 1949) is a straightforward approach that cannot represent nutrient luxury uptake since the model directly relates growth with available nutrients in the water column (Cerucci et al., 2010). The Droop model, while more complex, is generally a better predictor of nutrient-limited growth (Sommer, 1991). According to the Droop equation (Droop, 1973; Grover, 1991), the specific growth rate of cell i , μ_i , is given by:

$$\mu_i = \mu_{max,i} \left(1 - \frac{Q_{min,i}}{Q_i} \right) \quad (10)$$

where $\mu_{max,i}$ is the maximum specific growth rate of cell i , and Q_i and $Q_{min,i}$ are the current and minimum intracellular nutrient quota, respectively. Therefore, the specific growth rate of cell i increases with its intracellular nutrient content and becomes zero if its intracellular nutrient content has decreased to the minimum value $Q_{min,i}$ (Sommer, 1991). The Droop model can be incorporated into IBMs, but an obstacle to using the Droop model is that there are rarely measurements of cell quotas, and minimum cell quotas are more likely to be the theoretical values.

3.3. *Climate change and catchment-lake interactions*

Climate change has regional and local impacts on interdependent systems (e.g., weather, catchments, and lakes) that are typically modelled independently (Sharma et al., 2018). Large lakes with large heat capacity (low albedo), and small atmospheric roughness coefficients in comparison to their surrounding lands can modify regional weather and climate (Su et al., 2020). For example, lake surface temperatures in the Great Lakes are warmer than air temperatures in late fall and winter, leading to increased precipitation on the lee side of the lake, triggered by atmospheric instability. However, during summer, there may be downwind decreases in rainfall (Scott and Huff, 1996). On the other hand, climate variability and change can affect lake physics and, in turn, lake biology and biogeochemistry (Hadley et al., 2014). For example, the thermal structure of lakes is closely connected with the air temperature and wind speed (Magee and Wu, 2017). Warming air temperatures and decreasing wind speeds (atmospheric stilling) can lead to more long-lasting and stable thermal stratification (Magee and Wu, 2017; Woolway et al., 2017), favouring CyanoHABs (Paerl and Huisman, 2008). Lakes are influenced not only by the overlying atmosphere but also by neighbouring catchments (Sun et al., 2020) that exhibit two-way interactions with the atmosphere (Charney et al., 1975). Xue et al. (2017) developed a two-way coupling of FVCOM (Chen et al., 2003) with the Regional Climate Modelling system Version 4 (RegCM4) (Giorgi et al., 2012) in the Great Lakes region. As a result of providing a better representation of lake-atmosphere interactions, the two-way coupling increased the accuracy of simulated lake thermal structures and ice over previous studies that used hydrodynamic models in one-way offline simulations.

Future research exploring the impacts of climate change on CyanoHABs is recommended to incorporate climate-catchment-lake interactions using two-way coupled modelling systems. Climate change is expected to lead to a higher frequency and intensity of rainfall events,

leading to greater nutrient input into waterbodies during heavy rainfall events, thus resulting in conditions that are favourable for cyanobacterial growth (Reichwaldt and Ghadouani, 2012; Carpenter et al., 2015; Carpenter et al., 2018). Moreover, urban development or the widespread use of fertilizers for intensive farming can result in increased transfer of nutrients from catchments to receiving waters (Goyette et al., 2019), fuelling the growth of cyanobacteria. In addition, as discussed before, thermal stratification that suppresses turbulence and, in turn, allows buoyant cyanobacteria in the surface mixed layer to migrate upward and access sufficient light for growth is expected to be affected by climate change. Higher temperatures lead to more prolonged diurnal stratification in the surface mixed layer (Stetler et al., 2020), especially if atmospheric stilling (Woolway et al., 2017) also occurs. The interactions between the environmental drivers expected to be affected by climate change (e.g., more long-lasting and stable thermal stratification and altered nutrient loading) and cyanobacterial physiological processes (e.g., colony formation and buoyancy) will likely favour cyanobacterial dominance in most future climate scenarios (Carey et al., 2012). For example, warmer temperatures and higher phosphorus availability can lead to the formation of larger colonies of *Microcystis*, increasing surface scums (Duan et al., 2018). This strengthens thermal stratification (Kumagai et al., 2000; Ibelings et al., 2003; Jones et al., 2005; Rinke et al., 2010) and reduces momentum transfer from wind to water at low wind speeds (Wu et al., 2019), reinforcing conditions favourable for the development of CyanoHABs. Therefore, since climate change potentially influences CyanoHABs in several ways, incorporating two-way climate-catchment-lake interactions as well as cyanobacterial physiology into future CyanoHAB IBMs is essential to accurately predict the effects of climate change on CyanoHABs and thus develop effective management strategies to mitigate the impacts.

4. Summary and conclusions

IBMs can be used to improve predictions of CyanoHAB development and transport by capturing the key physical and physiological processes that interact in the formation and distribution of blooms. Here, we present a checklist of criteria that can be used to determine model type in future studies. IBMs are highly recommended when there is a considerable 1) strain-level diversity, 2) interspecific adaptive behaviour, and 3) intra-specific variability among individuals, or 4) individuals behave as a function of their previous environmental conditions. In addition, IBMs can be very useful to capture the interactions of individuals with each other and with their biotic or abiotic environment and the life cycles of individuals. A large array of complex processes lead to CyanoHABs, and incorporating them into CyanoHAB IBMs will be one of the most important challenges ahead. A step-by-step approach can be used to meet this challenge. First, it is recommended to pay particular attention to the physical characteristics of colonies, especially colony size. This is because the vertical migration velocity of a colony varies as an exponent of the diameter. As discussed earlier, the level of turbulence a colony encounters determines whether the colony can dis-entrain from turbulent mixing to form blooms which is related to the interaction of colony velocity and turbulence intensity. Colony size can vary among colonies and also vary dynamically with aggregation and disaggregation processes. Capturing variations in colony size is important for accurate predictions of the timing and magnitude of blooms. Second, individuals in CyanoHAB IBMs should carry a memory that reflects the previous physiological state such as light exposure history and nutrient status. For instance, if we wish to capture the effect of variations in irradiance on buoyancy regulation in cyanobacteria, then it would be necessary to consider the history of light exposure in individual cells or colonies. Future studies are also recommended to incorporate key processes in CyanoHABs of colony formation, overwintering, CCM, N_2 fixation, and luxury P uptake. Few models unite these processes, but some include formulations of the individual key processes that could form the

basis of a more comprehensive CyanoHAB IBMs. Finally, there are important dynamic feedbacks between CyanoHABs and their environment that can reinforce favourable conditions for CyanoHAB development. For example, surface blooms absorb heat and, in turn, strengthen thermal stratification that suppresses turbulence. This allows buoyant species, such as the cyanobacterium *Microcystis*, to migrate upward and outcompete other species for light. As a result, both thermal stratification and surface blooms can become progressively more intense, and sub-surface phytoplankton populations can be shaded by dense surface blooms. In the modelling context, online coupling of an IBM to a Eulerian hydrodynamic-ecological model could capture the two-way interaction between cyanobacteria and their environment. The combination of incorporating physiological processes into IBMs and online coupling could advance the ability of IBMs to identify the underlying mechanisms controlling CyanoHAB distribution and abundance.

An accurate CyanoHAB IBM requires a comprehensive dataset for model initialisation, boundary conditions and calibration and validation. Ideally, the combination of automated high-frequency monitoring and remote sensing is required. Advanced statistical approaches for model calibration and validation are also recommended when extensive datasets are used. In addition, since different complex processes are incorporated into a CyanoHAB IBM, it is advisable to assess whether the interactions among different mechanisms in the ecosystem are correctly captured by conducting process validation, wherever possible.

Climate change is likely to impact weather, catchments, and lakes, i.e., major environmental drivers of CyanoHABs related to thermal stratification and nutrient loads. High-resolution, integrated climate-catchment-lake modelling systems should therefore be used to simulate the potential effects of climate change on CyanoHABs and more fully test if climate change will favour cyanobacterial dominance, including considerations of the frequency, intensity duration and species composition of CyanoHABs.

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Declaration of competing interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

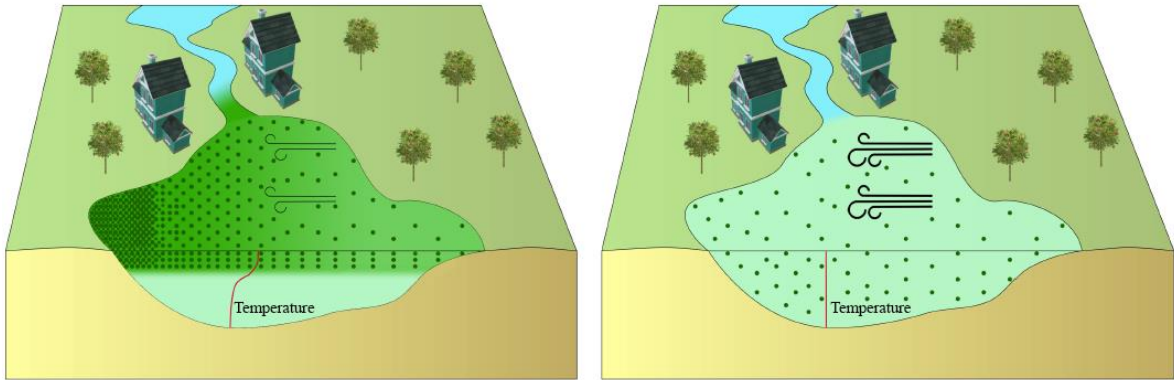
☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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Credit Author Statement

MHR: Conceptualization, Methodology, Writing - Original Draft, and Visualization; DPH: Conceptualization, Methodology, Writing - Review & Editing, and Supervision; AE: Methodology, Writing - Review & Editing, and Supervision; FH: Writing - Review & Editing, and Supervision.

Graphical abstract



Highlights

- Predicting cyanobacteria harmful algal blooms (CyanoHABs) is of crucial importance.
- Physical and physiological processes interact in the formation of CyanoHABs.
- Individual-based models (IBMs) can capture the key processes leading to CyanoHABs.
- IBMs, coupled with Eulerian models, can improve predictions of CyanoHABs.