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Review

Phytoplankton functional type modelling: Running before we can walk? A critical evaluation of the current state of knowledge

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ABSTRACT

In the context of aquatic biogeochemical modelling, there is an increasing pressure to explicitly treat multiple biogeochemical cycles and to increase the functional diversity of biotic communities. In this study, we evaluate the capacity of 124 aquatic biogeochemical models to reproduce the dynamics of phytoplankton functional groups. Our analysis reinforces earlier findings that aquatic ecosystem modellers do not seem to consistently apply conventional methodological steps during the development of their models. Although there is an improvement relative to earlier critiques, significant portion of published studies did not properly assess model sensitivity to input vectors; aquatic ecosystem modellers are still reluctant to embrace optimization techniques during model calibration; and assess the ability of their models to support predictions in the extrapolation domain. We also found significant variability with respect to the mathematical representation of key physiological processes (e.g., growth strategies, nutrient kinetics, settling velocities) as well as group-specific characterizations typically considered in the pertinent literature. Cyanobacteria blooms are a major concern for water industries as they represent high risk for human health and economic costs for drinking water treatment, and thus one of the outstanding challenges is to offer credible modelling tools that can serve as early warning systems to assist with the operational control of cyanobacteria blooms. Our study suggests that the derivation of distinct functional groups from fairly heterogeneous planktonic assemblages poses challenging problems. Because of the still poorly understood ecology, we do not have robust group-specific parameterizations that can support predictions in a wide array of spatiotemporal domains. In this context, we argue that the most prudent strategies are the gradual incorporation of complexity, where possible and relevant, along with an open dialogue on how we can mathematically depict the interconnections among different phytoplankton subunits or even how we can frame the suitable data collection efforts.

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> "*. . .Inadequacies and dysfunctionalities in models are not compensated for by the collection and use of data describing only part of the story. The devil is indeed in the details; nutrient-phytoplankton-zooplankton (NPZ) models get away with an awful lot by not exploring the details. If we are going to open Pandora's box to explore the details, then we had better be ready to handle the demons that escape from it. . .*"
>
> Flynn, 2006, J. Plankton Res. 28, p. 875.

1. Introduction

It is more than 40 years ago, when Chen (1970) proposed a general set of differential equations for describing key physical, chemical, and biological processes of aquatic ecosystems with site-specific parameters, initial conditions, and forcing functions, which were then used to address water quality problems (Fulton et al., 2004; Friedrichs et al., 2006). The philosophy and basic set of equations originally proposed remain the core of the current generation of mechanistic aquatic biogeochemical models, although advances in scientific understanding and improvements in methods of numerical analysis have brought significant progress in regard to the accuracy and sophistication (Ward et al., 2013). Early models were simple mathematical descriptions of aquatic systems that accounted for the interplay among nutrients, organic matter and aggregated biotic compartments, such as the generic "phytoplankton" and "zooplankton" state variables (Anderson, 2005). At higher aggregation levels, plankton communities exhibit satisfactory predictability and are often proposed as a paradigm for shedding light on the spatiotemporal patterns of complex natural systems (McCauley and Murdoch, 1987; Scheffer et al., 2003). Nonetheless, the aggregate plankton properties (total biomass, productivity) are also characterized by lower sensitivity to external perturbations (episodic meteorological events, invasion of exotic species, excessive nutrient enrichment) and may be unreliable indicators of structural ecosystem shifts (Schindler, 1990; Frost et al., 1995). Further, in the context of water quality management, one of the central issues revolves around the elucidation of the mechanisms that shape the composition of phytoplankton assemblages and the capacity to predict the occurrence of harmful algal blooms, such as toxin-producing cyanobacteria. Thus, it is not surprising that simple models are frequently perceived as inadequate (or even obsolete) management tools (Flynn, 2005, 2006; Le Quere, 2006), and modellers increasingly opt for more sophisticated constructs designed to explicitly represent multiple biogeochemical cycles, to accommodate the functional diversity of biotic communities, and to depict the interactions of plankton communities with the higher food web (Van Nes and Scheffer, 2005).

Delineating the optimal resolution level for phytoplankton modelling studies poses significant challenges, and thus far one of the most defensible strategies involves the concept of "functional grouping" relative to strategies that revolve around the specification of size classes, modelling of individual species, or stipulation of goal functions (Jorgensen, 1999; Reynolds et al., 2002). Founded upon the classification of species on the basis of their general morphological, physiological, and ecological characteristics, the functional grouping offers an intuitively plausible approach that accounts for different patterns of adaptive specialism, while accommodating the notion that external (seasonal forcing, resource availability) and internal (inter-specific competition, trophodynamics) factors may profoundly modulate the expected signals of phytoplankton community (Reynolds et al., 2002). In the typical modelling practice, the characterization of each phytoplankton functional group (*PFG*) postulates different degrees of specialization for limiting resources (nutrients, light) and/or environmental conditions (temperature), while purporting to reproduce inter-specific competitive interactions which – in reality – are characterized by an inconceivably wide array of physiological adaptations (mixotrophy, life stages) and sustained coexistence (Flynn, 2006; Thingstad et al., 2010). However, because of the poorly understood ecology, the literature debates to what extent we have robust group-specific parameterizations that can support predictions in a variable range of spatiotemporal domains. Modellers often use pre-conceived functional groups with subjective properties that are conveniently derived during the model fitting exercise to observed data (Thingstad et al., 2010). For example, preliminary efforts to incorporate plankton functional types into global biogeochemical models were based on speculative parameterization and – not surprisingly – resulted in unreliable predictions (Anderson, 2005). Likewise, Zhao et al. (2008) showed that the reproduction of seasonal succession plankton patterns in freshwater ecosystems is fairly sensitive and only occurs within a narrow window of the model parameter space. The latter study also pondered if it is "reasonable to expect single-valued data set-specific parameter estimates of artificially defined biotic entities to be extrapolated over wider geographical regions?" Thus, recognizing that the functional group modelling does not necessarily guarantee improved predictability, it is advised that the gradual incorporation of complexity, where possible and relevant, is the most prudent strategy and any such model development should be tightly coupled with rigorous assessment of the underlying uncertainty (Arhonditsis, 2010).

Given the importance of the topic, it is surprising the lack of published work to quantify the ability of *PFG* models in accurately reproducing the aggregated and compositional phytoplankton variability. In this regard, the present study evaluates the capacity of 124 aquatic biogeochemical models to reproduce the dynamics of phytoplankton functional groups across the range of temporal and spatial scales typically utilized. Following the practices presented in meta-analysis papers (Arhonditsis and Brett, 2004; Arhonditsis et al., 2006; Wellen et al., 2015), we first examine how consistently do modellers follow conventional methodological procedures, such as the quantification of goodness-of-fit, sensitivity analysis, and model validation in its broadest sense (predictive and structural confirmation, model transferability). We then evaluate the capacity of *PFG* models to reproduce seasonal succession patterns and structural shifts in phytoplankton communities in different geographical locations and environmental conditions. Along with the quantitative information, we also compile the most commonly used mathematical equations, parameter ranges and calibration methods used to reproduce phytoplankton functional groups, with special emphasis on cyanobacteria as one of the major threats to freshwater ecosystem health and integrity. Our intention is not to determine the most reliable way to refine the biotic resolution, but rather to assess the general performance of existing *PFG* models, to evaluate the methodological consistency during their development, to delve into how autotrophic organisms have been aggregated, and to pinpoint any major issues of model dysfunctionality. Our hypothesis is that the sizable number of modelling studies, which successfully passed the scrutiny of the peer-review process along with the experience gained from addressing a wide range of management problems, can objectively reveal systematic biases, methodological inconsistencies, and common misconceptions characterizing the field of *PFG* modelling. To the best of our knowledge, this is the first attempt in the literature to present a comprehensive assessment of the current generation of *PFG* models and examine the potential of improving the representation of phytoplankton adaptive strategies for resource procurement. It is our hope that this study will contribute towards an effective linkage of the variability at the organismal level with ecosystem-scale patterns.

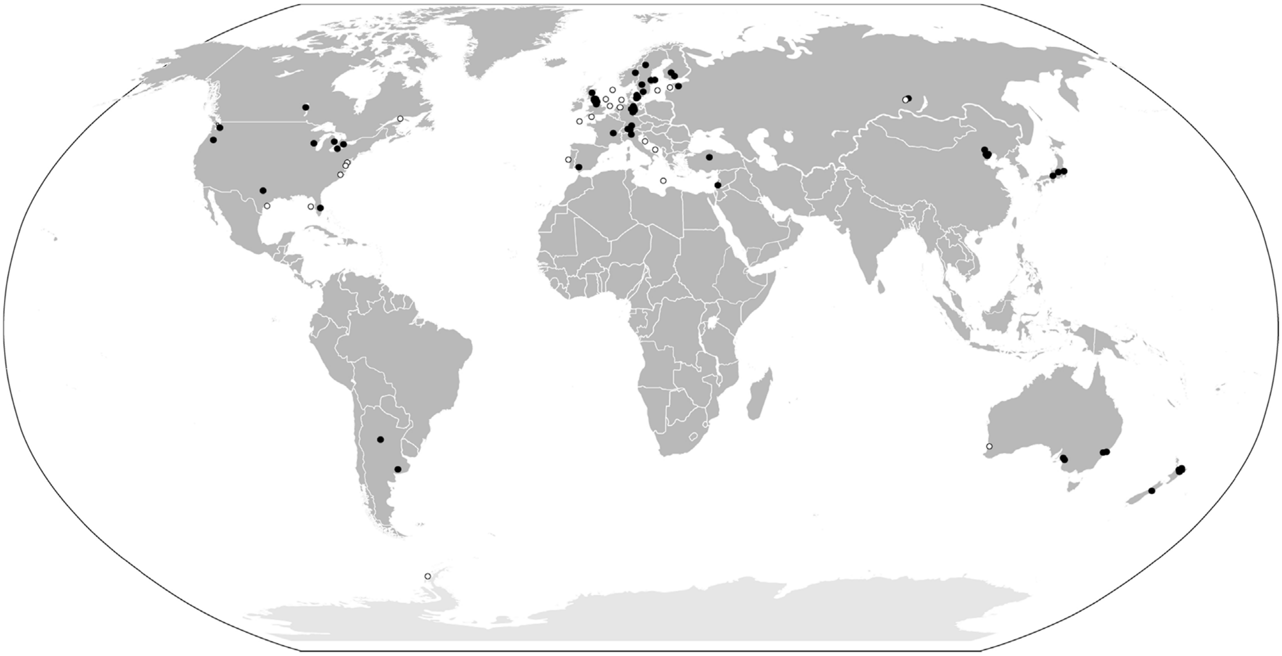

Fig. 1. Map of the locations modelled by the 124 studies included in our meta-analysis. Filled and non-filled circles represent freshwater and marine ecosystems.

2. Methods

In this study, we reviewed aquatic biogeochemical models that simulated multiple functional groups from 1980 to 2012, with special emphasis placed on conceptualizations and/or mathematical representations typically followed when modelling cyanobacteria. The literature was searched using the electronic databases: “ISI Web of Science”, and “Scopus” using the following keywords: “plankton functional group (*PFG*) or plankton functional type (*PFT*) model(l)-ing”, “phytoplankton model(l)-ing”, “cyanobacteria”, “biogeochemical model(l)-ing”, “lake ecosystem model(l)-ing”, “eutrophication model(l)-ing”. The criterion for a study to be considered in our meta-analysis was the explicit consideration of two or more phytoplankton groups within the original or modified (e.g., through addition of sub-models, reparameterization, coupling with hydrodynamics) ecosystem model. In this endeavour, we eliminated theoretical and laboratory (culture batch) studies to evaluate model performance, as our focus was on model capacity to simulate phytoplankton group dynamics in real world settings. The total number of studies investigated was 124 with broad geographic representation, although the majority of the studied locations were in the northern hemisphere; especially in European freshwater and marine ecosystems (Fig. 1; see also list of papers provided in Supporting Information section). 114 of the selected papers provided some type of information with respect to model performance by comparing simulated against observed phytoplankton dynamics either visually or quantitatively. This also includes model fit to aggregated phytoplankton variables, such as total phytoplankton biomass and chlorophyll *a*. 62 studies out of 114 selected studies provided only visual representation of model performance with time series, seasonal succession patterns, and spatial distribution of different functional algal groups. For the latter group of modelling studies, we digitized the relevant graphs to extract the original raw data and individually assessed their performance. We tested the magnitude of error that may stem from the digitizing processes by comparing the coefficients of determination (r^2) calculated from our digitized data and the values originally reported from the published studies (Fig. 2a). We found that our extracted estimates matched closely the reported model performance ($r^2 = 0.923$; $y = 0.945x + 0.038$, $n = 34$).

As previously mentioned, there were four main questions addressed through our analysis: How consistently do *PFG* modelling studies follow conventional methodological procedures during the development phase? How well do these models reproduce the dynamics of phytoplankton functional groups? What are the typical conceptualizations of different phytoplankton functional groups that influence their parameter specification? What are the differences between the characterizations of “cyanobacteria-like” state variables relative to other algal functional groups? The first two questions were intended to draw parallels with a previous meta-analysis of mechanistic aquatic biogeochemical models conducted by Arhonditsis and Brett (2004), which was based on 153 studies published in the peer reviewed literature from 1990 to 2002. Given that our analysis covers a longer period and comprises more recent papers, the present study indirectly offers an opportunity to evaluate if there is an improvement with respect to the methodological consistency (sensitivity analysis, goodness-of-fit, and validation) over the past decade. To quantify model predictive capacity, we calculated three dimensionless fit statistics; namely, the relative error $\left(RE = \sum \left|O - P\right| / \sum O\right)$, modelling efficiency $\left(MEF = 1 - \sum (O - P)^2 / \sum (O - \overline{O})^2\right)$, and coefficient of determination $\left(r^2 = \sum [(O - \overline{O}) \times (P - \overline{P})] / \sum (O - \overline{O})^2 \times \sum (P - \overline{P})^2\right)$, where O refers to observations, P refers to model predictions, $\overline{O}$ ($\overline{P}$) to the average of the observations (predictions). With the latter two commonly used metrics, higher values suggest better fit and 1.0 is indicative of perfect fit. A *MEF* of 0 indicates a model which predicts the observations as well as their corresponding average, while a negative *MEF* reflects a model which predicts more poorly than the average of the observations. Also note that the *MEF* penalizes for bias, whereas the r^2 does not penalize for linear bias.

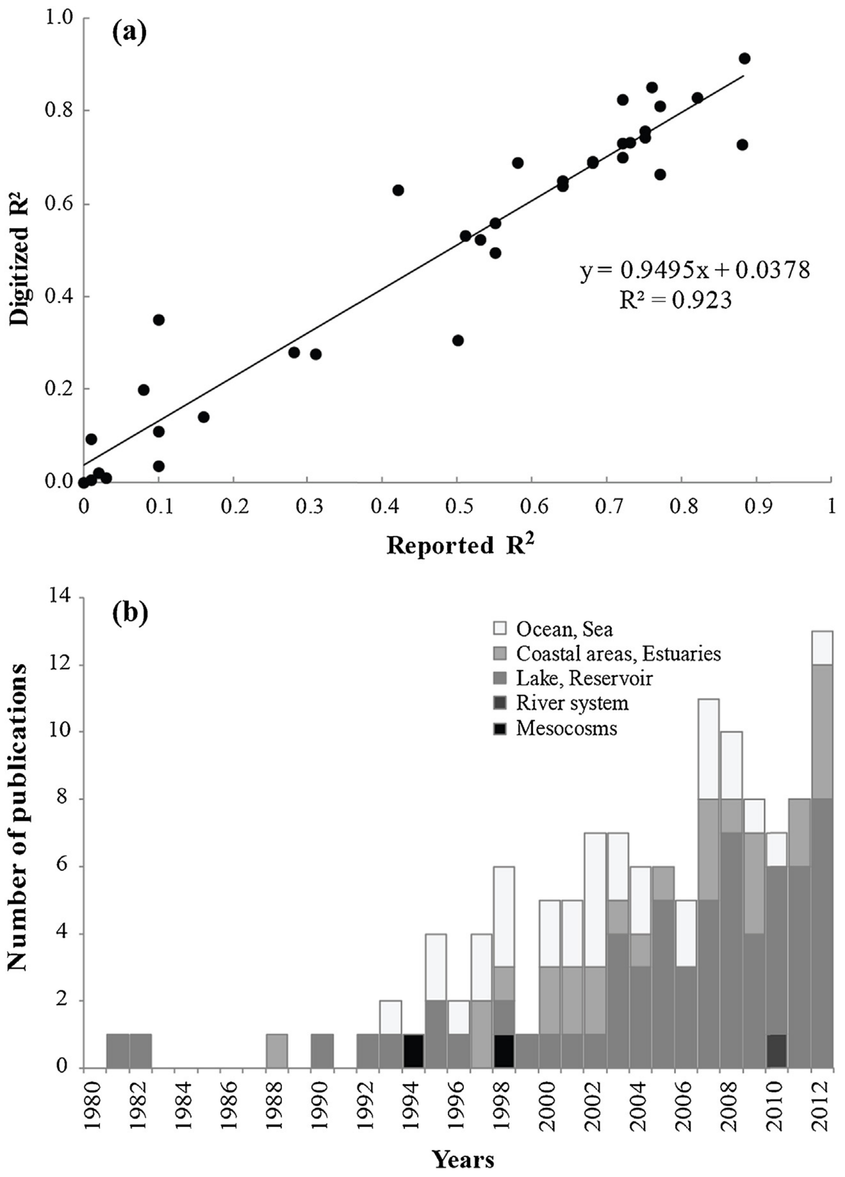

Fig. 2. (a) Digitization error associated with the assessment of model performance. Relationship between reported coefficient of determination (r^2) values and those extracted by the digitized data; and (b) ecosystems modelled per year of our study period.

3. Results and discussion

3.1. How consistently do PFG modelling studies follow conventional methodological procedures?

The number of mechanistic aquatic biogeochemical modelling studies, aiming to simulate multiple phytoplankton functional groups, has dramatically increased in the peer reviewed literature during the recent years (Fig. 2b). In particular, the average number of *PFG* models published towards the end of our study period (2010–2012) demonstrated a threefold increase relative to the 1990s. Counter to the predominance of oceanic modelling papers in the sample analyzed by Arhonditsis and Brett (2004), the present study is primarily based on aquatic biogeochemical models that have been developed in freshwater ecosystems (lakes, reservoirs, and rivers) to address eutrophication problems such as harmful algal blooms (Kim et al., 2014), and to evaluate the potential impact of climate change or other environmental changes on lake phenology (Adrian et al., 2009). The modelling literature emphatically argues the need for methodological consistency of the way models are being developed, highlighting the importance of several critical steps, such as sensitivity analysis, evaluation of goodness-of-fit after model calibration, and rigorous model validation (e.g., Chapra, 1997; Jørgensen and Bendoricchio, 2001). Nonetheless, Arhonditsis and Brett (2004) showed a surprising absence of a systematic methodological protocol widely followed by the aquatic ecosystem modelling community; namely, only 27.5% of the published studies identified the model components that needed to be estimated with greatest precision, whereas 45.1% did not report any results of sensitivity analysis whatsoever. In a similar manner, we here found that 47.5% of the *PFG* modelling studies did not provide any evidence of model sensitivity to various inputs, while 9.8% examined the influence of certain model structures (e.g., alternative formulations) or parameters without providing quantitative measures of model behaviour (Fig. 3a). The remaining 42.7% of the modelling studies did report results of sensitivity analysis, although a substantial portion of the latter group (25%) did not test the sensitivity of parameters relative to the phytoplankton functional groups simulated. Given the important insights gained for selecting the optimal model structure and

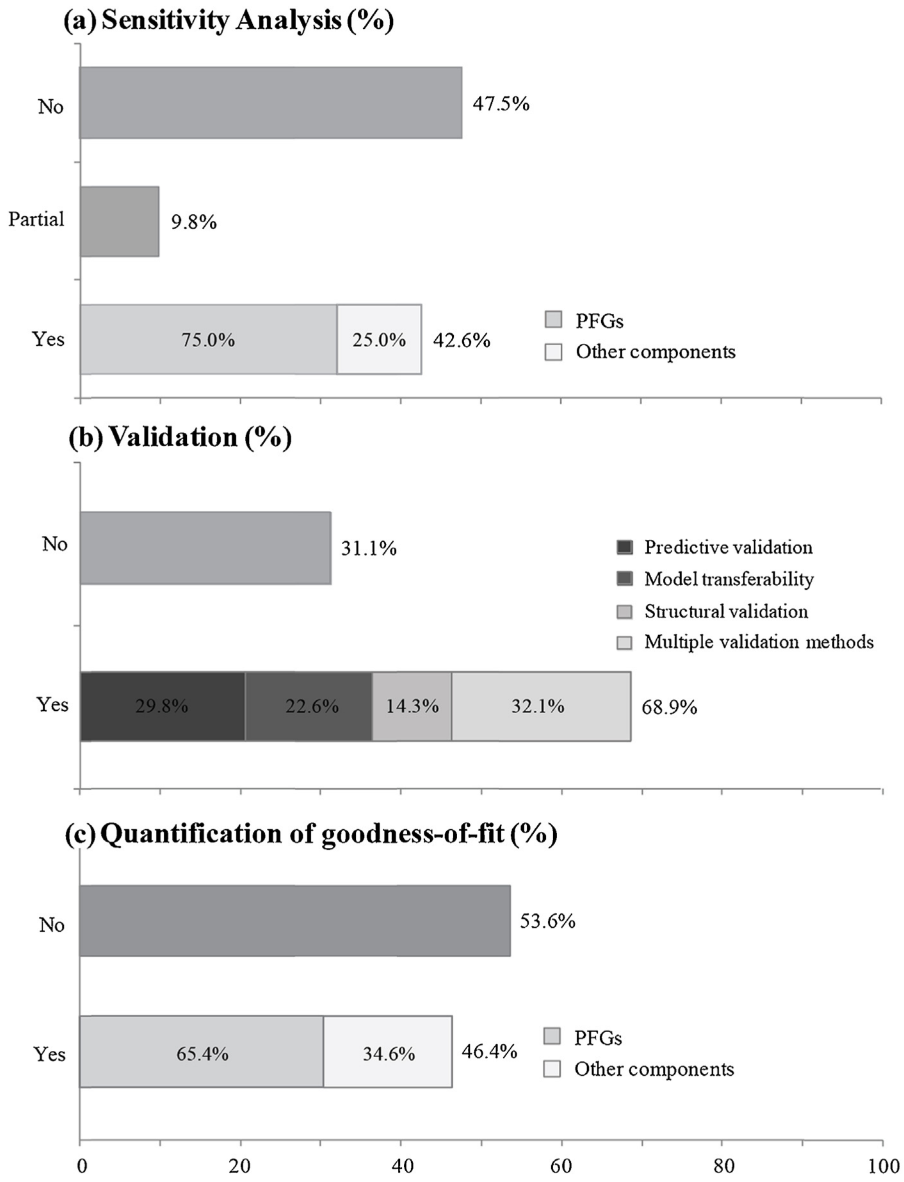

Fig. 3. Proportion of multiple functional group modelling studies that (a) performed sensitivity analysis, (b) performed different forms of model validation, and (c) quantified fit between simulated and measured data.

complexity, it is essential for modellers to perform (and explicitly report) different forms of sensitivity analysis when building their models.

The present meta-analysis paints a more favourable picture with respect to the proportion of modelling studies that performed model validation relative to Arhonditsis and Brett (2004). This finding partly stems from the fact that many of *PFG* models were developed by simply adding functional groups on existing aquatic ecosystem models (structural augmentation of existing modelling constructs). 68.9% of the papers reviewed, performed some type of validation during the model development phase (Fig. 3b). In particular, we considered the following types of validation: (i) predictive confirmation, defined as the evaluation of model-fit against independent data sets that were collected from the system after the model calibration (29.8%); (ii) model transferability to different locations or ecosystem types; and (iii) structural confirmation, defined as the assessment of the realistic reproduction of operational characteristics, causal relationships, and relative magnitudes of various ecosystem components (e.g., biological rates, derived quantities, mass fluxes associated with various ecological processes). In the same context, we also found that several popular model constructs (e.g., *CAEDYM*, *PROTECH*) have been applied to different locations (identified as model transferability exercises) as well as to different time periods with distinctive environmental conditions due to the increased availability of long-term data from the same system. Thus, these modelling studies were classified as having carried out multiple validation methods (32.1%). Finally, the remaining 31.1% of the published studies did not report any type of validation, which again compares favourably relative to the Arhonditsis and Brett's (2004) findings (see their Figure 2d).

Calibration is the procedure by which modellers attempt to find the best agreement between observed data and simulated outputs. In our analysis, we found that the most popular practice was the so-called "manual" or "trial and error" calibration by adjusting model parameters within the literature range until satisfactory fit was obtained. More recently though, modelling studies have applied automatic calibration procedures with objective criteria/goal

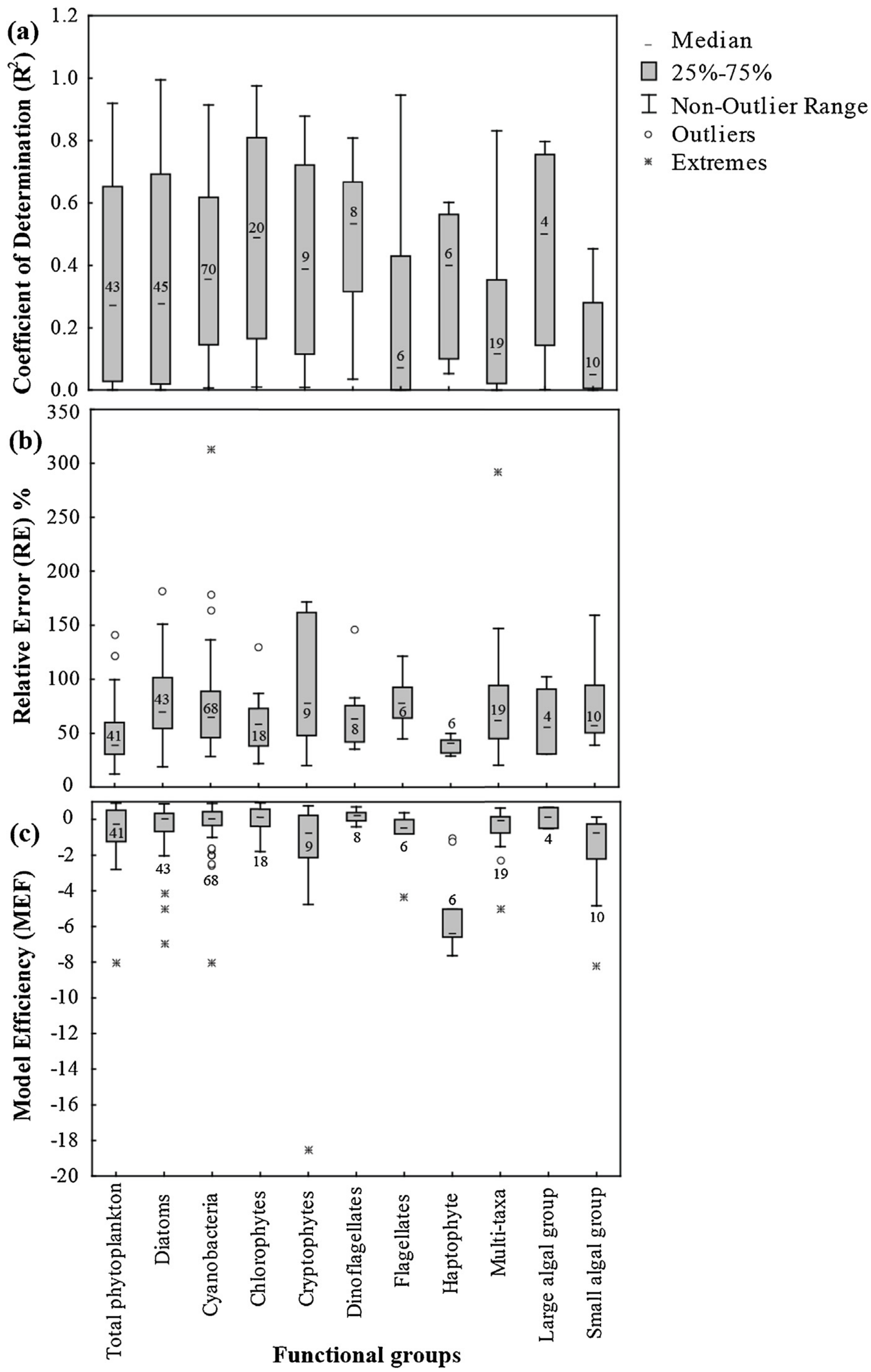

Fig. 4. Model performance for each phytoplankton functional group: (a) coefficient of determination, (b) relative error (%), and (c) model efficiency.

functions (Muller-Karulis and Aigars, 2011; Rigosi et al., 2011), and/or Monte Carlo and Bayesian inference techniques to estimate parameters based on prior knowledge and available data (Aldenberg et al., 1995; Bonnet and Poulin, 2002; Zhang and Arhonditsis, 2008). On an encouraging note, we found that a higher fraction of modelling studies reported fit statistics (Fig. 3c); 46.4% of the published studies (as opposed to 30.1% in Arhonditsis and Brett, 2004). However, we note that 34.6% of these studies reported fit statistics solely on simulations of aggregated phytoplankton variables, despite the fact that these models included individual functional phytoplankton groups as state variables. We hypothesize that the inconsistency between model structures designed and state variables targeted during calibration is that many study sites presumably lacked phytoplankton taxonomic data (see also following discussion).

3.2. How well do PFG models reproduce phytoplankton community dynamics?

Classification of functional/taxonomic phytoplankton groups in order to tabulate the corresponding model error was mainly derived from the original studies, although simulations of individual genera/species were assigned to more generic class categories (e.g., diatoms, chlorophytes, cyanobacteria). Cyanobacteria ($n = 70$)

Table 1
Maximum growth rates (day^{-1}) assigned to phytoplankton functional groups.

Functional groups	Count	Max	Min	Mean ± St.dev.
Cyanobacteria	67	4.60	0.02	0.93 ± 0.71
Diatoms	72	4.64	0.09	1.70 ± 0.79
Chlorophytes	30	3.60	0.54	1.43 ± 0.69
Chrysophytes	3	4.50	0.05	1.70 ± 2.44
Cryptophytes	8	1.48	0.70	1.06 ± 0.27
Dinoflagellates	21	1.60	0.30	0.84 ± 0.51
Other/combined functional groups	64	5.60	0.20	2.06 ± 1.09

and diatoms ($n = 45$) are the most commonly modelled taxonomic groups (Fig. 4). Generally, we were not able to identify phytoplankton functional groups with distinctly higher performance, only slightly better fit statistics with chlorophytes (median $r^2 = 0.49$, $RE = 59\%$, $MEF = 0.16$) and dinoflagellates (median $r^2 = 0.53$, $RE = 63\%$, $MEF = 0.24$). Simulations of aggregated phytoplankton had r^2 values ranging from 0.01 to 0.92 with median of 0.28, RE ranging from 12% to 141% with median value of 39%, and MEF values varying from −8.02 to 0.92 with median of −0.20. Although not directly comparable, total phytoplankton was characterized by slightly lower r^2 but also somewhat lower RE value relative to the Arhonditsis and Brett's (2004) findings (see their Table 1). Notably, moderate fit statistics were found for diatoms (median $r^2 = 0.31$, $RE = 70\%$, $MEF = 0.02$) and cyanobacteria (median $r^2 = 0.36$, $RE = 65\%$, $MEF = 0.06$). The worst performance among the phytoplankton functional groups simulated were recorded for cryptophytes (median $r^2 = 0.39$, $RE = 79\%$, $MEF = -0.74$), flagellates (median $r^2 = 0.07$, $RE = 78\%$, $MEF = -0.45$), and haptophytes (median $r^2 = 0.39$, $RE = 41\%$, $MEF = -6.36$), which may reflect our limited knowledge of their ecophysiological parameters compared to other well-studied functional groups. On a final note, a significant portion of the simulated cases had negative *MEF* values, suggesting that the predictive statements drawn from the models fared worse than the average values of the observed data. Compared with the performance of models in other disciplines (e.g., distributed watershed water quality modelling, see Wellen et al., 2015) or even the fidelity of simulations of nutrient dynamics (Arhonditsis and Brett, 2004), the *PFG* models demonstrate inferior ability to reproduce phytoplankton patterns.

3.3. *What are the typical PFG conceptualizations that influence their parameter specification?*

Given the heterogeneity of the modelling studies considered with respect to model complexity, type of ecosystem modelled, spatial and temporal scales, and model development objectives, we examined the presence of statistically significant trends of the parameter specification for different phytoplankton functional groups. We found the maximum growth rates (day^{-1}) assigned to diatoms ($\mu_{\max} = -0.034 \cdot \text{latitude} + 3.033$; $r^2 = 0.101$) and cyanobacteria ($\mu_{\max} = -0.018 \cdot \text{latitude} + 1.698$; $r^2 = 0.075$) demonstrated a weakly negatively relationship with the latitude in freshwater ecosystems, i.e., reduced maximum growth rates at higher latitudes for both functional groups and vice versa (Fig. 5a and b). This calibration practice is conceptually on par with the notion that water temperature gradually becomes an important regulatory factor of algal growth rate at higher latitudes. No statistically significant trend was found between phytoplankton maximum growth

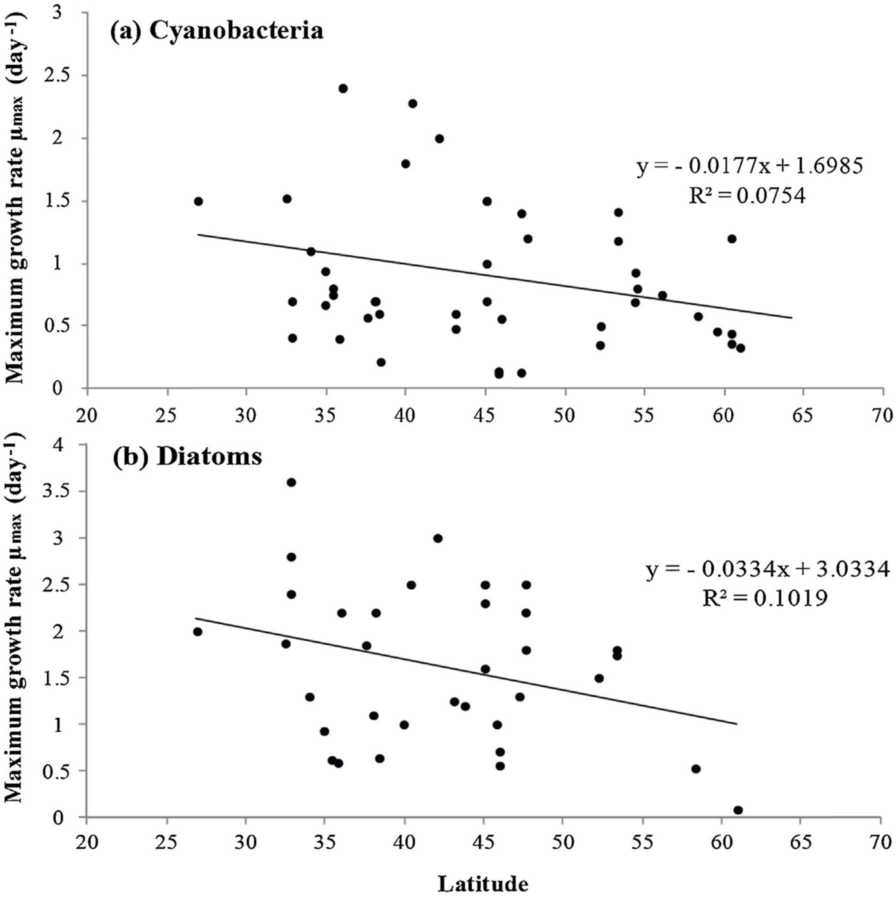

Fig. 5. Maximum growth rates assigned to (a) cyanobacteria and (b) diatoms over the latitude of the modelled ecosystems.

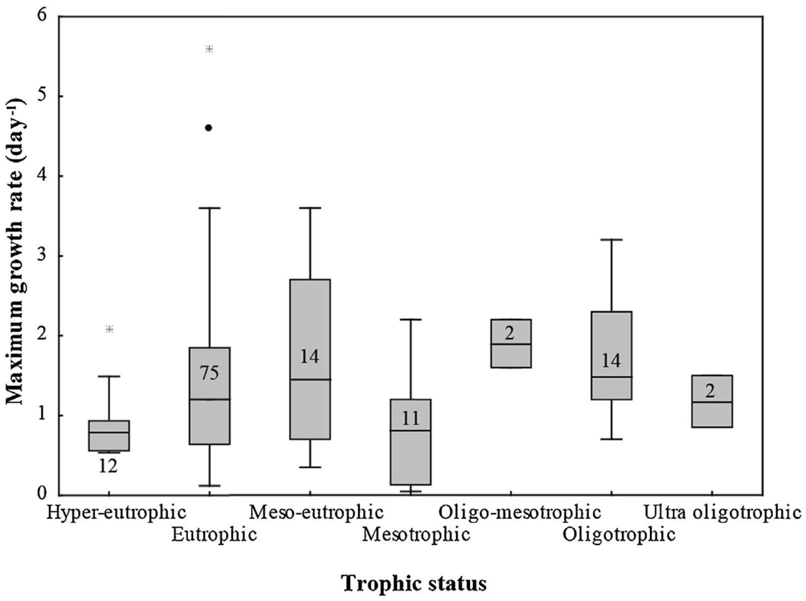

Fig. 6. Maximum growth rates assigned to phytoplankton functional groups against the trophic status of the modelled ecosystems.

rates and trophic states of the systems modelled (Fig. 6). Interestingly, maximum growth rates demonstrated wide variability in meso-eutrophic and eutrophic conditions, whereas the lowest values were assigned in hypereutrophic systems. Diatoms, 1.70 ± 0.79 day^{-1}, are typically assigned higher maximum growth rates relative to cyanobacteria, 0.93 ± 0.71 day^{-1} (Table 1 and Fig. 7), suggesting a general tendency to characterize the former group as *r* strategists, characterized by high growth and metabolic rates that typically exploit less-crowded ecological niches, and the latter one as *K* strategists, displaying traits that render competitive advantage at close to carrying capacity environments with slower growth and metabolic rates (Reynolds, 2006). Generally, the characterization of diatoms was relatively clear with high maximum growth rates and large sinking velocities (-0.81 ± 1.37 m day^{-1}), whereas a fairly wide range of sedimentation rates (0.17 ± 0.86 m day^{-1}) is typically assigned to cyanobacteria, with minimum and maximum values equal to -0.35 and 4.32 m day^{-1}, respectively (Tables 1 and 2). Notably, the rationale of positive settling velocity values is to mimic the buoyancy regulation of many cyanobacteria species that allows them to stay afloat and form surface scums (e.g., *Microcystis* spp), their capacity to control their cell density through carbon assimilation under photosynthetic activity and metabolic carbon loss through respiration, and the active motility of different species of dinoflagellates, cryptophytes, and chrysophytes (Burger et al., 2008; Rigosi et al., 2011; see also following discussion). Drawing parallels between the typical characterizations of diatoms and cyanobacteria in regard to their nutrient kinetics and intracellular storage properties, we can infer that cyanobacteria are assigned higher half saturation constants for phosphorus and lower for nitrogen, higher maximum phosphorus and lower minimum nitrogen cell quotas, whereas the majority of the simulations postulate that the two functional groups posses similar maximum nitrogen and phosphorus uptake rates (Table 3). [It is worth mentioning that the discrepancies between the half saturation constants for *DIN* and NH_4/NO_3 uptake represent the predominance of freshwater and marine algae, respectively.] On a final note, the relationships between maximum growth rate, and nutrient kinetics or sedimentation rates assigned during the *PFG* model calibrations were not statistically significant (Fig. 1 in Supporting Information), counter to popular notions in phytoplankton ecophysiology (Edwards et al., 2012).

3.4. *What are the differences between the characterization of "cyanobacteria-like" state variables relative to other algal functional groups?*

Cyanobacteria blooms in freshwater ecosystems are induced by intensifying agricultural land use and urbanization (Paerl and Huisman, 2008). Climate change has also been hypothesized to be a potential catalyst for more frequent cyanobacteria blooms in the summer (Legnani et al., 2005; Paerl and Huisman, 2008; Jöhnk et al., 2008). For example, the cyanobacteria outbursts during the extreme summer heatwave (locally 5 °C higher than average) of 2003 in Europe have been interpreted as a warning signal for a potentially important causal link between global warming and cyanobacteria dominance (Beniston, 2004; Jöhnk et al., 2008). Cyanobacteria blooms are a major concern for water industries as they represent high risk for human health and economic costs for drinking water treatment. Neuro- and hepatotoxins released by *Cylindrospermopsis*, *Microcystis*, and *Anabaena* can cause paralysis and liver damage (Carmichael, 1994). Thus, one of the outstanding challenges of *PFG* modelling is to offer credible tools that can serve as early warning systems to assist with the operational control of cyanobacteria blooms. Many hypotheses have been proposed to elucidate the ecophysiological traits of cyanobacteria that render competitive capacity and induce structural shifts in algal assemblages, such as higher temperature optima, low TN/TP ratios, buoyancy regulation, low light-energy requirements/higher tolerance to water turbidity, immunity to zooplankton grazing, nitrogen fixation, and superior kinetics for different nitrogen forms (Blomqvist et al., 1994; Dokulil and Teubner, 2000; Watson et al., 2008). Mathematical models have been developed to test these hypotheses and support short-term species-specific cyanobacteria forecasts. In this section, we review some of the mathematical representations proposed to represent key ecophysiological characteristics of N_2-fixers (e.g., *Aphanizomenon flos-aquae*, *Cylindrospermopsis raciborskii*), stratifying species (e.g., *Planktothrix rubescens*) with low-light tolerance and ability for buoyancy regulation, turbulent species (e.g. *Limnothrix redekei*, *Planktothrix agardhii*) that are usually well-mixed in the epilimnion, and colony forming species (e.g., *Microcystis* and *Aphanizomenon*) (Table 4).

Upon nitrogen limitation, several groups of cyanobacteria show the ability to differentiate between oxygenic photosynthesis

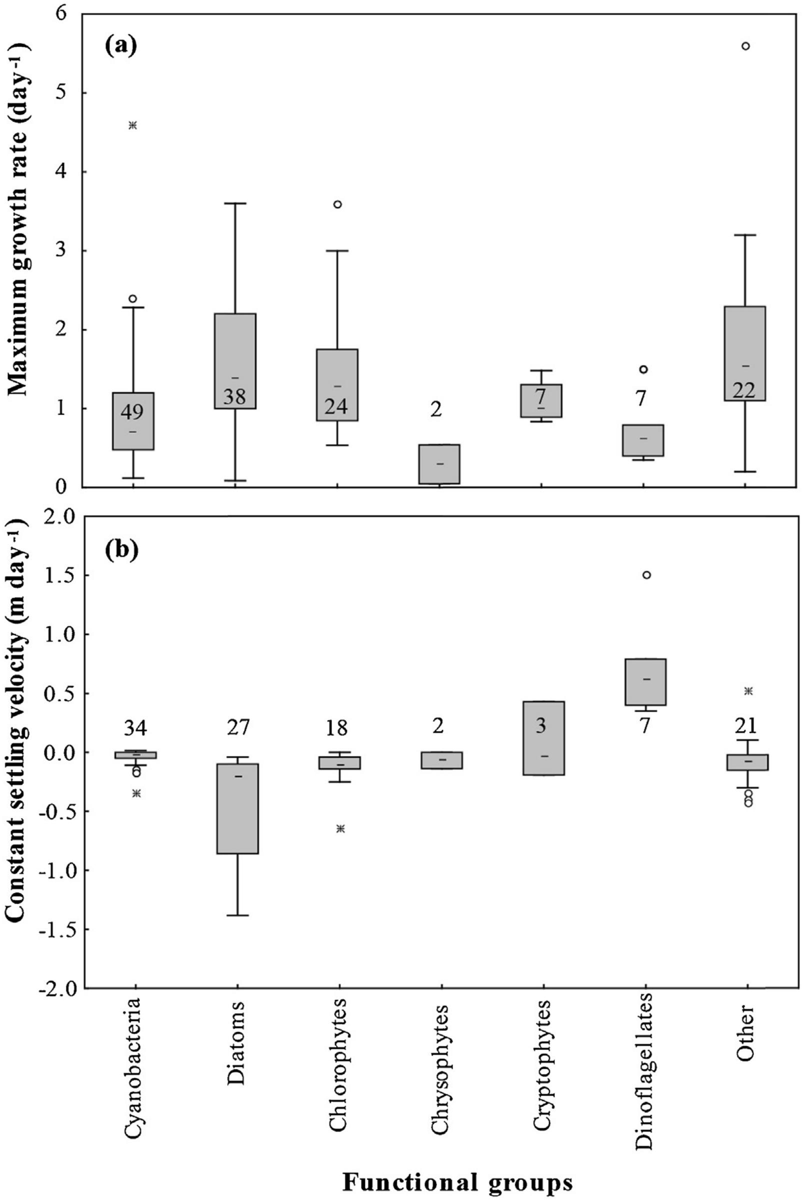

Fig. 7. (a) Maximum growth rate and (b) settling rates assigned to phytoplankton functional groups. Positive and negative values represent buoyant/floating and sinking phytoplankton. The “Other” group comprises cryptophytes, chrysophytes, and dinoflagellates.

Table 2
Settling velocity values (day^{-1}) assigned to phytoplankton functional groups.

Functional groups	Count	Max	Min	Mean ± St.dev.	Dynamic settling model[a]
Cyanobacteria	40	4.32	−0.35	0.17 ± 0.86	13
Diatoms	39	0	−5.81	−0.81 ± 1.37	9
Chlorophytes	19	0	−2.22	−0.27 ± 0.50	2
Chrysophytes	2	0	−0.14	−0.07 ± 0.10	0
Cryptophytes	4	0.43	−0.5	−0.07 ± 0.39	3
Dinoflagellates	9	8.65	−5	−0.15 ± 3.95	6
Other/combined functional groups	36	0.52	−1.5	−0.1 ± 0.29	7

[a] Number of *PFG* studies that presented dynamic settling submodels, i.e., settling velocity varies as a function of light, internal nutrients, cell density, effective colony diameter, and volume fraction of gas vacuoles in cells.

(in vegetative cells) and N_2 fixation (in the non-photosynthetic heterocysts). The latter cells have the ability to protect nitrogenase from inactivation by O_2 through several mechanisms, including high respiration rates and decreased permeability to O_2. Heterocysts do not evolve O_2 and cannot fix CO_2, so they rely on adjacent vegetative cells for a source of carbon. Non-heterocyst-forming cyanobacteria are usually based on temporal separation between N_2 fixation and photosynthetic O_2 production, and they typically fix N_2 in the dark and photosynthesize in the light (Bohme, 1998; Zehr, 2011); although there are exceptions that fix during the day, such as *Trichodesmium* (Staal et al., 2003). As previously mentioned, many aquatic biogeochemical modelling studies postulated that cyanobacteria have superior nitrogen kinetics by simply assigning low *N* half saturation constants and high maximum *N* uptake rates (Zhang and Rao, 2012). Building upon this assumption, there are attempts to accommodate the effects of N_2 fixation by considering a threshold value below which cyanobacteria are no longer *N*-limited; the source of *N* uptake is implicitly assumed to be the atmosphere and thus cyanobacteria do not remove any dissolved inorganic nitrogen from the water column (James et al., 2005). In a similar manner, *CAEDYM* applications consider nitrogen fixation to be maximized when both ambient dissolved inorganic nitrogen and internal nitrogen stores are depleted, while the growth rate and metabolic activity of algal cells is compromised as the rate of nitrogen fixation increases (Gal et al., 2009; Kara et al., 2012). A more detailed description of N_2 fixation explicitly accommodates the role of anoxic limitation, salinity, optimal temperature, and nutrient availability, and was originally formulated by Savchuk and Wulff (1996). With the same approach, the realized N_2 fixation is also determined by the nitrogen fixation capacity, which in turn is regulated by the ambient N:P ratio (Savchuk, 2002; Eilola et al., 2009). Nitrogen fixation can also be simulated in terms of cellular energetics, in that production of nitrogenase and fixation of nitrogen use *ATP* that would otherwise go towards production of chlorophyll or

Table 3
Characterization of phytoplankton functional groups with respect to nutrient kinetics and cell quotas.

	Count	Max	Min	Mean	St.dev.
Maximum P uptake (mg P mg C^{-1} d^{-1})					
Cyanobacteria	14	1.00	0.0010	0.1022	0.2667
Diatoms	12	0.50	0.0025	0.0814	0.1735
Chlorophytes	7	0.50	0.0010	0.0772	0.1865
Cryptomonas, chrysophytes, and dinoflagellates	4	0.01	0.0010	0.0039	0.0042
Other	12	0.05	0.0025	0.0137	0.0132
Maximum N uptake (mg N mg C^{-1} d^{-1})					
Cyanobacteria	10	210	0.0700	49.6	75.5
Diatoms	10	600	0.0025	164.5	221.5
Chlorophytes	5	200	0.0700	108.0	100.3
Cryptomonas, chrysophytes, and dinoflagellates	3	78	0.0448	26.1	45.0
Other	8	150	0.0025	31.3	59.4
Half saturation constant for P uptake (mg P m^{-3})					
Cyanobacteria	44	61.9	0.044	10.6	14.2
Diatoms	41	50.1	0.013	6.81	9.13
Chlorophytes	17	50.1	0.040	8.32	11.9
Cryptomonas, chrysophytes, and dinoflagellates	17	39.9	0.076	9.50	12.4
Other	25	77.3	0.279	14.0	20.3
Half saturation constant for DIN uptake (mg N m^{-3})					
Cyanobacteria	28	400	0.00	52.5	94.4
Diatoms	30	400	0.56	45.9	72.6
Chlorophytes	15	400	10.00	74.4	123.3
Cryptomonas, chrysophytes, and dinoflagellates	14	400	0.14	69.9	103.1
Other	14	100	0.14	32.8	26.8
Half saturation constant for NO_3 uptake (mg N m^{-3})					
Cyanobacteria	7	2.80	0.00	1.79	0.99
Diatoms	11	32.1	2.10	14.39	10.75
Cryptomonas, chrysophytes, and dinoflagellates	6	42.0	4.19	15.80	15.07
Other	16	100	0.70	19.42	31.12
Half saturation constant for NH_4 uptake (mg N m^{-3})					
Cyanobacteria	7	1.4	0.000	0.9	0.5
Diatoms	10	30.5	0.070	15.0	12.8
Cryptomonas, chrysophytes, and dinoflagellates	6	12.6	0.070	4.9	4.9
Other	13	100	0.070	19.8	35.3
Maximum phytoplankton internal P (mg P mg C^{-1})					
Cyanobacteria	14	1.300	0.0011	0.1345	0.3382
Diatoms	11	0.085	0.0021	0.0401	0.0268
Chlorophytes	7	0.042	0.0150	0.0303	0.0099
Cryptomonas, chrysophytes, and dinoflagellates	4	0.019	0.0021	0.0088	0.0078
Other	9	0.059	0.0250	0.0346	0.0128
Minimum phytoplankton internal P (mg P mg C^{-1})					
Cyanobacteria	15	0.016	0.0000	0.0054	0.0044
Diatoms	12	0.021	0.0005	0.0065	0.0057
Chlorophytes	8	0.008	0.0000	0.0039	0.0026
Cryptomonas, chrysophytes, and dinoflagellates	4	0.005	0.0003	0.0026	0.0026
Other	9	0.008	0.0001	0.0059	0.0025
Maximum phytoplankton internal N (mg N mg C^{-1})					
Cyanobacteria	10	0.24	0.0600	0.1505	0.0579
Diatoms	10	0.29	0.1125	0.1810	0.0449
Chlorophytes	5	0.23	0.1000	0.1800	0.0495
Cryptomonas, chrysophytes, and dinoflagellates	4	0.18	0.0700	0.1107	0.0472
Other	5	0.33	0.0900	0.1924	0.0911
Minimum phytoplankton internal N (mg N mg C^{-1})					
Cyanobacteria	12	0.08	0.0012	0.0475	0.0305
Diatoms	11	0.14	0.0249	0.0842	0.0360
Chlorophytes	6	0.08	0.0011	0.0508	0.0328
Cryptomonas, chrysophytes, and dinoflagellates	4	0.09	0.0100	0.0428	0.0324
Other	6	0.09	0.0051	0.0515	0.0315
Half saturation constant for Si uptake (mg Si m^{-3})	36	440	0	65.5	104.2
Half saturation constant for Fe uptake (mg Fe m^{-3})	19	1	0.00028	0.1	0.23

Table 4
Characteristic examples of mathematical representations of cyanobacteria ecophysiology.

Growth model	
• Growth rates based on cell morphology	Elliott et al., 2001, 2000; Reynolds et al., 2001 (PROTEC)
• Growth reduction coefficient under N_2 fixation	Gal et al., 2009; Kara et al., 2012 (CAEDYM)
Nutrient kinetics/nutrient limitation	
• No nitrogen limitation on uptake	Bierman and Dolan, 1981
• Low *N* half saturation constants and high maximum *N* uptake	Zhang and Rao, 2012
• No nitrogen limitation when inorganic nitrogen falls below a threshold value	James et al., 2005
• Dynamic internal nutrient stoichiometry (luxury uptake) with variant maximum and low minimum cell quotas	Gal et al., 2009; Kara et al., 2012 (CAEDYM)
• Size-dependent half saturation constant for nutrients	Gin et al., 1998; Sin and Wetzel, 2002
• N_2 fixation as a function of temperature, light intensity, and ambient N:P ratio.	Eilola et al., 2009; Savchuk and Wulff, 1996; Savchuk, 2002
Light limitation	
• Low half saturation constant for light (*Anabaena* spp.)	Malve et al., 2007
• Low light intensity saturation at maximum production (*Microcystis* spp)	Zhang et al., 2008
• Steele's photoinhibition function for *Planktothrix rubescens* growth: limited below and inhibited above optimum irradiance level	Copetti et al., 2006; Janse and Aldenberg, 1990; Omlin et al., 2001
Temperature limitation	
• High optimum temperature constant for growth	Estrada et al., 2009; Romero et al., 2004
• Asymmetric temperature function with minimum and maximum temperature to describe higher and wider optimal temperature range for cyanobacteria growth	Zhang et al., 2008
• Temperature sensitivity based on algal cell morphology	Elliott et al., 2001, 2000; Reynolds et al., 2001 (PROTEC)
• Sigmoidal temperature response function to reproduce faster cyanobacteria growth at high temperatures	Neumann et al., 2002
• Temperature limitation function on growth with high intercept value, higher temperature multiplier and higher optimum temperature for cyanobacteria	Robson and Hamilton, 2004
Buoyancy regulation	
• Lower settling velocity than other functional groups	Arhonditsis and Brett, 2005; Janse and Aldenberg, 1990; Romero et al., 2004
• Positive or neutral (=0) settling velocity	Burger et al., 2008; Lewis et al., 2004 (CAEDYM)
• Light intensity threshold to determine buoyant movement (positive settling velocity)	Elliott et al., 2001, 2000; Reynolds et al., 2001 (PROTEC)
• Modified Stokes' law for settling: settling velocity as a function of gravitational acceleration, colony diameter, cell density, viscosity of water with cell volume and colony volume ratio.	Guven and Howard, 2006; Islam et al., 2012
• Modified Stokes' law for settling: settling velocity is assumed to be proportional to the volume fraction of gas vacuoles in cells (%), represented by the collapsing of gas vacuole with increased turgor pressure due to increasing photosynthetic activity	Bonnet and Poulin, 2002
• Migration of non-N_2 fixing cyanobacteria is described by a net movement between the maximum migration velocity towards the optimum light and sinking during the restoration of internal nutrient storage	Gal et al., 2009; Kromkamp and Walsby, 1990
Grazing inhibition	
• No grazing: grazing term is deactivated for cyanobacteria	Elliott et al., 2001, 2000; Reynolds et al., 2001 (PROTEC), Allen, 1997; Allen et al., 1998a,b (ERSEM)
• Low grazing: a linear function of biomass with 1% removal of *Trichodesmium* population	Lenes et al., 2008
• Low feeding preference from zooplankton and low food quality for assimilation efficiency	Arhonditsis and Brett, 2005
• Grazing susceptibility is represented by reciprocal of the maximum longest cell diameter	Segura et al., 2013
Iron limitation	
• Michaelis–Menten function for iron limitation on algal growth	Lenes et al., 2012, 2008; Walsh et al., 2001
Salinity limitation	
• Salinity limitation above optimum concentration for freshwater cyanobacteria	Robson and Hamilton, 2004
Life cycle	
• Four life stages (vegetative cells, vegetative cells with heterocysts, akinetes, and recruiting cells) are determined by the stored cell energy and nutrient. Transition of each stage is determined by a set of threshold values that characterize the internal state.	Hense and Beckmann, 2010, 2006
• Change in the biomass of two life stages are described as a function of photosynthesis and respiration. Individual-based model describes the cell division when vegetative cell increase to twice the size of the initial cells and form akinetes	Hellweger et al., 2008 (individual-based model)
• Population dynamic model with two life stages of cyanobacteria, describing pelagic vegetative cell population and akinetes in the sediment. Formation of akinetes and germination are described as a function of light, temperature, and nutrients.	Jöhnk et al., 2011
Toxin production/allelopathic interaction	
• Cyanotoxin production is assumed to be proportional to the cyanobacteria population growth with production and decay terms. Allelopathy of cyanotoxins is represented by an inverse rectangular hyperbola.	Grover et al., 2010, 2012

other pigments, or cellular growth (Robson et al., 2013). In the same context, there are also conceptual advancements that are founded upon dynamical representations of the relationship between nutrient stores and chlorophyll, while explicitly accommodating the physiological status of cells and the effect of packaging of pigments within cells (Baird et al., 2013).

Cyanobacteria can regulate their buoyancy in response to changing environmental conditions based on three proposed mechanisms (Konopka, 1982; Reynolds et al., 1987; Bormans et al., 1999): (i) Collapse of gas vesicles under rising turgor pressure generated partly by photosynthetic production of low molecular weight (and osmotically active) carbohydrates and partly by light-stimulated uptake of potassium ions (Grant and Walsby, 1977; Allison and Walsby, 1981); (ii) kinetic regulation of gas vesicle synthesis (or cell growth relative to gas-vesicle production rates) that induces changes in buoyancy (Kromkamp et al., 1986; Konopka et al., 1987; Reynolds et al., 1987); (iii) accumulation of photosynthetically fixed carbon in the form of glycogen, acting as a “ballast” that adds to the excess cell density (Kromkamp et al., 1988; Reynolds et al., 1987). An equally important factor that regulates the accumulation of photosynthetic products is also their assimilation into proteins and other biopolymers, assuming that the internal nutrient reserves are adequate (Reynolds et al., 1987). In this context, there are four major strategies that have been used in the modelling literature to accommodate the patterns of cyanobacteria settling and vertical migration: constant settling velocity (typically lower relative to the values assigned to other functional groups); migration with or without photoinhibition; and settling velocity based on Stokes' sedimentation kinetics. Vertical migration without photoinhibition, largely based on the original model by Kromkamp and Walsby (1990), effectively postulates a dynamic balance between upward migration to irradiance and downward migration to refuel the intracellular nutrient stock. On the other hand, when the Stokes' formula is used to reproduce algal settling rates, cell density varies dynamically in response to carbohydrate synthesis (photosynthesis) and utilization (respiration) which in turn shapes the vertical velocity (Hipsey et al., 2006). A modification of the latter strategy was presented by Bonnet and Poulin (2002), based on the assumption that gas vacuoles are collapsing when the turgor pressure is increasing by the photosynthetic activity. The density of the cells is related to the volume of the gas vacuoles controlled by the turgor pressure (see their Table 3), and this buoyancy regulation model formed the basis to represent *Microcystis aeruginosa* vertical migration.

Colonial and filamentous cell formations may cause mechanical interference, toxicity and have inadequate biochemical nutritional value for consumers (Müller-Navarra et al., 2000); thus, they are typically parameterized as being an inferior food item for zooplankton growth (Perhar et al., 2012). For example, Arts et al. (1992) showed poor food quality of cyanobacteria may stem from their nutritional inadequacy, as consumers exclusively fed on cyanobacteria exhibited near-starvation traits. Further, freshwater cyanobacteria are reported to have high levels of myristic acid, very low levels of $n-3$ (omega-3) highly unsaturated fatty acids (making them very low quality food) as well as very low $n-3$:$n-6$ ratios (Perhar et al., 2012). A variety of parameterizations have been used to characterize their lower susceptibility (or even immunity) to grazing, including the lower grazing preference/palatability, lower assimilation rates, and inferior food quality (Arhonditsis and Brett, 2005). Moreover, recognizing the knowledge gaps related to the internal factors that could conceivably induce cyanobacteria blooms, Hense and Beckmann (2006) proposed a mathematical model to examine the dynamics of their distinctive life cycle, differentiating among four different stages: vegetative cells, vegetative cells with heterocysts, akinetes, and recruiting cells (including germinates). The model assumes that the transition between each stage is regulated by a set of internal energy and nitrogen quotas that act as threshold values for the cell to possess stage-specific physiological/ecological characteristics. For example, vegetative cells have high internal energy and nitrogen concentration and grow when nitrogen is available. Once nitrogen is depleted (i.e., below a threshold value), vegetative cells develop heterocysts that allow to grow further by nitrogen fixation. The two vegetative cell stages are considered to be in the form of filaments and are positively buoyant. The development of akinetes occurs towards the end of summer, triggered by the decreasing energy supply and reduced cell division rates which in turn is modulated by the internal cell quotas of energy and nitrogen. Thus, these resting spores break off from the filaments and sink down onto the sediments, where they take up nutrients and mature during the winter and most of the spring (Hense and Burchard, 2010). With the Hense and Beckmann (2006) model, cyanobacteria are assumed to inhibit zooplankton grazing due to their toxic characteristics, and therefore their mortality is expressed as a linear term. Along the same line of thought, Jöhnk et al. (2011) used a mathematical model to simulate the life cycle of *C. raciborskii* (*Nostocales*), thereby predicting their future development under varying environmental conditions. In coastal systems, salinity can also be an important factor regulating the production and germination of akinetes (Huber, 1985).

Other process-based submodels developed for the distinctive characteristics of cyanobacteria, include toxin production and allelopathic interactions with higher trophic organisms and/or other competing algal functional groups. The physiology and function of toxin production is still very poorly understood, as there are multiple competing theories that pose challenges in the development of reliable predictive tools (Vanderploeg et al., 2001). For example, several studies showed a positive relationship between nitrogen concentration and toxin-producing *Microcystis* strains or microcystin production (Murphy et al., 2003). In particular, urea is hypothesized to be an energetically favourable form of nitrogen and therefore a predominant stimulant of *Microcystis* blooms (Finlay et al., 2010). Others suggested that *TP* concentrations can explain most of the microcystin variability in embayments, rivers, creeks, ponds, nearshore and offshore sites in the Great Lakes, while other potentially reliable predictors include the concentration of micronutrients, *UV* radiation stress, chlorophyll *a* and Secchi disc depth (Makarewicz et al., 2009). In this regard, Grover et al. (2010) developed a model that considers cyanotoxin production during the blooms of the harmful alga *Prymnesium parvum*, which in turn inhibits the growth of other phytoplankton groups. Cyanotoxin concentrations were assumed to be proportional to the product of population density with the growth rate, while the allelopathic effects were introduced through an inhibition term that reduces the growth rates of the rest of the algal functional groups by 50%. In a subsequent model, Grover et al. (2012) added a population of small-bodied zooplankton, with their grazing rate on *P. parvum* similarly inhibited by the excreted dissolved toxins. The fundamental concepts of the model may have broader applicability to predict dynamics of other toxin-producing algal groups and to examine the importance of allelopathy and inhibition of zooplankton grazing in triggering major structural shifts in phytoplankton assemblages. Generally, a review of the pertinent modelling literature offers a number of interesting propositions on how mathematics can accommodate our ever-growing understanding of cyanobacteria ecophysiology. The questions arising though is are we ready to support reliable forecasts of harmful algal blooms or even to pinpoint what is missing in order to effectively support environmental management?

4. Concluding remarks and future perspectives

The documented challenges with mathematical modelling when addressing societally/scientifically important issues, such as drinking water, fisheries, and water use for recreational purposes, is often attributed to the fact that the field has advanced without the healthy dose of criticism required to obtain good science; partly because the "impenetrable" nature of mathematics has prohibited sober views from the modelling community, which in turn "has allowed modellers to carry their trade far beyond the limits of reality" (Pilkey and Pilkey-Jarvis, 2007). Indeed, the present analysis provided ample evidence that our capacity to reproduce the observed aggregated and compositional phytoplankton variability is limited, despite the plethora of mathematical expressions aiming to describe different ecophysiological facets of species populations. A significant portion of *PFG* modelling efforts published in the peer-reviewed literature reported model fit that was inferior relative to what we can achieve by merely using the average value of the corresponding calibration datasets!

Reviewing the recent literature, one can find several interesting recommendations in regard to the future of phytoplankton functional group modelling. For example, the series of "Horizons" articles hosted in the Journal of Plankton Research has offered many fresh ideas and pointers for progress (Anderson, 2005; Flynn, 2006; Le Quere, 2006). Challenging the trustworthiness of many models for addressing vexing aspects of water quality stewardship, one of the interesting propositions of this debate was to open the dialogue between biologists and modellers. According to Flynn (2005), the problem is that the latter group is not always supported by sound conceptual understanding, commonality in units, complete mass balance, and adequate empirical knowledge on the patterns of sentinel plankton organisms under environmentally relevant conditions. The same author further asserted that "*. . .we need data, and lots of them. But we do not need them just for the growth of individual organisms; vitally we also need data for combinations of organisms. What is becoming increasingly clear is that there are a whole host of interactions between members of the plankton that the vast majority of models do not even hint at. . .*" (Flynn, 2006). On the other hand, biologists claim that they do not get sufficient guidance on how data collection and experimentation could be optimized, while the profound oversimplifications of the current generation of ecological models do not allow rectifying the disconnect between empiricists and theoreticians (Flynn, 2005, 2006). Many of these assertions can be easily verified by anyone who is familiar with the *PFG* modelling literature.

From a technical standpoint, our analysis presented some encouraging trends relative to earlier critiques of the methodological practices typically followed in the field of aquatic biogeochemical modelling (Arhonditsis and Brett, 2004). Although far from "ideal", there is an increasing portion of the reviewed papers that does perform sensitivity analysis, quantify model performance, and (most importantly) attempt to present some type of structural and/or predictive confirmation. Of particular note is the fact that one third of studies that provided model performance measures did not evaluate the fidelity of algal functional group simulations. While a plausible explanation could be the aforementioned lack of suitable phytoplankton composition data, we also found that there were instances in which phytoplankton functional groups were added as state variables, even though they were not the actual focus of the study. Whatever the reason may be, this absence of data constraints on the *PFG* characterization is problematic and may reflect an ill-practice of treating the corresponding *PFG* parameters as "properties of convenience" that facilitate the fitting of models to observed data (Poulin and Franks, 2010). In fact, there are many examples in which the same phytoplankton functional group within the same system has been parameterized with very different properties, depending on the model considered (Kim et al., 2014). In this regard, our stance echoes skeptical views in the literature that raise concerns about the increasing model complexity and advice to seek parsimony rather than simplicity. We believe that the gradual incorporation of complexity, where possible and relevant, is the most prudent strategy and any such model development should be accompanied by rigorous assessment of the underlying uncertainty (Arhonditsis et al., 2007). Of equal importance is the establishment of a systematic methodological protocol specifically designed for *PFG* models along with performance criteria widely accepted by the modelling community. Even if the journals cannot enforce the submission of all the material required to reconstruct the mathematical models (Flynn, 2005), they can still demand the submitted modelling studies to meet certain criteria and ensure that the inclusion of state variables related to compositional variability is not used to provide additional degrees of freedom to fit aggregated phytoplankton variables (e.g., total chlorophyll *a* or algal biovolume).

On a final note, we could not agree more with Anderson's (2005) recommendation to integrate empirical *PFG* representations with process-based modelling. One such case could be the linkage of phytoplankton physiological processes with specific morphological features (i.e., cell volume, surface-to-volume ratio, shape). Founded upon concepts of allometric theory, the size and shape of organisms strongly influences their physiological rates and may shape their responses to external perturbations, the interspecific competition, and ultimately the composition of algal assemblages (Cyr and Pace, 1993). While far from being a flawless representation of the real world (Flynn, 2005), there are several important conceptual and technical reasons to consider the allometric scaling for the parameterization of plankton ecosystem model (Elliott et al., 2000; Sin and Wetzel, 2002; Kerimoglu et al., 2012; Wirtz, 2013). This strategy can effectively delineate model parametric uncertainty; namely, the literature-based ranges typically assigned to the calibration parameters are now replaced by the parameter standard error values and/or estimates of the residual variability of allometric equations (Shimoda et al., 2015). Considering the growing model complexity, this practice may be an excellent solution to the identifiability problem of complex over-parameterized model and may offer a reliable strategy to support model-based aquatic ecosystem management. The allometric scaling offers a different perspective towards the optimization of future data collection efforts. Model calibration is not solely perceived as a typical inverse solution exercise, constantly inviting the collection of data on model outputs and subsequently readjusting the parameters to obtain the best possible agreement between measurements and predictions. Rather, the effective model parameterization requires a more focused experimentation that revolves around the development (or further refinement) of the allometric characterization of model parameters (Shimoda et al., 2015). Moreover, depending on the nature of the dataset used (e.g., marine versus freshwater algae), the proposed strategy allows the potential users to identify the model domain in a straightforward way and determine to what extent a particular construct has site-specific or broader applicability. While Occam's razor is (and should be) the cornerstone of any modelling activity, we believe that the integration of process-based models and empirical parameter specification offers an appealing prospect from both methodological and ecophysiological point of view.

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Appendix A. Supplementary data

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PHYTOPLANKTON FUNCTIONAL TYPE MODELLING: RUNNING BEFORE WE CAN WALK? A CRITICAL EVALUATION OF THE CURRENT STATE OF KNOWLEDGE

SUPPORTING INFORMATION

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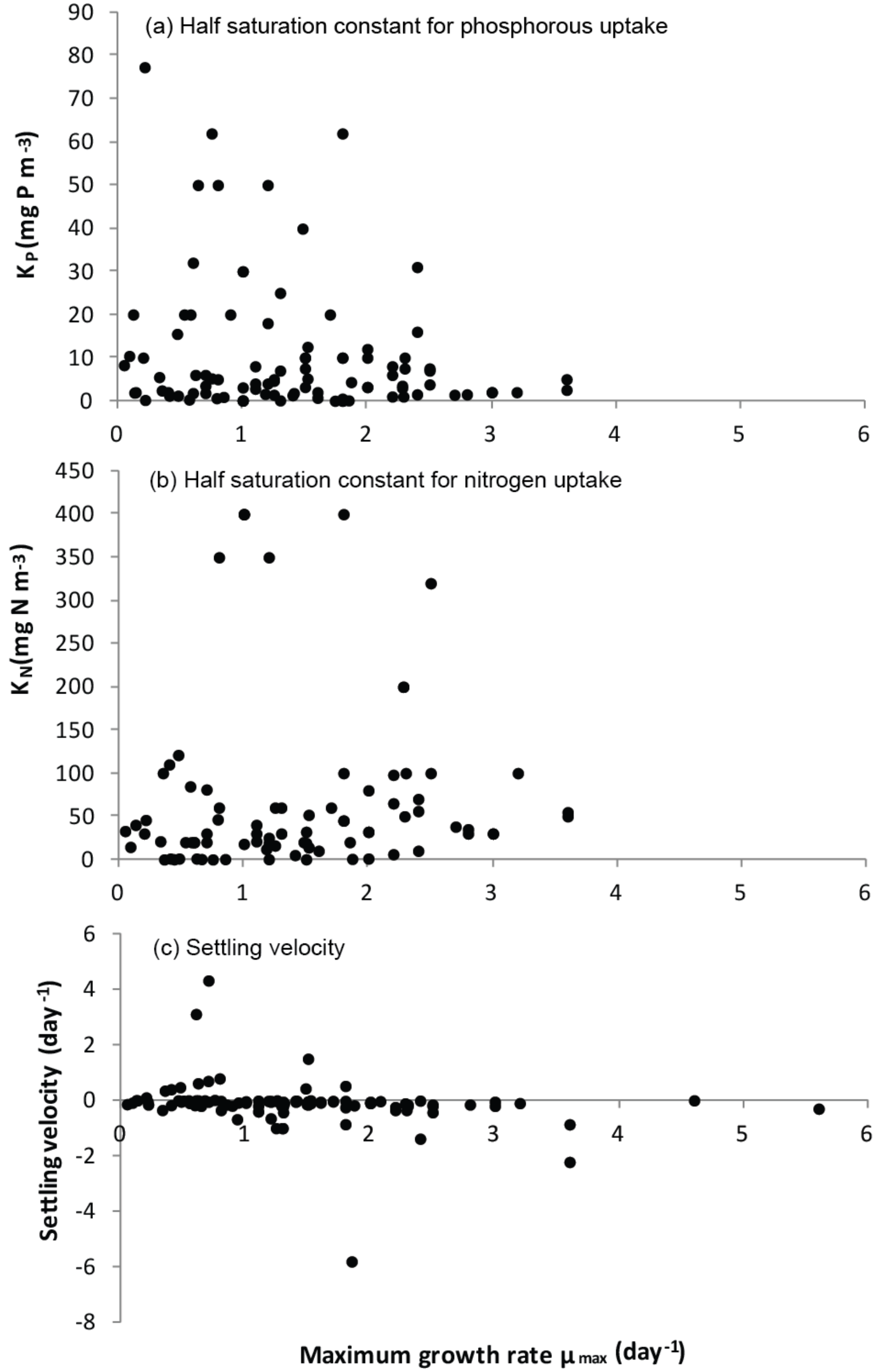

Figure 1: Relationships among parameters used for the characterization of phytoplankton functional groups: (*a*) maximum growth rate against half saturation constant for *P* uptake; (*b*) maximum growth rate against half saturation constant for *N* uptake; and (*c*) maximum growth rate against settling velocity.

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