Modelling phytoplankton, passengers and drivers of lake ecosystems

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The idea for my title stems from an essay on biodiversity by Walker (1992), who painted the picture of ‘passengers’ and ‘drivers’ of an ecosystem to illustrate that not all species have the same importance for ecosystem functioning.

“Ecologically, all species are not created equal. At one extreme, some are determinants, or ‘drivers,’ of the ecosystem of which they form a part. At the other extreme are those that are ‘passengers.’ Removing the former causes a cascade effect, but loss of the passengers leads to little change in the rest of the ecosystem.”

(Walker, 1992)

I adopted his illustration of the passengers and drivers and translated it to the role that phytoplankton plays in an ecosystem. Phytoplankton is driven by several factors, for example hydrodynamics, nutrient gradients and grazing pressure. On the other hand, it can drive the aquatic ecosystem by the provision of biomass to upper trophic levels or by changing light and nutrient gradients in the system.
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List of Abbreviations

**BELAMO**  Biogeochemical and Ecological LAke MOdel

**CAEDYM**  Computational Aquatic Ecosystem DYnamics Model

**doy**  day of year

**DYRESM**  DYnamic REservoir Simulation Model

**DYCD**  DYRESM-CAEDYM

**ENSO**  El Niño Southern Oscillation

**GCM**  General Circulation Model

**KDE**  Kernel Density Estimate

**NAO**  North Atlantic Oscillation

**PDO**  Pacific Decadal Oscillation

**PROTECH**  Phytoplankton RespOnses To Environmental CHange

**PSB**  phytoplankton spring bloom

**RCM**  Regional Climate Model

**SALMO**  Simulation of an Analytical Lake MOdel

**SML**  surface mixed layer depth

**VAR**  Vector-Autoregressive

**VG**  Vector-Autoregressive Weather Generator
General introduction

Freshwater lakes are important ecosystems worldwide and essential for humankind. Lakes supply humans with resources, e.g. drinking as well as irrigation water or nutrition through fishing. Beyond that, standing water bodies serve as recreational sites, they are used for energy generation and flood protection and they are important regulators for regional hydrology. Through the connection to their catchment and the open boundary to the atmosphere, lakes are exposed to frequent changes. These last over both long and shorter periods of time, from centuries (e.g. long-term climate change Smol & Cumming, 2000), to decades (e.g. eutrophication and re-oligotrophication, Jochimsen et al., 2013), to only a few days (e.g. storm events, Rinke et al., 2009b) or even hours (e.g. irradiance fluctuations, Marra & Heinemann, 1982).

To fully grasp the complexity of lake ecosystems and their dynamic response to these ongoing changes, a good mechanistic understanding is required. Mathematical models help to seize this complexity and to develop and test different hypotheses. By calculating scenarios with structurally different models (Refsgaard et al., 2006), different boundary conditions (Moenickes et al., 2012) or by keeping confounding factors constant, ecological models add to the analysis of long-term data and the understanding of ecosystems. In so-called ‘what-if’ scenarios (Hazeleger et al., 2015), forcing factors are changed and effects on lake system variables are analysed. For example, a model could be run multiple times with a fixed nutrient load, but with different mean air temperatures, in order to determine the impact on phytoplankton succession. Models thus also support lake management. In this respect, the Vollenweider model is one of the most prominent examples, relating chlorophyll concentrations to phosphorus load (Vollenweider, 1968). However, this empirical model is an example of static models, which are narrow in their application. To fully describe the dynamic physical and biogeochemical environment, dynamic process-based models are required (Robson, 2014b). In this field, two of the most recognised aquatic ecosystem models are DYRESM-CAEDYM (DYnamic REservoir Simulation Model–Computational Aquatic Ecosystem DYnamics Model, e.g. Romero et al., 2004; Bruce et al., 2006; Rinke et al., 2010) and PROTECH (Phytoplankton RespOnses To
Environmental Change, e.g. Reynolds & Irish, 1997; Elliott et al., 2010; Pätynen et al., 2014). While the former has a strong focus on the interaction between hydrodynamics and biological processes, the latter emphasises phytoplankton traits and community composition.

The adequate simulation of phytoplankton succession in lakes is one of the main issues in aquatic ecosystem modelling (Rigosi et al., 2010). This is due to the fact that phytoplankton has a key function in lake ecosystems as it is the trophic cornerstone of the pelagic food web. It provides biomass towards higher trophic levels like zooplankton and fish, and overall primary production in a given system reflects the water body’s trophic state. On a global scale, phytoplankton provides only about 1% of the total plant biomass, and yet phytoplankton accounts for 45% of global primary production (Falkowski et al., 2004). However, mass developments of algae in nutrient polluted systems are a major cause of water quality problems, especially with regard to harmful algal blooms (Heisler et al., 2008). Phytoplankton dynamics have consequently been intensively studied by aquatic ecologists over decades. Limnologists have been puzzled by the diversity in phytoplankton communities. This unexpectedly high diversity in apparently uniform water bodies has led Hutchinson (1961) to formulate the ‘paradox of the plankton’. He discusses the question as to how a large number of phytoplankton species can coexist in a system with relatively few nutrients without outcompeting each other. Although several answers have been found to Hutchinson’s question, the causes of the observed phytoplankton diversity are still under debate (Scheffer & van Nes, 2006; Clark, 2009). In order to grasp the dynamics leading to the observed phytoplankton diversity, modern approaches to phytoplankton community dynamics seek to substitute taxonomic diversity by functional diversity and trait-based approaches (Reynolds et al., 2002; Litchman & Klausmeier, 2008; Mieleitner et al., 2008; Pomati et al., 2013).

The functional diversity of the phytoplankton community, which acts on phytoplankton dynamics through competitive pressure (Tilman et al., 1982) or food quality (Elser & Urabe, 1999), functions as an internal factor of lake ecosystem dynamics. Internal factors emerge within the ecosystem. They also encompass food web complexity (e.g. regulating top-down versus bottom-up control, Kerimoglu et al., 2012b) or sediment-water interactions (e.g. internal loading, Nürnberg, 1984). External factors, on the other hand, impact on the lake ecosystem ‘from outside’. They include small-scale events like meteorological episodes (e.g. upwelling of nutrient-rich hypolimnetic water through strong wind events, Bocaniov et al., 2014), but also large-scale processes like changes in nutrient load from the catchment (causing a different trophy in the lake, Schindler, 1974; Jeppesen et al., 2005) or climate variability and climate change (Shimoda et al., 2011).

The latter two examples are particularly relevant to aquatic ecosystems, as they are both heavily influenced by anthropogenic activity. Nutrient load and consequent implications for lakes constituted the main area of limnological research from the early 20th century (for a review, see Hutchinson, 1973). In the second half of the 20th century, cultural eutrophication had led to large water quality problems, characterised by massive phytoplankton production and deep water anoxia. While many lakes in the developed world returned to their natural state (Anderson et al., 2005), the role of nutrients in lake ecosystems still remains a subject
of scientific debate (Lewis & Wurtsbaugh, 2008; Kolzau et al., 2014).

More recently, that is over the last decades, global climate change has been recognised as a potential threat to water quality and the functioning of lake ecosystems (see e.g. Goldman et al., 2013). By now, many studies have explored the effects of a warmer climate on aquatic ecosystems through experiments (e.g. Berger et al., 2007; Sommer & Lengfellner, 2008), field studies (e.g. Straile et al., 2010), data analyses (e.g. Livingstone, 2003; North et al., 2014), and modelling studies (e.g. Elliott, 2012a; Eder, 2013; Schlabing et al., 2014). Most lakes show increasing water temperatures (Adrian et al., 2009), with a more intense epilimnetic compared to hypolimnetic warming (Livingstone, 2003). The consequence is a stronger thermal stability and a more durable stratification (Shimoda et al., 2011). This may lead to a more frequent and longer occurrence of anoxia in lakes (North et al., 2014), a change in plankton phenology (Winder & Schindler, 2004b) and potential mismatch between different trophic levels (Winder & Schindler, 2004a). One of the main concerns is that toxic cyanobacteria are expected to benefit from increasing temperatures (Jöhnk et al., 2008; Elliott, 2012a), thus contributing to water quality deterioration.

Most climate research has focused on changes in average temperature (e.g. Straile et al., 2010; Elliott, 2012b) or large-scale synoptic indices like the North Atlantic Oscillation (NAO, e.g. Weyhenmeyer et al., 1999; Straile, 2000). Some modelling studies have analysed effects of other meteorological variables than air temperature. However, this has mostly been carried out using a simple sensitivity design, decreasing and increasing meteorological variables (e.g. Austin & Allen, 2011; Bueche & Vetter, 2014; Hadley et al., 2014). The apparent lack of studies focusing on the local effects of weather situations is surprising, since 20 years have passed since a group of limnologists called for a closer analysis of the effects of local meteorology on lake ecosystems. Only a few studies have emerged on this issue (e.g. George et al., 1998). There may be various reasons for the lack of detailed studies on regional meteorological effects and meteorological variability on lake ecosystems. The seminal paper by Livingstone (2008) calls for a new paradigm in limnophysics. He argues that lakes should not be regarded as individual systems that have a unique response to local weather conditions. Rather, they should be recognised as regional coherent systems since physical processes are predominantly driven by large-scale climatic forcing. Local meteorology is then merely the noise blurring this signal. Overall, there has been a trend for generalisation in climate impact studies, leading to a focus on the effect of large-scale synoptic indices like North Atlantic Oscillation (NAO), El Niño Southern Oscillation (ENSO) and Pacific Decadal Oscillation (PDO) (Stenseth et al., 2002). While all these studies provide insight into general patterns of climate effects, summarizing indices like NAO do not necessarily advance our mechanistic understanding of how meteorological variables affect lake ecosystems. Moreover, the role of extreme events for ecosystems has been recognised (Katz & Brown, 1992), necessitating a different approach to climate change studies (Jentsch et al., 2007) including intra- and interannual meteorological variability and the explicit inclusion of rare events.

The numerous model applications on climate impact demonstrate that forcing through external factors like meteorological variables is well incorporated into aquatic ecosystem mod-
els. In contrast, internal factors like community composition pose a challenge to complex ecological models. In the case of phytoplankton, Reynolds (2006) has estimated the number of different species of freshwater phytoplankton to be around 4,000. Falkowski et al. (2004) numbered about 25,000 different morphological forms of phytoplankton on Earth. Whatever the exact number, it is clear that mechanistic models cannot reproduce the species richness observed in lakes. However, to a certain degree it is necessary to cover biodiversity in lakes, as biodiversity influences ecosystem dynamics, e.g. with respect to resource usage efficiency or ecosystem stability (Cardinale et al., 2012).

Historically, biodiversity has often been quantified through species richness (Gotelli & Colwell, 2001). However, functional richness was more recently found to be more meaningful in the context of biodiversity and its importance to ecosystems (Hillebrand & Matthiessen, 2009). Functional richness arises from trait diversity, which for phytoplankton communities is defined e.g. by cell sizes and shapes, pigment composition, N₂-fixation capability, etc. (Pomati et al., 2013). This approach has been adopted by modellers, who have reduced species complexity by formulating different functional groups (König-Rinke, 2008; Mieleitner & Reichert, 2008; Rinke et al., 2009a) or by aggregating species information via a description of their traits (Wirtz & Eckhardt, 1996; Smith et al., 2014). PROTECH is an example of the latter, as from its inception it was built based on phytoplankton traits (Reynolds et al., 2001). In the model, different species or ‘trait groups’ are described through morphological and physiological traits.

In the previous paragraphs, internal and external factors of lake ecosystem dynamics are discussed as separate entities. However, depending on the combination of factors and the state of the system, either factor can influence the impact of the other. For example, light absorption by phytoplankton was found to change the thermal structure of deep lakes, with the extent of change being dependent on the trophic state of the system (Rinke et al., 2010). Thus, through its position within the aquatic food web and by being a major determinant of water quality, phytoplankton takes on a key function in lake ecosystems. Quantifying phytoplankton dynamics accordingly is crucial to grasping the complexity of lake ecosystems and to assessing the response of lake ecosystems to the variety of changes to which they are exposed.

### 1.1 Motivation

In this thesis, two complex lake models are applied to test ecological theory embedded in an ecosystematic view. A major focus is placed on the impact of climate change and meteorological variability on lake ecosystems. Future global change *per se* implies the use of models, as it requires an understanding of states that have not yet been experienced but are expected to occur under future conditions. Climate is an abstraction of local meteorology (for a definition of ‘climate’, see e.g. IPCC, 2013) and a change in climate and especially climate variability comes into play via changing meteorological conditions. A sound assessment of climate impacts on lake ecosystems therefore requires a mechanistic and quantitative under-
standing of the modes of action of the different meteorological drivers on these ecosystems. The change in climate variability, as predicted by the IPCC (2013), as well as the effect of meteorological extremes on lake ecosystems, have rarely been studied in a mechanistic way. Not many studies have analysed the effects of weather on lakes and the relative importance of different meteorological variables. In the first part of my thesis, I address this topic by coupling a process-based lake model with a statistical weather generator. I focus on the effects of a warmer climate as well as changed meteorological variability on lake ecosystems and especially on phytoplankton phenology. I analyse the dependence of phytoplankton spring bloom timing on meteorological conditions. This thesis aims to ascertain the relative importance of different meteorological variables for timing of cardinal events (i.e. stratification onset and phytoplankton spring bloom onset), and to identify the relevant time scales on which the variables have their impact.

In the second part of my thesis, I concentrate on phytoplankton traits and their interaction with the environment. As lakes are subjected to dynamic forcing (e.g. nutrient load or climate), the habitat for phytoplankton is not at steady-state but permanently changing. Phytoplankton shows a large variability in forms and thus possesses many different traits, which are beneficial only under certain conditions. Community composition changes as a result of these differences (Pomati et al., 2013). This presents a problem to phytoplankton modelling. Depending on the state of the system, different phytoplankton traits become important. If species or functional group composition is to be analysed with models, the importance of different traits must be reflected adequately. Furthermore, the ability of the model to capture variation in phytoplankton composition and function must be clarified in order to correctly describe changes in the lake ecosystem. My thesis therefore addresses the question as to how trait composition varies under different lake morphometries, climates and environmental scenarios and how this affects phytoplankton succession.

This question directs the focus from the lake ecosystem towards the phytoplankton community. Another aspect of phytoplankton modelling is introduced when considering how phytoplankton traits themselves affect their environment and thus the lake ecosystem. Previous studies have indicated that internal nutrient storage in phytoplankton cells may change the vertical distribution of resources (Benndorf, 1968). The amount of internally stored nutrients depends on the nutrient uptake and storage capability of cells and eventually on the trait composition of phytoplankton communities. Trait diversity thus will not only affect the temporal aspect of phytoplankton dynamics (i.e. phytoplankton succession); it also has the potential to act in the vertical and thus on the spatial dimension of lake ecosystems. Furthermore, trait diversity is influenced by both climate and nutrients (Elliott et al., 2006), indicating the interactive effect between external (nutrient and climate) and internal (community composition) factors. I was therefore especially interested in the feedback of phytoplankton dynamics on nutrient circulation within deep lakes and the potential of internal factors to shape the system. Accordingly, my study investigates how the traits of nutrient uptake and cellular storage capability change the nutrient distribution within deep lakes and whether they affect the whole lake ecosystem.
1.2 Dissertation outline

Chapter 2: Scientific background

This chapter will give a brief introduction to the scientific background relevant for the following chapters. The topics covered are phytoplankton ecology, nutrient cycling in lakes, the influence of climate change on lakes and hydrodynamic-ecological simulation of lakes.

Chapter 3: Use of a weather generator for simulating climate change effects on ecosystems: A case study on Lake Constance

The focus of this chapter is on the introduction and application of a new vector-autoregressive moving average weather generator (VG). The weather generator allows us to produce synthetic meteorological time series based on long-term meteorological observations from the past. During the generation process, disturbances can be added, e.g. an increase in mean air temperature. The time series of a changed climate can thus be generated and used as forcing for a lake model. Here, I tested the sensitivity of a large, monomictic lake to changes in mean air temperature, as well as changes in variability and a combination of both.

Chapter 4: Meteorological control of lake ecosystems: The (un)importance of air temperature

This chapter questions the strong bias of many climate impact studies towards changes in air temperature. The weather generator VG was used to produce multiple time series of the current climate. Results of the lake simulations were analysed to gain insight into which meteorological patterns cause stratification and phytoplankton spring bloom onset. The relative importance of different meteorological variables was assessed. The study further addresses the question of the time scales on which meteorological variables have their impact on the cardinal dates stratification onset and bloom onset.

Chapter 5: Predictive utility of trait-separated phytoplankton groups: A robust approach to modeling population dynamics

Unlike the other chapters, this chapter applies the ecological lake model PROTECH (Phytoplankton RespOnses To Environmental CHange). Phytoplankton succession is quantitatively described based on morphological and physiological traits. In a very generalised approach, the model was run for hypothetical lakes with different depths and located in different climates. Phytoplankton succession was analysed based on the sensitivity of traits in response to a range of environmental settings.
Chapter 6: Algal internal nutrient stores feedback on vertical phosphorus distribution in large lakes

This chapter compares two structurally different methods for the quantification of nutrient-dependent phytoplankton growth: The static P model prescribed a fixed cell stoichiometry, while the dynamic P model allowed for a flexible cell stoichiometry and thus enabled luxury uptake. The chapter evaluates how luxury uptake and internal nutrient storage affect phytoplankton dynamics and the spatial distribution of phosphate within lakes.

Chapter 7: General discussion

The final chapter summarises the results and discusses their implications, with an outlook for further research ideas.
Scientific background

2.1 Phytoplankton ecology

Phytoplankton is one of the simpler forms of life on earth and yet thousands of different species exist in marine and inland waters (Reynolds, 2006) with a diverse range of morphological and functional traits. Phytoplankton by definition is photoautotrophic. As a primary producer of carbon it is therefore located at the base of the lake food web and serves other trophic levels by the allocation of energy. This position assigns phytoplankton a key role in the food web and changes in phytoplankton phenology and composition will affect the whole lake ecosystem.

In the 1980s the plankton ecology group (PEG) model was developed (Sommer et al., 1986), a conceptual model describing the seasonal development of phyto- and zooplankton in both eutrophic and oligotrophic lakes in the temperate zone. Nowadays, many studies refer to the PEG model and it is an inherent aspect of limnological textbooks (e.g. Lampert & Sommer, 1999; Wetzel, 2001). Several papers have corroborated the single phases described in the model. In late winter/early spring, abiotic forcing prevails and phytoplankton growth is limited by light availability (e.g. Sverdrup, 1953; Talling, 1971). When the lake begins to stratify, a phytoplankton bloom develops (Huisman et al., 1999), mainly composed of light-tolerant fast-growing species (Reynolds et al., 2002). This intense growth brings about the depletion of nutrients, especially phosphorus. Additionally, grazing pressure by zooplankton increases (Tirok & Gaedke, 2007b). Both factors lead to a breakdown of the phytoplankton bloom (‘clear-water phase’, e.g. Winder & Schindler, 2004b). Subsequently, algae develop with a greater resistance to grazing pressure and a higher ability to compete for nutrients (Anneville et al., 2002). With the beginning of autumnal turnover, light becomes the limiting factor again and hampers phytoplankton growth. The PEG model concept was later refined and extended to other climatic zones (Sommer et al., 2012).

Phytoplankton has been classified in various ways (Anneville et al., 2002; Reynolds et al., 2002; König-Rinke, 2008; Mieleitner et al., 2008). Obvious classification criteria include size classes (femto-, pico- and nanoplanckton, see Sieburth et al., 1978) or taxonomy (families and
species, Reynolds, 2006). These classifications, however, are not very useful when studying the function of phytoplankton. The former is too unilateral, while the latter is too detailed and presents the problem of overdispersion (Kruk et al., 2010). Overdispersion means that phylogenetic close species occupy very different niches (Webb et al., 2002). This is why attempts have been made to describe phytoplankton based on characteristics determining their function and position in the aquatic ecosystem. Two alternative approaches divide phytoplankton into functional groups (Reynolds et al., 2002; Mieleitner et al., 2008) or describe a community based on its trait composition (Litchman & Klausmeier, 2008). Litchman & Klausmeier (2008) offers an instructive overview of phytoplankton traits by dividing the latter into different types and their various levels of importance for different ecological functions (see their Fig.1). Functional group and trait-based phytoplankton classifications are very useful for aquatic modellers. They allow the modeller to reduce the number of simulated groups to relatively few while at the same time keeping the model flexible enough to react to changing conditions within the lake. The different classification approaches are mirrored in the diverse range of phytoplankton models (Mooij et al., 2010; Rigosi et al., 2010).

2.2 Nutrient gradients and nutrient cycling

Although co-limitation with other nutrients exists (Sterner, 2008), primary production in most temperate lakes is mainly phosphorus limited (Wetzel, 2001). The deeper the lake, the more light becomes the limiting factor over longer periods of the year (Talling, 1971). Light levels and nutrient concentration are inverse to each other over depth. Close to the surface, where light is sufficiently available, phytoplankton growth leads to a strong depletion of nutrients. With increasing depth, light is attenuated, so that below a critical depth no positive net growth of phytoplankton populations is possible (Sverdrup, 1953). Thus, with larger depth, fewer nutrients are consumed to fuel growth. At the same time, nutrients resuspend from sediments, leading to higher concentrations close to the sediment surface. This results in nutrient gradients with higher concentrations at large depth and decreasing concentrations towards the water surface, which strongly influences phytoplankton dynamics. During the stratified period, nutrients in the epilimnion will only be replenished through excretion, recycling through the microbial loop, upwelling events or via input from the inflows. Due to the gradients in light and nutrients, the depth of the mixed layer and thus physical forcing becomes a crucial factor for phytoplankton (Diehl, 2002).

Phytoplankton is important as a source of energy, which is often described in ‘the currency’ of carbon (Reynolds, 1998). Nevertheless, the quality of phytoplankton as a food source has been increasingly recognised as being an important factor for nutrient turnover and zooplankton feeding (Lehman & Naumoski, 1985). Simplified, the stoichiometry of cells is used to express nutrient quality. For example, cells with a low C:P ratio are more valuable for zooplankton as fewer cells are needed to fulfil the zooplankton’s phosphorus requirement (DeMott et al., 1998). The basic concept of ecological stoichiometry is described in Sterner & Elser (2002).
2.3 Climate change

Since just over a century ago (1880 - 2012), the average global land and ocean surface temperature has increased by 0.85 °C (IPCC, 2013). This increase in global average temperature is attributed mainly to the ‘climate gases’ carbon-dioxide, methane and nitrous oxide. With the beginning of industrialisation, global CO$_2$ concentration has increased from 279 ppm in 1750 to some 391 ppm in 2011 (Stocker et al., 2013). This CO$_2$ concentration increase has the largest share of the radiative forcing with a value of about 1.82 W m$^{-2}$ during the industrial era (1750-2011, Stocker et al., 2013).

Global climate change has been traced in many lakes worldwide (Williamson et al., 2009; George, 2010; Goldman et al., 2013). One study has shown changes in observed water temperatures in lakes across the globe between -0.005 °C yr$^{-1}$ and 0.157 °C yr$^{-1}$ (Adrian et al., 2009). Ice cover break-up has occurred around 6 days earlier every 100 years (Magnuson et al., 2000) and main phenological events have shifted to earlier dates in the year (Winder & Schindler, 2004b; Thackeray et al., 2008). Besides recording changes in water temperature, the focus of climate impact studies on lake ecosystems has been placed on the occurrence and duration of anoxia (Fang & Stefan, 2009; North et al., 2014) and cyanobacterial blooms (Jöhnk et al., 2008; Elliott, 2012a). Both negatively affect water quality. Additionally, emphasis has been placed on temporal mismatch between trophic levels (Winder & Schindler, 2004a).

Besides shifts in average climate measures, climate variability is expected to change (IPCC, 2013), with a direct effect on the occurrence of extreme events (Katz & Brown, 1992). In the context of climate variability, a large number of studies have analysed correlations between different phenological metrics and the North Atlantic Oscillation (NAO, e.g. Straile & Geller, 1998; Weyhenmeyer et al., 1999; Gerten & Adrian, 2000). The NAO quantifies the pressure system between the Icelandic low and the Azores high (Hurrell & Van Loon, 1997) and serves as a measure with which to distinguish between mild and cold winters in central Europe. Variability is thus defined as interannual differences in synoptic scale weather patterns. Besides being mainly limited to variability in the winter season (Straile & Stenseth, 2007), the NAO is only to a limited extent suitable for gaining a mechanistic understanding of climate change effects. A different approach is therefore required to study the impact of climate and meteorological variability (Jentsch et al., 2007).

Statistical weather generators have been developed to generate synthetic time series of meteorological data (e.g. Mavromatis & Hansen, 2001; Dubrovský et al., 2004; Kilsby et al., 2007). With weather generators, ‘tales of a future weather’ (Hazeleger et al., 2015) can be played through, allowing for a mechanistic understanding while covering the inter- and intra-annual variability in meteorology.

Other modelling approaches in climate change impact studies on lake ecosystems comprise sensitivity studies, in which different meteorological variables are de- and increased (e.g. Austin & Allen, 2011; Kupisch et al., 2012; Bueche & Vetter, 2014) and studies which use the output from regional and global climate models to drive their lake model (Elliott et al., 2005;
Deep lakes are especially complex in their response to climate variability. Because of their large water volume, only parts of the whole water body are regularly in contact with the atmosphere. This leads to different warming rates in epi- and hypolimnion (Livingstone, 2003; Eder, 2013) and to irregular winter mixis (Straile et al., 2010) affecting oxygen concentrations in the deep water (Eder, 2013). The phytoplankton spring bloom in particular depends on stratification onset (Peeters et al., 2007b) and thus physical processes connected to meteorological conditions (Ollinger & Bäuerle, 1998). Consequently, phytoplankton phenology is expected to shift with a changing climate in the future (Thackeray et al., 2008). The phytoplankton spring bloom thus represents a highly sensitive ecological phenomenon particularly suitable for climate impact studies.

2.4 Lake ecosystem modelling

With growing computational power, modelling has become an increasingly important aspect of ecological research. In a strict sense, the term ‘model’ embraces different approaches, like conceptual, statistical or dynamic process-based models. Here I focus on dynamic process-based models, since my interest is in the mechanistic understanding of phytoplankton dynamics. In addition, a changing environment requires models that are dynamically responding and still valid under altered boundary conditions.

Mechanistic models span from simple population models with two to three state variables (Lotka, 1924; Volterra, 1926) to complex ecosystem models with many state variables and hundreds of parameters (e.g. Bruce et al., 2006; Omlin et al., 2001). While the first type of models, so-called ‘minimal dynamic models’ (Mooij et al., 2010), is used to conduct theoretical analyses on a chosen part of the lake ecosystem (e.g. population-regulating mechanisms), the latter type of models intends to describe whole ecosystems, comprising biological and chemical as well as physical processes. Complex ecosystem models are used to test management options (Trolle et al., 2008; Gal et al., 2009), calculate climate-scenarios (Elliott et al., 2005; Trolle et al., 2011) and to enhance our scientific understanding of lake ecosystems (e.g. Romero et al., 2004; Petzoldt & Uhlimann, 2006; Dietzel et al., 2013). While common critiques of complex models state that they are heavily overparameterised leading to a lack of identifiability (Brun et al., 2001; Beven, 2010), complex models have shown useful in many practical applications.

Many different aquatic ecosystem models have been developed through limnological research. Some of the most frequently used complex ecological lake models are DYRESM-CAEDYM, PROTECH, SALMO, BELAMO, CE-QUAL-W2 and PCLake (Trolle et al., 2012). During the last few years, this diversity of models has led to a movement in the scientific community of aquatic ecosystem modellers towards joining forces and a common framework with which to facilitate model development (Trolle et al., 2012). Comprehensive discussions on the different aquatic ecosystem models and their use can be found in Mooij et al. (2010); Rigosi et al. (2010) and Robson (2014b).

In this thesis, two dynamic ecological lake models were applied: DYRESM-CAEDYM (DY-
namic REservoir Simulation Model - Computational Aquatic Ecosystem DYnamics Model), developed by the Centre for Water Research in Perth, Australia and PROTECH (Phytoplankton RespOnses To Environmental CHange), developed by the Centre for Ecology and Hydrology in Lancaster, UK. Details on both models will be given in the following chapters.
2.4. LAKE ECOSYSTEM MODELLING
Use of a weather generator for simulating climate change effects on ecosystems: A case study on Lake Constance

D. Schlabing, M.A. Frassl, M.M. Eder, K. Rinke, A. Bárdossy


**Abstract**

We present a new vector-autoregressive weather generator developed to generate meteorological time series for climate impact studies on ecosystems.

As an example, the weather generator was applied in combination with a hydrodynamic-ecological lake model (DYRESM-CAEDYM). The effects of a warmer and more variable climate on hydrodynamics and phytoplankton in large monomictic lakes were analysed.

The weather generator reproduced dependency structures of measured meteorological data. Variability was altered at a time scale similar to lengths of synoptic disturbances, resulting in longer than day-to-day fluctuation changes.

Sensitivity of spring bloom development towards a warmer climate, increased climate variability and a combination of both was addressed. For this purpose, 500 meteorological time series per scenario were generated as input for the lake model. We found that onset and maximum of phytoplankton spring bloom are sensitive towards spring weather conditions and that an increase in variability favours early as well as late blooms.
3.1 Introduction

It is common understanding that climate change will have a huge impact on natural systems through changes in mean air temperature, but also changes in climate variability (IPCC, 2013). Uncertainty prevails on how ecosystems will respond to changes in climate. The application of ecosystem models informs about potential consequences of a changing climate. Yet a proper representation of the changed climate is not trivial. Many initial studies just applied meteorological time series with increased temperatures (often by +4 °C) (Trolle et al., 2011; Kupisch et al., 2012). This approach, however, completely neglects that also other meteorological factors will change within a warming climate and hence produces rather unrealistic meteorological time series. Another, more advanced approach is to take output from a General Circulation Model (GCM) (e.g. Diamond et al., 2013), which is based on a specific scenario for greenhouse gas emission. However, these outputs are given in a coarse resolution, exhibit biases and can therefore not be used directly as input for ecosystem models. They have to be bias-corrected and processed further by downscaling the data to the required scale (Maraun et al., 2010; Themeßl et al., 2011).

Alternatively, weather generators can be used to simulate synthetic time series. Weather generators have been used for agricultural modelling and are widely employed across the fields of water engineering design, flood risk analysis and hydrological modelling (Jack & Kelly, 2011; Mavromatis & Hansen, 2001; Dubrovský et al., 2004; Ivanov et al., 2007). They can be adapted for climate impact modelling by perturbation of their parameters.

Most weather generators have focused on precipitation and are based on the methodology developed by Richardson (1981). These weather generators combine a rain occurrence model based on Markov-Chains with separate models for dry and rainy sequences.

The approach has been developed further in diverse respects: e.g. multi-site simulation by Wilks (1999), gridded weather generators by Wilks (2009), better representation of extreme events in precipitation by Hundecha et al. (2009), finer time scales and inclusion of physically based dependencies by Ivanov et al. (2007), preserving low-frequency variability by Dubrovský et al. (2004); Mehrotra & Sharma (2007a,b). Other methods involve the use of non-homogeneous hidden markov models (Hughes et al., 1999), combinations of latent gaussian processes and general linear models (Kleiber et al., 2012) and general additive models for location scale and shape (Serinaldi & Kilsby, 2012). A different family of weather generators does not rely on parametric stochastic models but resamples measured data instead (Rajagopalan & Lall, 1999; Enke et al., 2005; Orlowsky et al., 2008).

Most of the established weather generators either reproduce past climate or are used to downscale GCM and Regional Climate Model (RCM) output. As the aim of this study is to investigate effects of changed mean and variability both separately and together, we developed a weather generator that is able to produce hand-tailored scenarios instead. The simple design of the weather generator allows guiding the scenarios through easy-to-grasp temperature-perturbations.

The fact that weather generators keep dependency structures between meteorological vari-
ables becomes crucial when a system is not only affected by temperatures, but also by other meteorological factors. Other meteorological factors may include cloud cover (Carbone et al., 2013), humidity influencing evaporation (Livingstone, 2003) and precipitation (Jentsch et al., 2007).

Another factor that has been ignored in many climate change studies, is the impact of extreme events on ecosystems (Jentsch et al., 2007). Since extreme climatic events are more sensitive to climatic changes than their mean values (Katz & Brown, 1992), the explicit inclusion of climatic variability and extreme events is important, particularly in the context of ecosystems (Wigley, 1985). While gradients in warming allow for adaptation of a community to these changes, extreme events have the potential to destabilize a system and even shift it into another steady state (Scheffer et al., 2001a). Capturing extreme events is restricted to few occurrences when using GCMs and RCMs. The possibility to increase meteorological variability with a weather generator and at the same time to produce several time series results in an increase in magnitude and quantity of extreme events. Therefore using a weather generator automatically allows the analysis of extreme events.

We use lakes as example ecosystems as they are sensitive to climate forcing and important ecosystems in terms of their usage as freshwater resources worldwide. Large-scale meteorological patterns were shown to affect the timing of cardinal events in plankton development (Weyhenmeyer et al., 1999; Straile, 2000; Winder & Schindler, 2004b). Air temperature is an important driver for lake ecosystems, as it affects the timing of stratification and mixing (Livingstone, 2003), leading to differences and shifts in phytoplankton phenology (Peeters et al., 2007a; Winder & Schindler, 2004a; Scheffer et al., 2001b). So far, just a few studies have explicitly examined interannual variability effects on lakes (Straile et al., 2010) and short-time weather effects on plankton development (Gaedke et al., 1998b).

For the simulation of phytoplankton phenology, coupled hydrodynamic-ecological lake models have been validated for different lake ecosystems (Bruce et al., 2006; Trolle et al., 2011; Dietzel et al., 2013). These models are especially well suited for running climate change scenarios and modelling weather effects on lakes as they require meteorological time series as input data.

The aim of this study is threefold. First, we develop a statistical weather generator that is able to generate consistent meteorological time series that preserve the correlations, distributions and annual cycles of measured data. Second, we produce meteorological time series for different climatic regimes. In particular we are interested in shifting temperatures (current climate vs. warmer climate) and in shifting variability in meteorological variables (current climate vs. more variable climate). Third, we apply the generated meteorological time series from the weather generator to a coupled hydrodynamic-ecological lake model. This last step highlighted the effects of different climatic regimes on ecosystems. We make use of the strengths of our weather generator and systematically study the response of lakes not only to warming but also to increased meteorological variability (and both factors together) in a stochastic approach with relatively high sample size.
3.2 Methods

Fig. 3.1 illustrates our modelling scheme: Time series for four different climate scenarios were generated by the weather generator VG (fitted on measured meteorological data). For each scenario, 500 realisations were run. They were then used to drive simulations with the hydrodynamic-ecological lake model (DYRESM-CAEDYM). In the following, each step is described in more detail.

3.2.1 Weather generator

The proposed weather generator employs a single Vector-Autoregressive (VAR) process. Here, the vector is the set of simulated meteorological variables at one time step. VAR processes capture the auto- and crosscorrelations in multivariate time series by separating them into a deterministic, linearly dependent and a random part. They assume that the time series have time-invariant means and standard deviations. Time series generated by stable VAR processes follow normally-distributed marginals.

The simulated variables are listed in Table 3.1. Rain was deemed as of minor importance for the thermal and volumetric budget of the lake. Compared to the large water volume of the model system, direct precipitation on the lake surface is negligible (Bäuerle et al., 1998). Rain was therefore not simulated, instead long term averages of daily precipitation measurement were used. The overall structure of VG is shown in Fig. 3.2.
Table 3.1: Meteorological variables generated by the weather generator VG. The last column lists the parametric distributions used for variable transformation (see section 3.2.1). “Empirical” refers to a kernel density estimation.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air temperature</td>
<td>θ</td>
<td>Normal</td>
</tr>
<tr>
<td>Short-wave radiation</td>
<td>Q_{sw}</td>
<td>Empirical</td>
</tr>
<tr>
<td>Incident long-wave radiation</td>
<td>Q_{lw(stat)}</td>
<td>Normal</td>
</tr>
<tr>
<td>Relative humidity</td>
<td>φ</td>
<td>Truncated Normal</td>
</tr>
<tr>
<td>Eastward wind speed</td>
<td>u</td>
<td>Empirical</td>
</tr>
<tr>
<td>Northward wind speed</td>
<td>v</td>
<td>Empirical</td>
</tr>
</tbody>
</table>

Figure 3.2: Structure of the weather generator VG. Boxes with grey background refer to computations in the standard-normal transformed domain.

Variable transformation

Meteorological variables show diverse marginal distributions and usually exhibit strong season-dependent means, standard deviations and further higher order moments. To address this non-stationarity, we employ a day-of-year (doy)-specific quantile-mapping to achieve stationary, standard-normal distributed variables.

Two approaches to attain an annual distribution function for quantile mappings are employed here: (1) approximating the annual cycle of parameters of theoretical distributions by Fourier series (annual distributions) and (2) pseudo-2-dimensional Kernel Density Estimation (annual KDE). Table 3.1 shows which distribution was chosen for each variable. Inserting the measured variables together with their doy into the distribution function $F_{doy}$ gives estimates for de-seasonalized quantiles. Those are then converted to standard-normal distributed variables by inserting them into the inverse normal distribution with zero mean and standard deviation of one.
The first case (fitting the annual distribution) consists of two steps. First, a set of parameters per \( \text{doy} \) is calculated by fitting a theoretic distribution to measurements of the \( \text{doy} \) and the neighbouring \( \text{doy}s \), resulting in a series of 366 parameter sets. These parameters closely follow the specifics of the dataset. In order to generalise, the parameter series was smoothed by approximating it with a Fourier series of order 4. In effect, the distribution parameters \( p_{1, \text{doy}}, \ldots, p_{k, \text{doy}} \) are given by a function of the \( \text{doy} \):

\[
p_{j, \text{doy}} = \frac{a_{j,0}}{2} + \sum_{n=1}^{4} \left[ a_{j,n} \cos \left( n \frac{2\pi}{\text{doy}} \right) + b_{j,n} \sin \left( n \frac{2\pi}{\text{doy}} \right) \right] 
\]

\( a_{j,n} \) and \( b_{j,n} \) are parameters that are obtained by discrete Fourier transform. In the case of air temperature (\( \theta \)), the distribution parameters are \( p_{1, \text{doy}} = \mu_{\text{doy}} \) (mean) and \( p_{2, \text{doy}} = \sigma_{\text{doy}} \) (standard deviation), i.e. the parameters of the normal distribution and the \( \text{doy} \)-specific distribution function becomes \( F_{\text{doy}}(X) = \Phi(X, \mu_{\text{doy}}, \sigma_{\text{doy}}) \) (\( \Phi \) is the distribution function of the normal distribution). This procedure allows for a smooth change of the variables throughout the year without introducing a large number of free parameters.

The second case (attaining a Kernel Density Estimate) is more data-centric and does not make any assumption that a measured variable follows a specific theoretic distribution. Short-wave radiation (\( Q_{sw} \)) and wind speed components (\( u \) and \( v \)) exhibited annual cycles that were hard to describe using trigonometric functions like Equation 3.1. Our variant of KDE gives a one-dimensional estimation of the probability density for each \( \text{doy} \), but takes values from neighbouring \( \text{doy}s \) into account:

\[
\hat{f}_{\text{doy}}(x) = \sum_{i \in \{ |\text{doy}_x - \text{doy}_{x_i}| < 15 \}} K_x \left( \frac{x - x_i}{h_{\text{doy}}} \right) \cdot K_{\text{doy}} \left( \frac{\text{doy}_x - \text{doy}_{x_i}}{15} \right)
\]

(3.2)

\( K_x \) is a Gaussian kernel for the dimension of the variable \( x \), \( K_{\text{doy}} \) is a triangular kernel for the \( \text{doy} \) dimension and \( h_{\text{doy}} \) the \( \text{doy} \)-specific kernel width of the \( x \) dimension. The number of \( x \)-values 15 \( \text{doy}s \) apart from measurement \( x \) is given by \( \#\{ |\text{doy}_x - \text{doy}_{x_i}| < 15 \} \). 15, the width of the \( \text{doy} \)-dimension, was chosen by hand to give a reasonable number of data points for each \( \text{doy} \) (usually \( 14 \cdot 2 + 1 \cdot n_{\text{years}} \)). \( h_{\text{doy}} \) was optimised by maximum likelihood, using the leave-one-out cross-validation approach. \( h_{\text{doy}} \) was further smoothed in the \( \text{doy} \)-domain to allow a greater abstraction from the data-set. Otherwise, back-transformed simulated values would follow the distinct short-term fluctuations (noise) inherent in the data-set. The distribution function \( \hat{F}_{\text{doy}} \) is attained by numerical integration of \( \hat{f}_{\text{doy}}(x) \).

**VAR fitting**

The VAR process is given in the form:

\[
y_t = \sum_{i=1}^{p} (A_i y_{t-i}) + \varepsilon_t + m
\]

(3.3)

\( y_t \) is a \( K \)-dimensional vector of transformed observations for the time step \( t \), \( A_i \) are \( K \times K \)
matrices containing the parameters of the process, \( \varepsilon_t \) is a \( K \)-dimensional vector containing the residual for time step \( t \). This means, that the weather of the current day \( (y_t) \) is depending on the weather of the preceding days \( (y_{t-i}) \), plus white noise \( (\varepsilon_t) \). \( m \) is an additional disturbance vector that is used to generate scenarios. The entries in \( A_i \) capture the correlations and cross- and autocorrelations of the dataset. To estimate the VAR parameters \( (A_i \) and the covariance matrix of \( \varepsilon_t \), the Least Squares Estimator was used (Lütkepohl, 2005, p. 70).

**Generation of time series**

Time series are generated by replacing the residuals \( \varepsilon_t \) with vectors drawn from a multivariate normal distribution in Equation 3.3 (for more details see Lütkepohl, 2005, p. 707). Because these values are normally distributed, they are transformed back into the measurement domain by using the inverse of the distribution functions \( (F_{\text{doys}}^{-1}) \) obtained in section 3.2.1, “Variable transformation”.

**Generation of scenarios with a changed mean**

The VAR process was further adjusted to allow for manipulation of key output statistics, i.e. simulating scenarios. The mean \( m \) of a \( K \)-dimensional VAR process of order \( p \), given in the form of Equation 3.3, can be adjusted through

\[
I - \sum_{i=1}^{p} A_i \right) \overline{y}. \tag{3.4}
\]

\( I \) is the \( K \times K \)-dimensional identity matrix and \( \overline{y} \) the vector of desired means. A design goal was to let the user define a change in air temperature mean \( \Delta \theta \) and have the weather generator set the means of the other variables accordingly. First, the change given in \( ^\circ \text{C} \) has to be converted to a change in the transformed domain. As \( \theta \) and \( \theta_{\text{trans}} \) are both normally distributed, with \( \sigma_{\theta, \text{doys}} \) (given by Equation 3.1) and \( \sigma = 1 \) respectively, this amounts to a simple division, namely \( \Delta \theta_{\text{trans}} = \Delta \theta / \sigma_{\theta, \text{doys}} \). Using the covariances between the transformed air temperature \( \theta_{\text{trans}} \) and the other variables \( \sigma_{\theta_{\text{trans}}, y_{\text{trans}}^i} \), the non-air temperature elements \( i \) of \( \overline{y} \) are obtained similarly to a linear regression:

\[
y_{\text{trans}}^i = \Delta \theta_{\text{trans}} \sigma_{\theta_{\text{trans}}, y_{\text{trans}}^i} \sigma_{\theta_{\text{trans}}}^{-1} \sigma_{\theta_{\text{trans}}, y_{\text{trans}}^i}. \tag{3.5}
\]

As the link between the desired temperature change \( \Delta \theta \) and all elements of \( m \) is established, all further scenario definitions can be expressed in terms of \( \Delta \theta \). By changing the theoretical mean of the VAR-process and keeping the rest of its parameters unchanged, we assume that the linear dependence structure of variables remains the same under changed climatic conditions.

**Generation of scenarios with higher variability**

In order to increase climate variability, the change of air temperature was applied non-stationary as \( \Delta \theta_{t} \).
22 3.2. METHODS

In the context of this study, climate variability is quantified by the statistics of periods in which daily average air temperatures deviates from the long-term average for this day of year. These episodes can be described by their duration in days and their deviation from the mean in °C. In the measured air temperatures of the reference period, episodes duration shows strong similarity to an exponential distribution with an average value of 5.3 days. Apart from a bimodality around 0 °C the amplitudes are approximately normally distributed with a standard deviation of 2.3 °C. Here, increasing climate variability means increasing duration and amplitude of the episodes.

In order to increase this episode variability, artificial episodes of \( \Delta \theta \) were generated. This is done by generating random numbers following an exponential distribution to be used as episode lengths and normally distributed random numbers to be used as episode amplitudes. These episodes are used to change the theoretical means of the underlying VAR-process.

Disaggregation

Short-wave radiation and the wind speed components were disaggregated to hourly values as we wanted to run the lake model with sub-daily meteorological input. The scheme to disaggregate short-wave radiation is deterministic and adds a typical daily cycle while maintaining the mean daily short-wave radiation generated by the weather generator. Wind speed components are disaggregated by resampling differences between daily and hourly values in the measured data. These differences are added to the daily simulated wind speed components in chunks of two days. This largely maintains the cross- and autocorrelations in the disaggregated time series. For the non-disaggregated variables, daily means are applied to each hour of the day.

3.2.2 Lake ecosystem model

For simulating the effects of changed meteorological conditions on large lakes, the coupled ecological-hydrodynamic model DYRESM-CAEDYM was used (V5.0.0; DYRESM 3.1.0-03; CAEDYM 3.1.0-06; Centre for Water Research, Australia). DYRESM (Dynamic Reservoir Simulation Model) is a one-dimensional lake model. It calculates the vertical distribution of temperature, salinity and density in a lake based on a Lagrangian layer structure (Imberger & Patterson, 1981). DYRESM allows dynamical coupling to the Computational Aquatic Ecosystem Dynamics Model (Hipsey et al., 2010), which simulates nutrient cycling, oxygen dynamics as well as primary and secondary production. DYRESM-CAEDYM requires meteorological input and inflow data as boundary conditions.

We have chosen this lake ecosystem model, as it has been applied successfully to a variety of different lakes (e.g. Gal et al., 2009; Rigosi et al., 2011; Frassl et al., 2014). Rinke et al. (2010) have validated DYRESM-CAEDYM for Lake Constance. They used visual comparison of the most relevant outputs (isotherms, timing of stratification and total chlorophyll a concentration pattern), summed squared error for calibration and linear regression analysis on measured data and model output, which are standard measures in this context (Bennett et al., 2013). In this study, the model configuration includes nutrient dynamics, four functional phytoplankton
groups and one zooplankton group. The analysis focuses on simulated total chlorophyll a concentration, which is the sum of all four functional phytoplankton groups. A full description of model parameters can be found in Rinke et al. (2010).

### 3.2.3 Definition of scenarios

We defined 4 scenarios in a 2 x 2 matrix of the two factors increased mean air temperature and climate variability (Table 3.2). The scenario $T_C$ (“current temperature”) was used for comparing simulation results under current climate conditions to measured data. This scenario is the reference scenario for the remaining climate change scenarios. For the scenarios with future climate ($T_F$ “temperature future” and $V_F$ “variability future”), mean air temperature was increased by 4 °C. This increase is within the likely range of temperature increase until 2081-2100 for several IPCC scenarios (Stocker et al., 2013).

For the scenarios with higher climate variability ($V_C$ “variability current” and $V_F$ “variability future”), we let VG add artificial episodes with mean episode length of 7 days and standard deviation of amplitude of 5 °C.

The effects of changed meteorological conditions were studied by applying the generated meteorological input data to DYRESM-CAEDYM. For each of the four scenarios 500 realisations were generated by VG and used as input data. Simulations were run over four years, results are only shown for the last year in order to account for a spin-up time of the model. To ensure that simulated effects on the lake ecosystem are attributed to changed meteorological conditions, inflow volume and inflow concentration were kept identical for each simulated year. That is, we took a year with balanced water budget and repeated this year of daily inflow and outflow data four times. Due to the lake’s large surface area, heat import and export by throughflows are negligible in comparison to heat exchanges with the atmosphere (Bäuerle et al., 1998).

For each scenario, the means of simulated water temperature and total chlorophyll concentration over the upper 20 m were calculated. From these depth-averaged values, the median and 5th and 95th percentile per day of year were calculated and compared between scenarios.

In order to statistically analyse model results and to assess influences of air temperature

<table>
<thead>
<tr>
<th>mean air temperature</th>
<th>climate variability</th>
</tr>
</thead>
<tbody>
<tr>
<td>unchanged (C-scenarios)</td>
<td>$T_C$ “current temperatures”</td>
</tr>
<tr>
<td>+ 4 °C (F-scenarios)</td>
<td>$T_F$ “future climate”</td>
</tr>
<tr>
<td>increased (V-scenarios)</td>
<td>$V_F$ “future climate with higher variability”</td>
</tr>
<tr>
<td>unchanged (V-scenarios)</td>
<td>$V_C$ “current temperatures with higher variability”</td>
</tr>
</tbody>
</table>

#### Table 3.2: Climate scenarios generated by the weather generator (VG)
on lake characteristics, cardinal dates of stratification and plankton succession were derived from the model results. The beginning of lake stratification was described by the day of year at which the temperature difference between 0 and 20 m is larger than 1 °C (doy_{strat}). Start of spring bloom development was defined as the day of the year at which mean total chlorophyll concentration in the upper 20 m is larger than 3 µg L^{-1} (doy_{chla}) (Peeters et al., 2007a). To obtain a comparable metrics for air temperatures, the day of the year was calculated at which the sum of daily air temperature, starting at the 1st of January, surpassed 300 °C (doy_{spring}). A value of 300 °C was chosen, as it ranges in a similar time of the year as doy_{strat} and doy_{chla}.

### 3.2.4 Study site

Lake Constance is a large, deep (>250 m), monomictic lake, situated at the northern boundary of the central European Alps, between Germany, Switzerland and Austria (47° 37.440’ North, 9° 22.528’ East) at 395 m a.s.l.. With phosphorus concentrations of around 10 µg L^{-1}, the lake is currently classified as oligotrophic (Güde et al., 1998).

Lake Constance is an interesting and important study system for climate warming effects. First, Lake Constance is an important source for drinking water. About 5 million people in Germany and Switzerland get their drinking water from Lake Constance. Second, the lake is located in an area where both higher air temperatures and increased climate variability have been projected (Stocker et al., 2013; Schär et al., 2004).

### 3.2.5 Data

For this study, VG was fitted on a data set of hourly meteorological measurements for the reference period 1980–2000 (measurement station Konstanz, Germany, National Meteorological Service (DWD)).

Gaps in the data measured by the DWD have been filled by linear interpolation where single values were missing. Longer periods of missing values were replaced by values from neighbouring stations (Guettingen, Federal Office of Meteorology and Climatology MeteoSwiss; Friedrichshafen, DWD). In total, 0.546% of values were missing.

As long wave radiation is not measured directly at Konstanz meteorological station, it was calculated from air temperature, humidity, and cloud cover, using an empirical formula set up by Iziomon et al. (2003) for a nearby measurement station (in the Upper Rhine plain 212 m a.s.l., distance to Konstanz: approx. 120 km).

The reference period is a period of relatively strong temperature increase. A linear regression on the air temperature data yields a gradient of 0.0746 °C a^{-1}, i.e. an increase of 1.566 °C within the whole period.
CHAPTER 3. WEATHER GENERATOR SIMULATIONS

3.3 Results

3.3.1 Direct validation

To achieve parsimonious parametrisation, selection of the autoregressive order $p$ was done with the Schwarz (Schwarz, 1978) and the Hannan-Quinn (Hannan & Quinn, 1979) information criterion. The first suggested $p=2$ and the latter $p=4$. $p=3$ was chosen for better representation of the autocorrelation.

The residuals of the fitted VAR-process were tested on their whiteness on a 5% significance level. Except for the third and fourth lag of the autocorrelation of the residuals of relative humidity, all other autocorrelations up to lag 7 can be considered as being those of a white noise process. Third and fourth lag of relative humidity slightly fail the test. Note, however, that about 2 of the 36 tests (6 variables and 6 lags) are expected to fail even when the hypothesis is true given a 5% significance level.

Apart from a few exceptions, distributions of measured and simulated values generally match (see Fig. 3.3). The weather generator underrepresents higher eastward wind speeds. Lower tail values in relative humidities are smaller than their respective measured values. Also some low values of the air temperature are not reproduced.

Correlation matrices of measured and simulated values are shown in Fig. 3.4 and agree
3.3. RESULTS

The ability to extrapolate was tested by using the years from 1984 to 1987 as calibration and the years 1992 to 1995 as validation period. Those periods were chosen because their difference in temperature mean (1.3 °C) was the highest for all combination of 4-year slices. The weather generator was fitted to the data of the calibration period. Afterwards a scenario with a mean increase of 1.3 °C was produced. As seen in Fig. 3.5, distributions of projected and observed values agree well. The temperature increase is propagated to other variables that show a correlation to air temperature - notably long-wave radiation. Wind speed component distributions were not changed much compared to the calibration period, as is expected from their weak dependence to air temperature. Relative humidity shows changes in the upper quantiles between calibration and validation period. During the validation period a lot of the values are exactly one, indicating a possible change in instrumentation.

3.3.2 Generated data

Generated air temperatures show a clear annual pattern with strong daily fluctuations. They are clearly separated into two groups: scenarios with current air temperatures (\(T_C, V_C\)) and scenarios with warmer mean air temperatures (\(T_F, V_F\), Fig. 3.6, Table 3.3). In each of these groups, the annual course of the median is the same. The median of the warmer scenarios is shifted by 4 °C, the band width of both groups stays the same: the average difference between 95th and 5th percentile is 11.29 °C for both \(T_C\) and \(T_F\), and 17.41 and 17.46 °C for \(V_C\) and \(V_F\).

While median air temperatures are clearly separated from each other between \(T_F\) and \(T_C\), the 95th quantile \(T_C\) and the median of \(T_F\) overlap (accordingly their median and 5th quantile). The same accounts even stronger for both scenarios with higher variability (\(V_C, V_F\)).
Figure 3.5: QQ-Plots to illustrate extrapolation skill. The grey line shows observed against simulated data during the validation period of 1992 to 1995. Simulation is based on the calibration period of 1984 to 1987. The black line shows measured validation against calibration period values. Where the black and 1:1-line meet, the according quantile did not change from calibration to validation period. Where grey and 1:1-line meet, the according quantile is equal in simulation and the validation period, i.e. the change was projected correctly.

In Table 3.3, the change in median and range between 5th and 95th percentile is shown for all meteorological variables. To account for the yearly cycle, all numbers have been calculated for each day of the year separately. The values given in Table 3.3 are the averages over the yearly cycle. While for $\theta$ and $Q_{lw}(\text{in})$, median and range (variability) can be changed separately, this does not completely hold true for those of the other variables which have physical upper or lower boundaries: for $Q_{sw}$, an increase in variability decreases the median. For humidity ($\phi$), an increase in mean temperature decreases the median, but increases the range. This is due to the fact, that these two variables have physical upper boundaries. As a measure for the relative change in median, the percentile in $T_C$ that corresponds to the absolute value of the median in the specified scenario is given in Table 3.3.

For the evaluation of the episode statistics, a set of scenario data with the same length as the measurement data set (1980 to 2001) was generated. In $T_C$ and $T_F$, VG reproduces, due to the realistic representation of the autocorrelations, the climate variability of the measured data: The standard deviation of amplitudes is the same (2.3 °C), the mean episode length is slightly lower (5.1 instead of 5.3 days). In the scenarios with higher variability ($V_C$ and $V_F$), mean episode length is increased by 1.1 day, and the standard deviation of amplitudes by 0.7 °C. (See Table 3.4)
Figure 3.6: Simulation results for the four climate change scenarios for current temperature ($T_C$, blue line), higher mean air temperature ($T_F$, red line), current temperature with higher climate variability ($V_C$, green line) and higher mean air temperature with higher variability ($V_F$, turquoise line). Shown are mean air temperature per day (A), mean water temperature of the upper 20 m (B) and mean chlorophyll concentration of the upper 20 m (C). For each variable the median, 5th and 95th percentile of 500 realisations per scenario are depicted.
Table 3.3: Statistical properties of the generated data: change in median compared to $T_C$ and range between 5th and 95th percentile (averaged over yearly cycle).

<table>
<thead>
<tr>
<th></th>
<th>Difference to $T_C$</th>
<th>Range (95th - 5th percentile)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$V_C$</td>
<td>$T_F$</td>
</tr>
<tr>
<td>$\theta$ [°C]</td>
<td>0.05</td>
<td>4.02</td>
</tr>
<tr>
<td>percentile in $T_C$</td>
<td>50.0</td>
<td>87.8</td>
</tr>
<tr>
<td>$Q_{sw}$ [W/m²]</td>
<td>-1.49</td>
<td>18.08</td>
</tr>
<tr>
<td>percentile in $T_C$</td>
<td>50.0</td>
<td>61.0</td>
</tr>
<tr>
<td>$Q_{lw}$ [W/m²]</td>
<td>0.15</td>
<td>18.52</td>
</tr>
<tr>
<td>percentile in $T_C$</td>
<td>50.6</td>
<td>76.0</td>
</tr>
<tr>
<td>$\phi$ [-]</td>
<td>0.00</td>
<td>-0.03</td>
</tr>
<tr>
<td>percentile in $T_C$</td>
<td>49.8</td>
<td>38.4</td>
</tr>
<tr>
<td>$U$ [m/s]</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>percentile in $T_C$</td>
<td>50.6</td>
<td>50.8</td>
</tr>
</tbody>
</table>

Table 3.4: Climate variability: Episode statistics in measured data and VG scenarios.

<table>
<thead>
<tr>
<th>Measurements</th>
<th>$T_C$</th>
<th>$V_C$</th>
<th>$T_F$</th>
<th>$V_C$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean episode length [days]</td>
<td>5.3</td>
<td>5.1</td>
<td>6.2</td>
<td>5.1</td>
</tr>
<tr>
<td>$S_{amplitude}$</td>
<td>2.3</td>
<td>2.3</td>
<td>3.0</td>
<td>2.3</td>
</tr>
</tbody>
</table>

3.3.3 Indirect validation

During the process of direct validation small imprecisions of the weather generator became apparent. The purpose of an indirect validation is to assess whether these imprecisions affect the studied variables of the lake model (Dubrovský et al., 2004). A comparison of a simulation with measured meteorological input data (reference run) and simulations with generated meteorological time series ($T_C$) is shown in Fig. 3.7. Measured air temperatures stay well within the range of generated temperatures (500 realisations). The same holds true for simulated water temperatures. Chlorophyll concentrations in the reference run show a large variability from year to year but are nonetheless within the range of the weather generator driven model runs.

Cardinal dates of the reference run are a bit lower than but still in line with those from the $T_C$-scenario. The mean of the 4 available years of $doy_{spring}$ in the reference run is 95.0 compared to 99.0 in $T_C$. This is reflected in $doy_{strat}$ and $doy_{chla}$, too. In the reference run, the mean of $doy_{strat}$ is 112.5 compared to 117.6 in $T_C$. The mean of $doy_{chla}$ is 117.5 in the reference run and 123.6 in $T_C$. Based on a two-sided t-test at a 5% level of significance, it can be rejected that any of the means of the reference run is lower than their respective mean of the $T_C$-scenario.

3.3.4 Lake scenarios

In the scenario simulations water temperatures lag behind air temperatures (upper and middle panel in Fig. 3.6). Air temperature minima occur in mid January in all scenarios, whereas
3.3. RESULTS

Figure 3.7: Indirect validation. Black line in the top plot is measured data of air temperature, grey lines are 500 realisations from VG ($T_C$). The lower two plots show mean water temperatures and chlorophyll concentrations of the upper 20 m over four years, simulated by DYRESM-CAEDYM. Black lines are results from a simulation based on measured meteorological variables. Grey lines are model outputs based on the VG realisations ($T_C$). All black lines refer to data or simulations from 1994–1997. Each grey line refers to a $T_C$ realisation of 4 years produced by VG that was fitted on data from 1980–2001.
water temperature minima are reached in the end of February (C-scenarios) and mid February (F-scenarios).

Water temperatures show less fluctuation on a daily basis than air temperatures. The medians within current temperature scenarios (T_C, V_C) lie one upon the other, as is the case for the increased temperature scenarios (T_F, V_F). The same insensitivity of the median to changed variability can be seen in the air temperatures. Regarding the confidence band (5th to 95th percentile) in temperatures, an interesting contrast appeared between air and water temperatures. For air temperatures, the confidence band for current and future climate largely overlap (irrespective of variability) over the entire year. This is not the case for water temperatures, where confidence bands of F- and C-scenarios are rather separated in winter while they clearly overlap during summer. This means, that warming of the lake is in a statistical sense stronger in winter. The minimum difference between C- and F-scenario medians occurs in the middle of August with about 1.7 °C, the maximum difference is about 3.6 °C at the beginning of May. The variability effect is reflected in the confidence band. The average difference between 95th and 5th percentile is 2.3 and 2.4 °C for T_C and T_F and 3.1 and 3.4 °C for V_C and V_F.

Another effect of increased variability is a higher standard deviation of the cardinal dates, making early and late dates of stratification more frequent. The standard deviation of cardinal dates of stratification increases from 10.9 to 15.6 days for T_C to V_C and from 13.7 to 18.9 days for T_F to V_F (see density plot in Fig. 3.8). This effect of climate variability is strongly reduced in comparison to cardinal dates of air temperature (doy_{spring}). There, standard deviation changes from 12.0 to 23.3 days from T_C to V_C and from 11.2 to 18.7 days from T_F to V_F.

The timing of phytoplankton spring bloom shows a clear differentiation between C- and F-scenarios. The peak in the F-scenarios is shifted by approximately three weeks from the end of May to the beginning of May (Fig. 3.6). The day of year when the threshold of 3 µg L^{-1} is surpassed in the upper 20 m (doy_{chla}) is shifted by approximately three weeks from the beginning of May to the middle of April, as well (Fig. 3.8).

A similar shift is observed for the day of year, when the water temperature difference between surface and 20 m depth surpassed 1 °C (doy_{strat}): the median date is April 29 and 27 in the T-scenarios (T_C and V_C) compared to April 13 and 9 in the F-scenarios (T_F and V_F). The onset of the phytoplankton bloom is correlated with the onset of stratification (doy_{strat} vs. doy_{chla}: r^2 = 0.49). Similar relationships were found between doy_{spring} and doy_{chla} (r^2 = 0.52) and to a lesser extent for doy_{spring} and doy_{strat} (r^2 = 0.29), respectively.

While the 95th percentile of chlorophyll concentrations in spring does not vary much between scenarios, the 5th percentile of the peak production is influenced by climatic variability (Fig. 3.6). This means that low chlorophyll maxima are more likely in the V-scenarios compared to the T-scenarios. The V-scenarios are also associated with a generally higher variability in the spring bloom onset (Fig. 3.6). Accordingly, the combination of higher variability and warmer temperatures (V_F) shows a higher probability of very early phytoplankton blooms.
Figure 3.8: Relationship between measures of cardinal dates for chlorophyll concentrations and air and water temperature. Scatter plots show the day of the year where the temperature sum surpassed 300 °C (doy$_{spring}$, x-axes in upper and lower left plots), the day of the year where the difference of water temperature between 0 and 20 m depth is larger than 1 °C (doy$_{strat}$, y-axis in upper and x-axis in lower right plot) and the day of the year where the mean chlorophyll concentration of the upper 20 m is above 3 µg L$^{-1}$ (doy$_{chla}$, y-axes in both lower plots). The outer figures show the kernel densities of these value per scenario. Colours reflect the different scenarios. The grey line marks the 1:1 line.
As for $doy_{spring}$ and $doy_{strat}$, the standard deviation of $doy_{chla}$ also increases in the V-scenarios (from 7.8 to 9.6 days in $T_C$ to $V_C$ and from 11.2 to 13.2 days in $T_F$ to $V_F$).

While in some cases of C-scenarios, phytoplankton growth continues until late November, increasing mean air temperature in the F-scenarios shows a general trend towards a third phytoplankton peak in the months October – November. In the 95th percentile of the F-scenarios, this peak in late autumn exceeds the magnitude of the summer peak.

### 3.4 Discussion

We created a new scheme for statistical weather generators based on a vector-autoregressive process combined with disturbances for scenario generation. It is well suited for producing meteorological time series for environmental modelling studies such as the one described here.

#### 3.4.1 Weather generator

Our weather generator has a different structure than weather generators employing a resampling scheme such as the ones of Sharif & Burn (2006) or Orlowsky et al. (2010). Those methods reorder historic observations and are therefore greatly limited in their output possibilities (Lee et al., 2012). VG also differs from almost all previously introduced weather generators in that rain is not simulated. While being a serious limitation at first glance, the exclusion allows a structure that is simpler because of the absence of a rain occurrence model.

Increasing variability was achieved by adding artificial episodes during the generation of the time series. As these disturbances are propagated from air temperature to the other variables, this is different from changing standard deviations on fixed time scales for each simulated variable, as it is done for example in Kilsby et al. (2007). The use of disturbances is different to other weather generators adapted for a climate impact context, where the parameters of weather generators are usually changed (e.g. Fatiči et al., 2011), conditioned on an external variable like a weather type (Maraun et al., 2010). In this work, adding a disturbance and fixing the parameters of the stochastic process is done so that a change in one variable (air temperature) is passed on to the others. This method was tested by extracting a calibration and validation set from the available data. Though not all variables changed much between the two sets, the ones that did were successfully projected by a change in air temperature. It has to be noted that the correlations between the wind speed components and the rest of the variables is low. This does not mean that generated time series will be unlike the measured data, but that scenarios with changed air temperature will not produce much different wind conditions. Nonetheless, including wind has the advantage of it being different from realisation to realisation. While not directly relevant to this study, wind direction is simulated in VG implicitly by generating the wind speed components. There are few weather generators that simulate wind direction (e.g. David et al., 2010).

Indirect validation showed that the properties of the weather influencing the outcome of stratification and plankton bloom phenology were captured by the weather generator. The fact that the reference run could just as well be a run driven by weather generator output gives
DISCUSSION

confidence that scenario runs give a plausible range of possible outcomes. It is assumed that this is also true under changed climatic conditions. Some weather generator studies contain an indirect validation (e.g. Chen et al., 2010; Hirschi et al., 2012), while in some publications weather generator output is compared directly to observations and applicability in diverse fields is claimed (e.g. Birt et al., 2010; Ivanov et al., 2007). We believe that the applicability in a given field has to be tested, but are confident that possible necessary adaptations can be easily implemented in VG. For instance, new variables with nearly arbitrary marginal distributions can be added easily.

VG was deliberately designed so that modellers can easily define climate scenarios of their own. This enables “what if” experiments that help to understand processes. VG is flexible in terms of definition of scenarios and offers the possibility to study effects of changed means and variability independently. It is not practical or even possible to produce the same kind of scenarios with the help of a RCM.

3.4.2 Water temperatures and stratification

The course and cycle of water temperatures illustrates the buffered and lagged reaction of the lake to the meteorological input. Short fluctuations in weather shown by the fluctuations of air temperatures are smoothed away in the water temperatures. The epilimnion reaches its coldest state about one month after the coldest air temperatures occurred. This points to the fact that meteorological variability must occur on a longer than daily scale, in order to have an impact on the water temperature.

Warming in water temperature is stronger in winter than in summer, even though the same air temperature difference is applied over the whole year. We hypothesize that the explanation of this season-specific warming is the non-linear energy loss by evaporation and long-wave emission. Both loss rates increase disproportionally strong with temperature and therefore reduce the warming effect in summer. Differently to Peeters et al. (2007a), our results show a stronger warming of the upper 20 m in winter than in summer. This difference likely results from the fact that VG takes dependency structures between meteorological variables into account. Eder (2013) simulated climate scenarios for Lake Constance with the 3D-model ELCOM-CAEDYM, observing a stronger warming in winter as well.

3.4.3 Phytoplankton phenology

Due to improving light conditions, phytoplankton bloom occurs quickly after stratification and is in this sense indirectly dependent on the weather conditions (Sommer, 1986). In that sense, climate warming and increasing climatic variability affect plankton development via influencing the stratification (Winder & Schindler, 2004b). That means that a warmer climate causes an earlier phytoplankton bloom and a more variable climate increases the number of extremely early and late blooms.

As another effect in the biological response to changed climatic conditions, the occurrence of weaker phytoplankton blooms is favoured by higher variability regardless of the actual
warming. This can be easily missed, because aggregating over all realisations barely changes the median chlorophyll a concentration at the time of maximum bloom. The cause may lie in the phenology of phyto- and zooplankton. Phytoplankton development is strongly controlled by light availability while zooplankton growth is strongly affected by temperature. This may result into years having a low spring maximum in phytoplankton due to higher zooplankton abundances during the time of the spring bloom. This effect of higher grazing pressure by zooplankton has been assumed by other modelling studies (Müller-Navarra et al., 1997).

The maximum of the spring chlorophyll concentration (taken as the 95th percentile) is the same over all four scenarios. Thus, it seems to be unconnected to the changed meteorological input. The reason might be the fixed amount of available nutrients in the lake, which is the same over all scenarios. Thereby, the yield has an upper limit and this carrying capacity is probably reached in a number of realisations within all scenarios. Therefore, the maximum chlorophyll concentration in all four scenarios remained at a similar value.

Our results are in line with other studies, showing a shift of phytoplankton spring bloom towards earlier dates with increasing mean air and water temperatures (Berger et al., 2007; Peeters et al., 2007a). In this context, also the interplay with radiation and cloudiness is important, as these were shown to affect the timing and magnitude of spring phytoplankton bloom (Townsend et al., 1994).

One important characteristic of the weather generator applied in this study is the possibility of generating time series with a higher variability. The effect of different weather patterns in spring and the impact on plankton development has been studied before (Gaedke et al., 1998b), showing a strong dependency of spring bloom phenology on water temperatures (Elliott et al., 2006; Thackeray et al., 2008) and on strong wind events early in the year (Tirok & Gaedke, 2007a). These different meteorological spring conditions are reflected in the generated time series. We were able to show that an increase in variability potentially leads to even earlier spring bloom onset, adding to effects by a warmer climate. Nevertheless, a detailed analysis of single years still needs to be addressed.

3.4.4 Advantages of using a weather generator

As the coupling of a weather generator to an ecosystem lake model is new, this study is just a first step.

We demonstrated that an added 4 °C can mean a plethora of outcomes. Each of the realisations is a plausible future because VG preserves key statistical properties from the measured time series. In contrast to this, using a measured time series and adding 4 °C, as done in many previous studies (e.g. Peeters et al., 2007a), gives only one possible future. We consider this particular possible future as insufficient, because air temperature is related to the other meteorological input variables.

Weather generators can be used to produce synthetic time series of unlimited lengths that are all consistent with a specific projected large-scale climate change (Wilks, 2010). This is useful when modelling the effect of a changed climate on an ecosystem, as one has a range of possible outcomes according to an uncertain input.
3.4.5 Limits of our approach

As a statistical approach, using a weather generator brings with it certain assumptions of stationarity (Themessl et al., 2011). This stems from the fact, that a common goal was to reproduce some of the statistical properties of the measured time series. However, it is unknown whether, under changed climatic conditions, the dependency structure of the variables remains the same.

Our weather generator has a number of limitations. It is a single-site weather generator, suitable for providing input to a one-dimensional model like DYRESM. However, for a large lake as Lake Constance, the meteorological conditions are not uniform all over the surface area. This is true especially for wind. In the current version of VG, the dependency structure is assumed to be stationary during the year. For the disaggregation of daily to hourly wind velocity values, a resampling algorithm is used. This implies, that the difference of hourly to daily average wind speed can not exceed the highest value from the reference period. Also rain is not simulated by VG. This limits the application of the current version of the weather generator to ecosystems with weak dependency on precipitation.

We chose to simulate four years, while using the last year for analysis. In many scenario-based applications of lake models a spin-up time for the model is included in the simulation scheme (e.g. 10 years as in Gal et al., 2014). Spin-up times should be chosen in a way that the model outputs show a stabilized pattern and are independent of the initial conditions. As we are using the model in a probabilistic framework with randomized meteorological time series, i.e. each year differs from the other; the simulation never approaches a stabilized state. The weather generator keeps the model constantly in a transient state and a spin-up time of 3 years is believed to be sufficient to minimize any influence from the initial conditions. We are convinced that the general outcome of our simulation would not have changed if a prolonged spin-up time had been applied.

3.4.6 Outlook

Seasonally changing dependencies could be taken into account. Whether an ecosystem like a lake is sensitive to this aspect could be a question for further research.

The present study assumed a changed climate in which each scenario itself was stationary. It is, however, not foreseeable that the climate reaches a steady state in the current century. Therefore, it would be interesting to estimate the impact not of a changed, but of a changing climate on lakes. Input time series could be applied to the lake model with a trend component. As ecosystems are in principle able to adapt, the interesting question is: how fast can they adapt? And can they adapt to a trend towards higher variability?

The experiment consists of 2000 realisations in total. It would be wrong to say that every aspect of the produced data was documented here or even analysed by the authors. A lot more could be done. Some realisations caused very early plankton blooms for example. Some realisations triggered a third peak in fall. It would be interesting to look at single realisations and find out what kind of weather caused these extremes.
After having used freely adjustable climate scenarios a possible next step is to design a closer connection to global or regional climate model output. The ability to set the process mean at every time step (Equation 3.4) provides the interface to do that. Results of this step towards downscaling are important for decision makers, because they have a stronger predictive quality. Furthermore, the weather generator could be used in studies concerning other ecosystems. A prerequisite for this is, however, the inclusion of rain.

This study could show that the combination of a weather generator and an ecosystem model provides new insights into a system’s responses to changed meteorology. For large deep lakes, we showed that phytoplankton phenology is sensitive towards both increasing mean air temperature and higher climate variability.

The developed weather generator provides a flexible tool that allows the generation of hand-tailored “what-if”-scenarios with independent changes of specific weather characteristics. It therefore has the potential to add valuable information to climate impact studies on a variety of different ecosystems.

Acknowledgements

We would like to thank the German Meteorological Service (DWD) for providing meteorological data. For providing lake data, we thank the IGKB (Internationale Gewässerschutzkommission für den Bodensee), the ISF (Institut für Seenforschung, Langenargen, Germany) as well as Dietmar Straile from the Limnological Institute, University of Konstanz. The Centre for Water Research at the University of Western Australia is thanked for providing the model DYRESM-CAEDYM.

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Analysis, data-processing and generating the figures was done with the programming language Python (Jones et al., 2001) and the statistical software R (R Core Team, 2012).

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Meteorological control of lake ecosystems: The (un)importance of air temperature

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submitted

Abstract

Annual plankton succession in lakes follows regular patterns and the phytoplankton spring bloom (PSB) is a cardinal event in temperate lake systems. Our current knowledge about this cardinal event clearly documents the importance of climate and many studies repeated the simplified message that the PSB takes place earlier in a warmer world. In favour of simplicity, however, it is ignored that phenology is not driven by a factor ‘climate’ directly; rather it is driven by the (probably complex) interplay of some highly dynamic meteorological variables acting over yet unknown time scales. In essence, we do not quantitatively understand how the different meteorological variables (particularly others than air temperature) act on PSB timing. By using several hundreds of meteorological time series produced by a weather generator in a probabilistic simulation of lake ecosystems we tackle this question and challenge the prevailing predominance of temperature. We tested the role other meteorological variables may play and on which time scales they are effective. We were able to show that meteorological variability causes a large spread in stratification and PSB onset timing, which cannot be explained by one meteorological variable alone. Increasing air temperature, shortwave radiation and decreasing wind, when analysed separately, led to an earlier onset of the spring bloom. Against expectations, we showed that wind speed had the strongest effect on timing, while air temperature was less influential. We found that the effective time scales over which meteorological variables act on stratification and spring bloom onset were shorter for wind than for air temperature and shortwave radiation. We conclude that climate impact studies on lake ecosystems should not only focus on changes in air temperature. Moreover, changes in
overall weather situations and the impact of several meteorological variables, including wind, have to be taken into account.

4.1 Introduction

Phytoplankton spring blooms are cardinal events in lakes and the ocean. Their timing is crucial for the general phenology of the annual succession of plankton communities (Sommer et al., 1986, 2012) and important for the resource supply to upper trophic levels (Edwards & Richardson, 2004). Different environmental factors have been discussed as influential on spring bloom formation, e.g. air temperature (Sharples et al., 2006), duration of ice cover in winter (Gerten & Adrian, 2000), solar radiation (Siegel et al., 2002), grazing pressure (Behrenfeld & Boss, 2014) and stratification onset (Winder & Schindler, 2004b). Factors influencing the spring bloom have been studied by mesocosm experiments (Berger et al., 2007), in the field (Thackeray et al., 2008) and through modelling (Ollinger, 1999). By now, the importance of physical factors on spring phytoplankton development is beyond dispute. The dependence of phytoplankton growth on solar radiation, mixing depth and light attenuation has been recognised as a major prerequisite for the onset of positive net growth (Huisman et al., 1999; Fischer et al., 2014). Sverdrup’s principle introduced a theory for the onset of phytoplankton growth in spring (Sverdrup, 1953). According to his theory, the mixed layer needs to become shallower than a critical depth so that the effective light availability for phytoplankton is sufficient to outbalance respiration losses and support positive net growth. Later, Sverdrup’s theory was revised to include different turbulence conditions in the water column (Huisman et al., 1999). However, the mechanisms and processes leading to the occurrence and timing of spring phytoplankton blooms are still under debate (Mahadevan et al., 2012; Behrenfeld & Boss, 2014; Ferrari et al., 2014), and a quantitative conclusion regarding the timing of the event remains difficult.

Many studies on climate change shed light on the effects of larger meteorological phenomena like the North Atlantic Oscillation (NAO, Weyhenmeyer et al., 1999) or the El Niño Southern Oscillation (ENSO) and Pacific Decadal Oscillation (PDO, Arhonditsis et al., 2004b). Even though it has been discussed repeatedly that short-term meteorological events entail direct ecological responses in lakes (Reynolds, 1990; Jennings et al., 2012), the effect of regional weather and related meteorological variables on spring bloom timing has rarely been quantified (Gaedke et al., 1998b; Ollinger, 1999; Blenckner & Chen, 2003; Peeters et al., 2007a; Schlabing et al., 2014). This might result from the difficulty of non-matching time-scales: while weather changes on an hourly or day-to-day basis, plankton community dynamics proceed at a slower rate and are usually monitored at weekly or even biweekly intervals. To track changes in phytoplankton and its interactions with meteorological drivers, however, dynamics would need to be measured at a higher frequency, at best at sub-daily intervals. In contrast, large-scale meteorological phenomena (e.g. NAO) or average meteorological
conditions (e.g. monthly means of meteorological variables) are aggregated information at a low sampling frequency, corresponding conveniently with the time-resolution of most existing long time series for plankton (Winder & Schindler, 2004b; Jochimsen et al., 2013; Thackeray et al., 2013). As a consequence, existing analyses focus mostly on interannual patterns and often refer to aggregated meteorological or climatological information fitting to the observation frequency in their lakes and therefore systematically ignore short-term meteorological effects.

In conclusion, for a sound empirical analysis of phytoplankton phenology with respect to regional meteorology, highly resolved time series of phytoplankton succession and meteorology are required over many years (Adrian et al., 2012). Such a data set would allow us to separate effects acting on different time scales and gain new insights into the importance of the different meteorological drivers. Although high frequency measurements of phytoplankton have been initiated in several lakes worldwide (Weathers et al., 2013) existing time series are rather short and still insufficient for such a statistical analysis.

This is where theoretical studies using hydrodynamic-ecological models can provide a valuable approach. They allow for simulations with small time steps and thus track changes on a day-to-day or even hourly basis. Boundary and initial conditions can be kept constant between different scenarios in order to exclude interference from confounding factors. Finally, the effect of meteorological variables on phytoplankton development can be studied by applying original meteorological observations (Ollinger & Bäuerle, 1998) or – leaving the observational standpoint – by using artificially generated meteorological input from climate models (Elliott et al., 2005), from observed time series multiplied by a constant factor (e.g. Trolle et al., 2014), or from weather generator data (Schlabing et al., 2014).

Previous studies in Lake Constance have investigated the impact of different meteorological variables on PSB timing through a combination of modelling and statistical analysis (Peeters et al., 2007a,b). However, these studies neglected the dependency structures between meteorological variables and did not quantify the relative importance of the different meteorological variables.

Here, we used the output of a stochastic weather generator (VG) in combination with a one-dimensional lake ecosystem model (DYRESM-CAEDYM) to analyse the effect of regional meteorology on the timing of the phytoplankton spring bloom in a large, monomictic lake. For this purpose, 500 meteorological time series of the current climate were generated and used as input data for the lake model. To exclude other abiotic and biotic influences (e.g. nutrient limitation, grazing pressure or winter meteorology), initial conditions and inflow boundary conditions were the same for each simulation scenario.

We hypothesise that the timing of phytoplankton spring blooms in deep lakes is mainly driven by stratification onset. When the emergence of a spring bloom is potentially possible, i.e. mixing depth or active mixing is shallow enough, we further hypothesise that short-term meteorological events either speed up or delay blooming. We expect relevant time scales to span a few days. We further expect exceptionally quick blooming when the optimal combination of high irradiance values, high air temperature and low wind speed is prevailing. Although the basal effect of any single meteorological variable on stratification or bloom onset,
respectively, is clear based on first principles, the prediction of these cardinal dates for any given meteorological time series will be difficult. On the one hand, accelerating effects in one variable (e.g. high shortwave radiation) might be offset by decelerating effects in another variable (high wind velocity). On the other hand, accelerating conditions may turn into decelerating conditions within a few days and the overall effects of these quickly alternating situations of favourable and unfavourable conditions are not easy to predict. We therefore also expect a large scatter in the correlations between single meteorological variables and cardinal dates in spring phytoplankton succession.

4.2 Materials and methods

4.2.1 Site description

Lake Constance is located at the borders of Germany, Switzerland and Austria (47° 37.4400’ North, 9° 22.528’ East). It has a surface area of 472.3 km² and a maximum depth of 253 m (Tab. 4.1). The lake usually mixes once a year, in late winter. Detailed information about Lake Constance can be found in the literature (Bäuerle et al., 1998; Güde & Gries, 1998; Wessels, 1998).

After a phase of re-oligotrophication beginning in the 1980s, Lake Constance has now reached an oligotrophic state. During the reference period of this study (1994), total phosphorus concentration during mixis was about 29 mg/m³. Phytoplankton development in the lake is characterised by a distinct spring bloom, followed by a clear water phase and moderate algal concentrations thereafter.

Table 4.1: Characteristics of upper Lake Constance

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume</td>
<td>47.637 km³</td>
<td>Wessels (1998)</td>
</tr>
<tr>
<td>Surface area</td>
<td>472.3 km²</td>
<td>Wessels (1998)</td>
</tr>
<tr>
<td>Maximum depth</td>
<td>253.3 m</td>
<td>Wessels (1998)</td>
</tr>
<tr>
<td>Altitude (mean water level)</td>
<td>101 m</td>
<td>Wessels (1998)</td>
</tr>
<tr>
<td>Catchment area</td>
<td>395.3 m a.s.l.</td>
<td>Wessels (1998)</td>
</tr>
<tr>
<td>Outflow (Seerhein, mean 1961-1991)</td>
<td>10.976 km³ yr⁻¹</td>
<td>Bäuerle et al. (1998)</td>
</tr>
<tr>
<td>Drinking water abstraction</td>
<td>0.139 km³ yr⁻¹</td>
<td>Bäuerle et al. (1998)</td>
</tr>
</tbody>
</table>

4.2.2 Generation of meteorological input data (VG)

The Vector-Autoregressive Weather Generator (VG) was developed by Schlabing et al. (2014) as a tool to produce synthetic time series as input for ecological models. It is a multi-variate, single-station weather generator that consists of a VAR process at its core:

\[ y_t = \sum_{i=1}^{p} (A_i y_{t-i}) + \varepsilon_t + m_t \]  

(4.1)
where \( y_t \) are the transformed observations for time step \( t \), \( A_i \) are the matrices containing the parameters of the process, \( y_{t-i} \) is the weather of the preceding day, \( \varepsilon_t \) is the residual vector and \( m_t \) is an additional disturbance vector used to generate scenarios with a changed climate.

The weather generator uses parametric and non-parametric transformations to translate between the statistical distributions of the measured data and the theoretical distribution of the process variables. Unlike global or regional climate models, weather generators easily allow for the generation of a high number of time series, reflecting interannual variability for one climatic situation.

In addition to the configuration used in Schlabing et al. (2014), the current study also took into account the intra-annual changes in the dependency structure between the meteorological variables. Generally speaking, this additional degree of freedom can account for the fact that the covariation between meteorological variables, for instance in late winter, might be different from that in early spring. This was done similarly to the estimation of annually changing distribution parameters in the previous study (Schlabing et al., 2014). In a first step, a VAR process was fitted to the values of each day of the year (doy) by including only values of the respective doy and its neighbourhood. This resulted in a series of 365 values for each VAR parameter. The second step consisted of approximating each of those series with a 4th order harmonic function (Eq. 4.2) attained with the help of the Fourier transform. That is, each element \( a_{i,doy}^{j,k} \) of the \( A_i \) matrices in Eq. 4.1 is given by:

\[
a_{i,doy}^{j,k} = \frac{c_{i,0}^{j,k}}{2} + \sum_{n=1}^{4} c_{i,n}^{j,k} \cos \left( n \frac{2\pi}{doy} \right) + d_{i,n}^{j,k} \sin \left( n \frac{2\pi}{doy} \right) \tag{4.2}
\]

where parameters \( c_{i,0}^{j,k} \) and \( d_{i,n}^{j,k} \) are obtained by discrete Fourier transform. The same procedure is done with the elements of the covariance matrix of \( \varepsilon_t \).

The weather generator was used to produce 500 time series with the length of one year characterising the current climate. Generated variables were: air temperature, wind speed, longwave and shortwave radiation as well as relative humidity. For precipitation input, the long-term mean per doy was calculated from measured data.

### 4.2.3 Lake model

For the simulations, the one-dimensional lake ecosystem model DYRESM-CAEDYM was used (V5.0.0; DYRESM 3.1.0-03; CAEDYM 3.1.0-06; Centre for Water Research, Australia). DYRESM (DYnamic REservoir Simulation Model) simulates the dynamics of temperature, salinity and density along the vertical axis. Its calculations are based on a Lagrangian layer structure (Imberger & Patterson, 1981). DYRESM is coupled with the ecological model CAEDYM (Computational Aquatic Ecosystem DYnamics Model, Hipsey et al., 2010), which simulates nutrient and oxygen concentrations, as well as primary and secondary production. In this study, the model was configured with four functional phytoplankton groups and one zooplankton group. The parameterisation for this study was taken from Rinke et al. (2010) who provided a validated model setting for Lake Constance.
4.2.4 Simulations

In a base scenario (Fig. 4.1) the model was run 500 times over the course of one year; beginning on January 1st with a fully mixed water column at a homogeneous water temperature of 4.3 °C, a typical temperature during winter mixing in Lake Constance. Meteorological input for 500 realisations was produced by the weather generator, whereas inflow and outflow data were taken from measurements in the year 1994 and sustained for all simulations. From each model run, the daily means of simulated water temperature and total chlorophyll concentration over the upper 20 m were calculated. This depth corresponds roughly to the euphotic depth where most of the phytoplankton dynamics take place. Phytoplankton spring bloom onset was characterised by the day of the year (doy) on which mean total chlorophyll concentrations in the upper 20 m exceeded 3 µg L⁻¹ (doy_{chla,3}) (Peeters et al., 2007a). To further characterise the spring bloom, the same criterion was calculated with a threshold of 1 µg L⁻¹ (doy_{chla,1}). However, to exclude phases with much fluctuation around very low chlorophyll concentrations, doy_{chla,1} was taken as the last day before the spring bloom when the threshold 1 µg L⁻¹ was surpassed. We refer to ‘bloom formation’ for the time needed by the phytoplankton to grow from doy_{chla,1} to doy_{chla,3}.

Additionally, surface mixed layer depth (SML) were calculated from each simulation. The criterion for SML was chosen as the depth at which the water temperature surpassed a threshold of 0.5 °C difference from the surface water temperature (Peeters et al., 2007a).

From the evaluation of the base scenario, two further scenarios arose: in the ‘stratification scenario’, the long period of winter mixing was excluded to quantify short term effects of meteorological conditions on stratification onset. In the ‘bloom scenario’ the effect of stratification onset was excluded to analyse the direct effect of weather on phytoplankton growth and phytoplankton spring bloom (PSB) timing. Compared to the base scenario, only the initial conditions and starting day were changed (Fig. 4.1), while model forcing remained the same. The new start dates, initial temperature profile and initial salinity profile were derived from the base scenario. That is, for the stratification scenario, for each of the 500 simulations from the base scenario, the day of the year was calculated on which the water column was fully mixed for the last time before stratification established (doy_{SML,250}). From these days, the 10th quantile was calculated and defined as the simulation start date (doy 88). Initial water temperature and salinity values were derived by averaging temperature and salinity profiles at the 100 earliest doy_{SML,250}, resulting in a homogeneous temperature profile of 4.1 °C. These conditions characterise the setting in Lake Constance during the end of the winter mixing phase.

For the initial conditions in the bloom scenario, the day of the year was calculated for each simulation in the base scenario on which SML became shallower than 30 m (doy_{SML,30}). To avoid days with inverse stratification, only days after March 15th were taken into account. From these days, the 10th quantile was calculated and defined as the simulation start date (doy 109). The initial temperature and salinity profile were determined by extracting the temperature and salinity profiles at doy_{SML,30} from the 100 earliest doy_{chla,3} and calculating the median profile from this subset of realisations (Fig. 4.9). These conditions characterise
the setting in Lake Constance during the full establishment of the vernal stratification.

In a third simulation step, we systematically analysed the effect of single meteorological variables on stratification onset and PSB timing, using the respective initial conditions of the above mentioned stratification and bloom scenario (Fig. 4.1). We manipulated the meteorological input for the variables wind speed, shortwave radiation and air temperature separately at a magnitude corresponding to the 25 and 75 percentile of the 500 generated time series of the respective meteorological variables. In other words, we scaled the relative changes in the respective meteorological variables according to their variability in long-term records in order to identify their effect sizes in situ. These scaling factors were calculated based on quantiles of daily meteorological values. That is, for each day of the year, the ratio between 25th quantile and median as well as 75th quantile and median of daily values was calculated. Afterwards the
mean of these values was taken; both resulting values from the upward and downward change were averaged and applied as the factor for change. Wind speed was altered by multiplying and dividing the time series by 1.28, shortwave radiation by 1.37 and air temperature (here expressed in Kelvin) by 1.0081, leading to another 6x500 simulation runs. When changing air temperature, cloud cover and relative humidity were kept unchanged while longwave radiation and vapour pressure were adjusted to the altered temperature values using formulas by Iziomon et al. (2003) and the WMO (2008). Applying the above mentioned factors led to an average change of ± 0.8 m/s, ± 41.2 W/m\(^2\) and ± 2.3 K in the hourly values of wind speed, shortwave radiation and air temperature.

4.2.5 Analysis

We defined different metrics to characterise potential explanatory variables of phytoplankton spring bloom onset (\(doy_{\text{chla,3}}\)). Stratification onset was defined as the day of the year on which SML became shallower than 20 m (\(doy_{\text{SML,20}}\)). The influence of surface irradiance on PSB timing was described by the day of the year on which cumulated daily irradiance surpassed a value of 1.17 \(\cdot\) 10\(^9\) J m\(^{-2}\) (\(doy_{\text{I,surf}}\)). Finally, we calculated a metric to approximate the light history of phytoplankton cells within the surface mixed layer (SML). First the average light in the SML per day \(I_{\text{SML}}\) was calculated (Riley, 1957):

\[
I_{\text{SML}} = \frac{I_0}{z_{\text{SML}} \varepsilon} \left(1 - e^{-\varepsilon z_{\text{SML}}} \right), \tag{4.3}
\]

\(I_0\) is the daily averaged surface irradiation (W/m\(^2\)), \(z_{\text{SML}}\) is the depth of the surface mixed layer (m) and \(\varepsilon\) is the light extinction coefficient (0.27 m\(^{-1}\)). From \(I_{\text{SML}}\), the cumulated sum was taken and the day of the year calculated on which a value of 8.6 \(\cdot\) 10\(^7\) J m\(^{-2}\) was surpassed (\(doy_{\text{I,SML}}\)). Threshold values for the different metrics were found by optimising the \(r^2\) value of a linear regression model of the metrics and \(doy_{\text{chla,3}}\).

In a second approach, the effect of the weather conditions on phytoplankton growth was analysed by applying a tree model (Ripley, 2014) to the generated meteorological and simulated total chlorophyll data of the base scenario. For this analysis only the relevant window of opportunity for PSB initialisation was taken into account. That is, the utilised time span from every single realisation was beginning on April 1st, as no positive net phytoplankton growth took place before this date, and ending on \(doy_{\text{chla,3}}\) in the respective simulation. Chlorophyll concentrations were transformed into a Boolean variable, with a value of 1 for concentrations > 1 \(\mu\)g L\(^{-1}\) and 0 otherwise. In this transformed data space, days without blooming phytoplankton are assigned with a zero, while those days right before bloom onset (bloom formation, i.e. chlorophyll concentration between 1 and 3 \(\mu\)g L\(^{-1}\)) are assigned with a value of 1. In tree models binary recursive partitioning is applied to classify data into a dichotomous decision tree. We used the above mentioned Boolean variable of chlorophyll blooming as response variable and meteorological data (averaged by a seven day moving average) as explanatory variables. In tree models, the dichotomous partitioning proceeds over the given explanatory variables until no more minimisation of deviance can be achieved or the number
of data points within the group is too small. This defines critical thresholds in the explanatory values, which form decision chains (‘branches’). The final node of each branch quantifies the occurrence of the response variable following the splitting rules of that branch and represents the mean of the response variables within that last group (Crawley, 2013), which in the case of Boolean variables corresponds to a probability.

Multiple linear regression was carried out to assess the importance of each single meteorological variable for the timing of stratification and PSB bloom onset. Prior to analysis, meteorological data were deseasonalised by calculating the anomalies, i.e. subtracting the mean per \textit{doy} over all 500 realisations from the value of the meteorological variable. We averaged these anomalies over different number of days before stratification and bloom onset in order to identify the most decisive time scale for each meteorological variable. This step is similar to the analysis by Peeters \textit{et al.} (2007a). However, since our analysis is based on simulation results with a daily output, we could move backwards from stratification and bloom onset on a daily time step. Additionally, the relative importance of the meteorological variables (shortwave radiation, air temperature and wind speed) was calculated using the R software package \textit{relaimpo} (Grömping, 2006) and the function \textit{pmvd} (proportional marginal variance decomposition, Feldman, 2005). The relative importance quantifies the proportionate contribution of each explanatory variable to the coefficient of determination (Johnson & LeBreton, 2004). In other words, their sum equals exactly the coefficient of determination of the respective multiple linear model.

4.3 Results

4.3.1 Base scenario

Medians of generated meteorological variables followed observed averaged conditions. They showed the typical seasonal course for air temperature and shortwave radiation (Fig. 4.2), whereas median wind speeds revealed only a slight seasonality with higher wind speeds during winter. Intra-day variability of these meteorological variables remained fairly constant for air temperature, while wind speed and shortwave radiation variability showed an opposing seasonality. Wind speeds varied most strongly in winter with a skew towards high wind speeds. Shortwave radiation had a larger interquartile distance in summer, reflecting the variability between sunny and cloudy days.

Simulated water temperatures and chlorophyll concentrations showed a high variability, as well, which in this case was solely caused by meteorological variability (Fig. 4.2). Water temperature followed the course of air temperature. Stratification varied strongly in winter, due to the range between complete mixing and inverse stratification. In summer the lake is stratified, and surface mixed layer depth therefore varied only slightly. Chlorophyll concentration followed a typical seasonal cycle with a distinct spring peak, a subsequent clear water phase and lower concentration afterwards. Timing of stratification onset (\textit{doy}_{SML,30}) varied between \textit{doy} 89 and \textit{doy} 142 (mean = 119, standard deviation = 8). Spring bloom onset (\textit{doy}_{chla,3}) varied between \textit{doy} 110 and \textit{doy} 152 (mean = 129, standard deviation = 7).
Figure 4.2: Median, 5th and 95th quantiles and range of generated meteorological variables air temperature (a), wind speed (c) and shortwave radiation (e) and simulation results for mean water temperature 0-20 m (b), surface mixed layer (d) and mean total chlorophyll concentration 0-20 m (f) of the base scenario. The grey area marks the range of phytoplankton spring bloom onset (\text{doy}_{chla,3}) in the base scenario.
Surface shortwave irradiation alone did not explain spring bloom onset properly; \( \text{doy}_{\text{surf}} \) explained only 27% of the variability in spring bloom onset (Fig. 4.3c). A better explanation was given by surface mixed layer depth \( \text{doy}_{\text{SML,20}} \) \( (r^2 = 0.71) \) and the corresponding cumulated light \( \text{doy}_{\text{SML}} \) \( (r^2 = 0.73) \). Nevertheless, in 6% and 38% of all realisations, phytoplankton already reached the 3 \( \mu \text{g} \cdot \text{L}^{-1} \) threshold before \( \text{doy}_{\text{SML,20}} \) and \( \text{doy}_{\text{SML}} \) respectively (Fig. 4.3a,d). Changing the thresholds to deeper SML (Fig. 4.3b) moved all points above the 1:1 line, but necessarily reduced the explanatory power. No bloom occurs, for example, as long as the SML is deeper than 30 m.

![Figure 4.3: Relationship between phytoplankton spring bloom onset (\( \text{doy}_{\text{chla,3}} \)) and different explanatory variables derived from the base scenario: day of the year on which the surface mixed layer becomes shallower than 20 m (\( \text{doy}_{\text{SML,20}} \), a) and 30 m (\( \text{doy}_{\text{SML,30}} \), b); day of the year on which the cumulated daily irradiance surpasses \( 1.17 \cdot 10^9 \) J m\(^{-2} \) (\( \text{doy}_{\text{surf}} \), c); day of the year on which the cumulated sum of the average available light in the surface mixed layer surpasses \( 8.6 \cdot 10^7 \) J m\(^{-1} \) (\( \text{doy}_{\text{SML}} \), d). The dotted line is the bisecting line.](image)

Results from a tree model, considering the time period from April 1st until \( \text{doy}_{\text{chla,3}} \) identified a bloom formation (i.e. days when chlorophyll concentrations are between 1 and 3 \( \mu \text{g} \cdot \text{L}^{-1} \), see methods) at different combinations of meteorological variables (Fig. 4.4). The highest probability of occurrence for bloom formation is at high shortwave radiation and high air temperature (66% of all days within this category). Conditions acting negatively on phytoplankton growth, e.g. light limitation, can be counterbalanced by conditions acting positively. For example, low irradiance could still support a bloom onset at high temperatures and low wind conditions (43% of values are larger than 1 \( \mu \text{g} \) chl-a \( \mu \text{L}^{-1} \)) of that leaf). Combinations of low shortwave radiation with either low temperature or high wind speed impede spring blooming (probability for bloom onset below 15%).
Figure 4.4: Results from the tree model applied to simulation results from the base scenario. The response variable ‘mean total chlorophyll of the upper 20 m’ was treated as a logical variable, with concentrations > 1 µg L\(^{-1}\) set to 1 and to 0 otherwise. Decision criteria at the nodes of the tree are air temperature (\(T_a\)), wind speed (\(U\)) and shortwave radiation (\(Q_{sw}\)). The size of the green circles and the numbers below denote the proportion of cases with concentrations > 1 µg L\(^{-1}\) within that group.

Table 4.2: Linear model derived from results of the base scenario, explaining the duration of bloom formation (time span between \(\text{doy}_{\text{chla},1}\) and \(\text{doy}_{\text{chla},3}\)). Meteorological variables shortwave radiation (\(Q_{sw}\)), air temperature (\(T_a\)) and wind speed (\(U\)) were averaged over the period of bloom formation and tested as explanatory variables. The multiple linear regression model explained 57.9% of the observed variation, with the relative importance of \(RI_{Q_{sw}} = 0.156\), \(RI_T = 0.072\) and \(RI_U = 0.352\).

<table>
<thead>
<tr>
<th>Explanatory variable</th>
<th>intercept</th>
<th>slope</th>
<th>(r^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Q_{sw})</td>
<td>19.45***</td>
<td>-0.05***</td>
<td>0.173</td>
</tr>
<tr>
<td>(T_a)</td>
<td>15.48***</td>
<td>-0.45***</td>
<td>0.105</td>
</tr>
<tr>
<td>(U)</td>
<td>-5.78***</td>
<td>5.20***</td>
<td>0.346</td>
</tr>
</tbody>
</table>

Another effect of the three studied meteorological variables of wind speed, air temperature and shortwave radiation was found for the duration of spring bloom formation (time between \(\text{doy}_{\text{chla},1}\) and \(\text{doy}_{\text{chla},3}\)). Bloom formation was fast (i.e. short time span between \(\text{doy}_{\text{chla},1}\) and \(\text{doy}_{\text{chla},3}\)) when irradiance and temperature were high and wind speeds low (Tab. 4.2). Remarkably, the wind conditions turned out to explain most variability, while air temperature was the weakest predictor. At the same time, a regression between the time span and \(\text{doy}_{\text{SML},30}\) showed a negative slope (\(\text{doy}_{\text{SML},30} = -0.35 \times T_{\text{chla3} - \text{chla1}} + 51.97\), \(r^2 = 0.31\), \(p < 0.001\)), i.e., it will take longer for a bloom to develop when it occurs earlier in the year.
4.3.2 Simulations with changed initial date: Stratification scenario & bloom scenario

Although the period of winter mixing had been ruled out in the stratification scenario, stratification onset \((\text{doy}_{\text{SML},30})\) still showed a large spread (mean = 118, standard deviation = 8). The onset of the phytoplankton spring bloom in the bloom scenario showed a narrower distribution (mean = 138, standard deviation = 5.6; Fig. 4.10).

Averaging deseasonalised meteorological variables over the period from simulation start until the timing of \(\text{doy}_{\text{SML},30}\) and \(\text{doy}_{\text{chla},3}\), respectively, resulted in significant correlations with onset timing (Fig. 4.5). Again, stratification and blooms began earlier with higher irradiance, higher air temperature and lower wind speeds. In the stratification scenario, air temperature and shortwave radiation showed a similar explanatory power \((r^2 = 0.23\) and 0.21), while wind speed had the lowest coefficient of determination \((r^2 = 0.16)\). In the bloom scenario, however, wind speed and shortwave radiation had a similar correlation with PSB timing \((r^2 = 0.31\) and 0.32), and air temperature the lowest \((r^2 = 0.23)\). Nevertheless, the scatter in all six regression models remained high.

Averaging meteorological conditions over the whole simulation period until the timing of stratification or bloom onset, however, is a suboptimal statistic as it does not allow the differentiation between effective time scales of the meteorological variables. We, therefore, systematically tested the explanatory power of the three meteorological variables over a range of time scales before the onset of stratification and blooming, respectively.

Explanatory power of all meteorological variables increased steeply with longer time scales of averaging and either showed an optimum or levelled off towards larger time scales (Fig. 4.6). In general, relevant time scales were shorter for stratification onset compared to bloom onset (also in the base scenario, not shown). This indicates that the establishment of stratification in most cases is a relatively fast process and a few days of favourable conditions are sufficient to establish a thermal stratification. The formation of the vernal algal bloom, however, proceeds slower and requires a longer period of favourable conditions as the increase in algal biomass is slower than the increase in surface temperature at this time of the year. The relevant time scale for wind forcing was shorter than the corresponding time scale for air temperature or shortwave radiation. The same patterns were identified when evaluating the base scenario (not shown).

Including all three meteorological variables into a multiple linear regression model and taking into account the respective optimum time scale for averaging explained up to 70% of the variability in stratification and bloom onset timing (Tab. 4.3). In all models the interaction terms were not significant and consequently removed from the model.

Taking the best regression model of each scenario and comparing the relative importance of the meteorological variables always indicated wind speed to have the largest importance. For bloom onset, for example, 70.2% of the observed variability was explained by the multiple regression model and wind alone contributed 37.3% to this value. That is, wind forcing accounted for roughly half of the explanatory power of the multiple regression model (Tab. 4.3). A similar pattern was found for stratification onset. The relative importance of shortwave
Figure 4.5: Relationship between stratification onset ($doy_{SML,30}$) and bloom onset ($doy_{chla,3}$) and averaged meteorological variables in the stratification scenario (a, c, e) and the bloom scenario (b, d, f). Meteorological variables in each realisation were averaged over the entire period from simulation start and the timing of stratification onset ($doy_{SML,30}$) and bloom onset ($doy_{chla,3}$), respectively. The dotted line shows the linear regression.
CHAPTER 4. PHYTOPLANKTON SPRING BLOOM

Figure 4.6: (a) Explanatory power (coefficient of determination) of the linear regression between the deseasonalised meteorological variables shortwave radiation (black), air temperature (blue) and wind speed (green) and stratification onset (doy$_{SML,30}$, stratification scenario) for different time scales of averaging. The x-axis shows the number of days before doy$_{SML,30}$ over which the explanatory variables were averaged. Filled symbols denote time scales where all 500 realisations were used for averaging. Open symbols denote time scales where some realisations had been removed because stratification onset in these cases had been faster than the given number of days. (b) The same graph for the results of bloom onset (doy$_{chla,3}$, bloom scenario).

Table 4.3: Multiple linear models explaining the onset time in the different scenarios. RI is the relative importance of the single explanatory variables. Averaging of meteorological variables was done over the whole simulation period (i.e. simulation start until stratification onset (doy$_{SML,30}$) and bloom onset (doy$_{chla,3}$), respectively), unless denoted by a subscript, which refers to the days before doy$_{SML,30}$ and doy$_{chla,3}$ over which the meteorological variable was averaged.

<table>
<thead>
<tr>
<th>Model</th>
<th>$r^2$</th>
<th>AIC</th>
<th>RI$<em>{Q</em>{sw}}$</th>
<th>RI$_T$</th>
<th>RI$_U$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stratification scenario</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>doy$<em>{SML,30} = 117.68 - 0.14 Q</em>{sw} - 1.68 T + 7.07 U$</td>
<td>0.436</td>
<td>3224</td>
<td>0.144</td>
<td>0.155</td>
<td>0.137</td>
</tr>
<tr>
<td>doy$<em>{SML,30} = 118.44 - 0.11 Q</em>{sw,20} - 1.62 T_{18} + 7.79 U_7$</td>
<td>0.672</td>
<td>2953</td>
<td>0.119</td>
<td>0.207</td>
<td>0.346</td>
</tr>
<tr>
<td><strong>Bloom scenario</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>doy$<em>{chla,3} = 138.55 - 0.11 Q</em>{sw} - 0.95 T + 8.92 U$</td>
<td>0.607</td>
<td>2681</td>
<td>0.232</td>
<td>0.190</td>
<td>0.266</td>
</tr>
<tr>
<td>doy$<em>{chla,3} = 138.58 - 0.11 Q</em>{sw,20} - 0.91 T_{23} + 9.67 U_{19}$</td>
<td>0.702</td>
<td>2542</td>
<td>0.217</td>
<td>0.112</td>
<td>0.373</td>
</tr>
</tbody>
</table>
radiation and air temperature differed between $doy_{SML,30}$ and $doy_{chla,3}$ with air temperature being more important for stratification onset (about 20%) and least important for bloom onset (about 11%). In summary, wind was identified to be the most relevant meteorological variable for the timing of stratification and bloom onset.

### 4.3.3 Simulations with changed meteorological variables

Increases in shortwave radiation and air temperature advanced stratification onset by 7 and 5 days on average and spring bloom onset by 6 and 5 days on average, whereas increased wind speeds delayed stratification onset by 17 days and spring bloom onset by an average of 13 days (Fig. 4.7). Conversely, a decrease in shortwave radiation and air temperature delayed stratification by 8 and 5 days and PSB onset on average by 7 and 3 days, whereas a decrease in wind speed resulted in stratification taking place an average of 11 days earlier and PSB onset on average 8 days earlier. Again, wind speed turned out to have the most powerful influence on stratification and PSB onset while air temperature had weaker effects.

### 4.4 Discussion

In the past, most climate impact studies on lakes concentrated on the temperature shift between the current and future climate (e.g. De Senerpont Domis et al., 2007; Elliott, 2012b; Trolle et al., 2014) or analysed warm anomalies in the current climate (e.g. Jöhnk et al., 2008; Straile et al., 2010). Our study emphasises that climate impact has more aspects than just...
the effects mediated by temperature. We even question whether temperature is the most important meteorological variable for the dynamics in lentic ecosystems. In fact, several modelling studies have started to test the sensitivity of lakes to other meteorological variables (e.g. Austin & Allen, 2011; Hetherington et al., 2015). However, in those studies meteorological variables were analysed independently from each other and the extent to which the variables are responsible for initiating the plankton succession in lakes has not been quantified. Other studies on Lake Constance have shown the importance of stratification onset for the beginning of the PSB (Ollinger, 1999; Peeters et al., 2007b) and have analysed the effect of meteorological conditions on that lake (Ollinger & Bäuerle, 1998; Gaedke et al., 1998b; Peeters et al., 2007a). However, the modelling studies analysed only few years and changed meteorological variables independently from each other. Peeters et al. (2007a) added a statistical analysis of long-term data on PSB onset to their study. While this analysis gave insight into effects of air temperature and wind speed on PSB timing, it did not resolve the relative importance of these variables. Furthermore, the analysis is based on a coarse measurement interval of weekly to biweekly sampling, making the precise timing of PSB onset problematic. In comparison, our simulation study allowed us to analyse meteorological effects based on a high number of years with a high temporal resolution. The model set-up enabled us to quantify the relative importance of different meteorological variables and to differentiate between separate periods in spring where meteorology has an effect on PSB timing.

Our two main outcomes are depicted in Fig. 4.8 and can be summarised as follows: First, besides air temperature also shortwave radiation and wind velocity play a crucial role for the succession start in lake ecosystems, with wind being by far more important for the timing than the other two variables. Second, we identified the relevant time scales over which these meteorological variables effectively act on lake ecosystems. These relevant time scales were shorter for wind velocity than for the other two variables and they were generally shorter for stratification onset compared to bloom onset.

Our results point to the fact that a reliable assessment of climate change effects on lake ecosystems requires a sound prediction of future wind conditions. However, due to large uncertainties on the global scale (Hartmann et al., 2013), such coherent projections for wind conditions on the regional scale are rather difficult to achieve. Our findings furthermore indicate that many previous studies on climate change effects on lakes with the focus on warming of a few centigrade (mostly 1...6 K temperature increase), may contain larger uncertainties than previously expected because these studies did not take future changes in wind velocity into account.

4.4.1 Phytoplankton spring bloom timing

The plankton succession in lakes is initiated when positive net growth of algae is maintained over a sufficiently long period. This start of succession can be seen as a two-step sequence in deep water bodies (Fig. 4.8): First, a stable thermal stratification establishes. Once this state is attained, favourable meteorological conditions initiate the second step and speed up algal growth giving rise to the PSB. The importance of stratification for the onset of
Figure 4.8: Conceptual scheme for the sequence of stratification and bloom onset and the relative importance of different meteorological variables. The width of the onset boxes reflects the respective variation in the timing of stratification and bloom onset. The colour gradient in stratification and bloom onset boxes refers to the respective density distribution, with the darkest colour at the mean onset time. The arrows indicate the relative importance of the meteorological variables (arrow width) and the most effective time scale (arrow length) for explaining stratification and bloom onset.

The phytoplankton spring bloom (PSB) is well documented in lakes (Ollinger, 1999; Peeters et al., 2007b) and the ocean (Fischer et al., 2014). Our study revealed, too, that the timing of stratification is a good predictor of the PSB onset timing. The causal mechanism is light limitation of phytoplankton as long as vertical mixing takes place over the whole water column. As soon as stratification has started to build up, algal cells are not mixed deep into the water column anymore and gain a better average light supply. The window of opportunity for stratification onset was rather broad in our study and in the range of several weeks (from doy 89 to 142). Once stratification has established, the phytoplankton achieves an ‘explosive state’ since favourable meteorological conditions immediately give rise to ‘explosive’ phytoplankton growth. This growth can be very fast. In our simulations the shortest time recorded to grow from 1 to 3 $\mu g$ L$^{-1}$ was just five days. The majority of simulations, however, revealed a range between 5 and 15 days. In fact, there are many possible combinations of environmental conditions for sustaining the formation of a PSB. When the depth of the SML is quite shallow, for example, already intermediate shortwave radiation suffices for algal growth. When on the other hand the SML depth is quite deep, algal growth can only take place if shortwave
radiation is at very high levels. During this phase, the ecosystem is also highly susceptible for perturbations, particularly by wind.

A detailed analysis of individual scenarios revealed that wind-induced perturbations (e.g. deepening of the SML by a storm event) are an important element in the phenology of phytoplankton dynamics during early spring and it appears that this mechanism is the main cause for the dominating importance of wind for the timing of the PSB onset.

4.4.2 Changed meteorological conditions

Changing the meteorological forcing underpinned the effects of the studied meteorological variables. Shortwave radiation, air temperature and wind speed all showed an effect on bloom timing. Comparing the effect of different meteorological variables on spring bloom timing with each other is rather difficult due to different scales and units. We tried to achieve a comparative approach, by applying factors calculated from fixed percentiles (25% and 75% quantiles) of each variable’s distribution.

Our approach showed that air temperature changes had a relatively weak effect on PSB timing compared to shortwave radiation and wind speed changes. Despite the arguably difficult quantitative comparison of the effects, it was made evident that air temperature is only one of three possible important drivers of PSB timing and clearly less important than wind (Fig. 4.8).

The probability of high wind speeds is larger during winter than during summer (Fig. 4.2). Since stratification onset strongly depends on turbulence, generated by wind forcing, the occurrence of storm events with the potential to destroy emerging stratification is more likely early in the year. A shift towards earlier stratification onset by increased air temperatures might be outbalanced by the higher probability of high wind speeds earlier in the year. Additionally, shortwave radiation is an important ingredient for stratification onset because the required heat input can only be achieved at sufficiently high radiative fluxes. Therefore, even if PSB onset is shifted towards earlier dates by increasing air temperature alone, the counterbalancing or reinforcing effects of other meteorological variables should be taken into account, too. These compensatory and reinforcing effects were shown by Schlabing et al. (2014), who found a widening in the distribution of PSB onset with changed climate.

Many climate change studies on aquatic ecosystems have a strong bias towards temperature change (e.g. Trolle et al., 2014) or summarizing measures like the NAO (e.g. Gerten & Adrian, 2000). Only a few studies directly included other meteorological factors (e.g. Peeters et al., 2007a) and even less assessed the relative importance of these driving factors (e.g. Arhonditsis et al., 2004a). The interplay of different meteorological variables can only be analysed by looking at different combinations of meteorological conditions and taking the variability in meteorological drivers into account. Hence, our methodology of choosing a probabilistic approach using several hundreds of meteorological realisations contributes to a more sophisticated analysis of climate impacts on ecosystems that goes beyond plain changes in individual meteorological variables. In our study, the covariance present between the variables in the observed meteorological data was conserved by the weather generator, making
each realisation statistically reasonable but different in detail. This allowed a comprehensive assessment of the variability present in meteorological variables.

Coupling the stochastic weather generator with a deterministic lake model filled a gap in climate impact studies on lentic ecosystems. With this ‘modelling lab’ we reproduced inter and intra-annual variability and excluded disturbing factors from hydrology or nutrient supply. This meteorological variability alone led to a high variability in PSB onset timing. The importance of wind velocity for the timing of the PSB lets us question the strong focus on air temperature effects on aquatic systems in many current climate change studies on lakes. Admittedly, it is unlikely that other meteorological variables as irradiance or wind speed increase unboundedly together with air temperature, because of physical constraints. However, this fact just stresses the urgent need for a higher certainty in predicting changes in wind speeds and irradiance (including effects from changing cloud cover).

Acknowledgements

For providing data for model validation we thank the German Meteorological Service (DWD), the Limnological Institute at the University of Konstanz, the IGKB (Internationale Gewässerschutzkommission für den Bodensee) and the ISF (Institut für Seenforschung, Langenargen, Germany). The Centre for Water Research at the University of Western Australia is thanked for providing the model DYRESM-CAEDYM. We thank Wendy Anne Kopisch for proofreading large parts of the manuscript. M.F. and D.S. were financially supported by the DFG (Deutsche Forschungsgemeinschaft, grant Ri 2040/1-1 and grant BA 1150/14-1) and the IMPRS (International Max Planck Research School) for Organismal Biology. M.F. would like to thank Barbara Helm, Kathryn Elmer and the Haggis group for their marvellous writing course.
4.5 Supplements

Temperature profiles extracted from the simulations at \( \text{doy}_{\text{SML},30} \) revealed a relatively narrow temperature range (Fig. 4.9). The median calculated from those realisations with the 10% earliest \( \text{doy}_{\text{chla},3} \) resulted in a steeper profile with colder temperatures above 190 m than the median of all realisations. The median profile from the late bloom realisations showed warmer temperatures.

**Figure 4.9:** Water temperature profiles from each realisation at the day of the year on which the surface mixed layer became shallower than 30 m, \( \text{doy}_{\text{SML},30} \) (grey lines). Median profile of all realisations (thick black line), median of early blooms, defined as those realisations within the 10th quantile of \( \text{doy}_{\text{chla},3} \) (red line), median of late blooms, defined as those realisations above the 90th quantile of \( \text{doy}_{\text{chla},3} \) (blue line), base scenario.

**Figure 4.10:** Distribution of phytoplankton spring bloom onset, \( \text{doy}_{\text{chla},3} \), (a) and the time needed by the phytoplankton to grow from \( \text{doy}_{\text{chla},1} \) to \( \text{doy}_{\text{chla},3} \) (b) for the simulations starting with a stratified temperature profile.
Predictive utility of trait-separated phytoplankton groups: A robust approach to modeling population dynamics

Reynolds, C.S., Elliott, J.A., Frassl, M.A.


Abstract

We explore here the sensitivity and predictive power of quantified morphological and physiological properties of phytoplankton. We have adopted groups of species, distinguished by the clear morphological- and physiological-traits (Kruk *et al.*, 2010; Litchman *et al.*, 2010), and simulated their growth in various environments, using the model PROTECH (Phytoplankton RespOnses To EnvironmenTal CHange). This well-tested model uses equations fitted to optimal growth performances of various (“real”) phytoplankton species, described in terms of their functional attributes. Thus, we are able to reconstruct successional series in a range of shallow and deep lakes, situated at set latitudes (temperate or “Mediterranean”). All sequences are initiated at equal biomass levels but they soon become dominated by Groups which responded positively to the changing environmental conditions. We show the selection of small algae under conditions of good light and resource abundance and their subsequent collapse, especially as a consequence of zooplankton consumption. We show the advantages accruing to larger organisms that escape grazing but may also be motile and better defend assembled biomass against loss. Lengthening of cells or filaments of many cells increases organismic size but preserves the high surface-to-volume ratios that aid optimal interception of underwater light in turbid, mixed layers. Nitrogen-fixing capability confers to appropriately adapted species the opportunity to dominate when diminishing supplies of nitrogen limit the growth of other algae. Models founded on trait-separated phytoplankton demonstrate the value of these properties to the description and interpretation of phytoplankton succession.
5.1 Introduction

The desire to understand the assembly of the dominant phytoplankton in lakes and seas and to predict the compositional responses to supposedly driving events has been implicit from the earliest papers on the subject (reviewed in Reynolds, 2006). As knowledge has been developed and technology has been refined, it has been recognized that the prediction of outcomes at the species levels is difficult, perhaps even impossible, owing to the vast variability in environmental influences (Reynolds, 2000). In recent times, there has been progress in resolving compositional responses by reference to groups of alternative species, some of whose members happen to be present at the same time, essentially because they also share similar relevant morphological or physiological pre-adaptations, or traits (see review of Naselli-Flores & Barone, 2011). For instance, the species that are able to grow the fastest in-situ are also particularly small and whose cells have relatively large surface areas in relation to their volumes to enable the rapid exchange of resources and wastes across their surfaces. Equally, the capacity to reduce (“fix”) uncombined gaseous nitrogen in solution offers nitrogen-fixing Cyanobacteria (heterocystous Nostocales) a considerable dynamic advantage over other, non-adapted autotrophs which can be constrained by severely depleted stocks of combined nitrogen.

The recent interest in recognizing traits and defining trait-separated groups of species has been increasing, at least since the publication of Reynolds’s (1984) exploratory paper. Notable recent attempts to categorize and give identities to the so-called functional types include those of Padisák et al. (2009) and Kruk et al. (2010, 2011). Beyond merely describing natural phytoplankton assemblages, attempts have also been made to simulate the dynamics of their selection and assembly using models to predict the compositional response of the phytoplankton (see the review of Mooij et al., 2010). Unfortunately, there is no universal agreement about how to reconstruct population dynamics. Many authors have built anabolic models, invoking well-established components relating to photosynthesis and resource uptake; but, as pointed out by Reynolds & Irish (1997), these tend to exaggerate specific in-situ growth rates. These authors ventured that the predicted specific growth rates are subject to resource saturation and to critical depletion and that the corresponding relationships could be used to determine the extent to which growth rate is impaired. This approach was incorporated into the simulation model PROTECH (Phytoplankton RespOnses To Environmental CHange; see Reynolds et al., 2001) specifically to quantify the subtractive impairment of growth caused by inadequate resources (including temperature, daily insolation and depletion of critical nutrient resources) on specific performances. Moreover, the model invokes certain morphological properties of named species, certain specific specialisms (e.g. requirement for skeletal silicon or the ability to fix nitrogen) and to the buoyant, sinking and swimming behavior. PROTECH has been used extensively over the last decade (Trolle et al., 2012) to simulate, reconstruct and predict the dominant phytoplankton in a wide range of physical environments (for a recent overview, see Elliott et al., 2010).

In this paper, we use model solutions to focus on the power and sensitivity of selected
morphological and physiological traits of phytoplankton that we would expect to govern their
dynamic performances in natural environments, responding to seasonal or stochastic fluctu-
ation. The algae have no identities, saving the morpho-functional groupings to which we
ascribe them. The functional traits that we give them are strongly influenced by the papers
of Litchman & Klausmeier (2008), Litchman et al. (2010) and of Kruk et al. (2010). Being
easy to recognize, we have first distinguished seven morphological forms, and then introduced
physiological caveats where these were necessary or appropriate. An eighth group is added
to separate nitrogen-fixing Cyanobacteria. We have then introduced this model phytoplank-
ton assemblage to each of a range of simulated environmental scenarios in order to test and
express their functional traits.

5.2 Methods

The PROTECH model (Elliott et al., 2010) was used to simulate the dynamics of the assem-
bly of phytoplankton in two different kinds of water body (“shallow”, “deep”) in two different
latitudes (“temperate”, 52.8 °N and “Mediterranean”, 32.5 °N). These types of lakes were
selected because in the past the model has already been successfully tested and applied to
real lakes which were similar to the hypothetical ones presented in this study (e.g. Elliott
et al., 2000; Lewis et al., 2002; Moreno-Ostos et al., 2007; Elliott, 2010, 2012b). PROTECH is
set up to simulate events in lakes described by their morphometries, defined by the summed
areas of successive layers, each 0.1 m deep, forming the complete water column. Water is
exchanged by depth-specific inflow which may be integrated by known or given levels of wind
stress on the surface, subject to the Wedderburn density resistance induced by measured or
calculated heat fluxes across the surface, and included in the PROTECH model. Thus, simu-
lated columns can stratify, remain stratified or be mixed to depth again. The transparency of
the water is expressed by the vertical extinction coefficient of the alga-free water ($\varepsilon_w$), albeit
as affected by colored solutes and suspended particulate matter (tripton) represented by a
notional constant background extinction coefficient. The impact on algal growth is repre-
sented by a variable product owing to the morphology and existing concentration of biomass
of each species modeled (see Reynolds et al., 2001, for details). Growth-sustaining nutrients
are introduced with the inflow and distributed with depth according to the mixing. Algal
species or types are allowed to grow and accumulate in each layer of the simulated column,
at species-specific daily rates that are sensitive to temperature, to the probabilistic time of
exposure to saturating light and to the concentrations of each nutrient continuing to saturate
or limit proportionately the specific growth requirement, i.e. growth limitation occurs when
concentrations are below 3 mg m$^{-3}$ SRP, 80 mg m$^{-3}$ NO$_3$ or 550 mg m$^{-3}$ SiO$_2$, depending
on the needs of the alga. Where relevant, algae may move vertically (sink, float or swim) in
the water column, in accord with species-specific rules. Algae smaller than 50 µm are subject
to removal by grazers, according factors based upon the changing abundance of zooplankton
(modeled on responses of Daphnia) and invoking temperature, growth dynamics and the con-
tinued nourishment of the feeders. For full details of the constants and variables invoked, see
Reynolds et al. (2001).

We have not assumed continuously benign growth conditions with regard to the weather conditions for the modeled lakes. Data on air temperature and cloud cover were derived from the German meteorological service (DWD). We chose two stations representing two different climate zones, according to a classification scheme by Schultz (2000): one temperate climate (station Magdeburg, Germany), and one Mediterranean climate (station Haifa, Israel). Climate data were given as monthly means from the reference period 1961–1990. These monthly means were linearly interpolated using the statistical software R (R Core Team, 2012) to provide low-variance synopses of seasonal weather patterns to drive the simulations. From these interpolated data, daily values were derived and used as input data for PROTECH. To provide a pattern of seasonal stratification for the simulations, daily wind speeds were set to be constant for the shallow and deep lakes (3 and 6 m s\(^{-1}\) respectively). Similarly, daily discharge into and out from the lakes was set at a constant value to give a 182.5 day hydraulic retention time for both the shallow and the deep lake (Table 5.1). Thus, although these driving conditions are somewhat artificial, they are purely there to produce a varying seasonal pattern that allows new ecological niches to be expressed in the model environment.

Table 5.1: Summary of the lake habitat characteristics utilized for the PROTECH simulation runs.

<table>
<thead>
<tr>
<th></th>
<th>Temperate shallow</th>
<th>Mediterranean shallow</th>
<th>Temperate deep</th>
<th>Mediterranean deep</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latitude</td>
<td>52.8 °N</td>
<td>32.5 °N</td>
<td>52.8 °N</td>
<td>32.5 °N</td>
</tr>
<tr>
<td>Depth (m)</td>
<td>10</td>
<td>10</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>Volume (10^6 m(^3))</td>
<td>20</td>
<td>20</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Hydraulic exchange (10^6 m^3 d(^{-1}))</td>
<td>0.1096</td>
<td>0.1096</td>
<td>0.548</td>
<td>0.548</td>
</tr>
</tbody>
</table>

Initial concentrations: 200 mg MRP m\(^{-3}\), 1000 mg DIN m\(^{-3}\), SRSi 3500 mg m\(^{-3}\), except as stated. Daily inflow concentrations: 500 mg MRP m\(^{-3}\), 5000 mg DIN m\(^{-3}\), SRSi 5000 mg m\(^{-3}\), except as stated. The water is ascribed a background light-extinction coefficient (\(\varepsilon_w\)) of 0.1 m\(^{-1}\), prior to the introduction of any algae, unless otherwise stated (see text). Note that there is no unique euphotic depth; the light compensation of growth is solved independently for each Group in the model according to its morphological traits.

Characteristic traits accorded to the eight species adopted (Groups I–VIII) are set out in Tables 5.2 and 5.3. The selection is based on the morphological categories of Kruk et al. (2010) which includes organisms covering a wide variety of sizes and shapes of flagellate, buoyancy-regulating and non-motile species, as well as obligate consumers of dissolved silicon and a facultative nitrogen fixer. To populate the Groups, we have selected morphometric data pertaining to individual species from the PROTECH phytoplankton library which we consider to be representative of that particular function type. Organismic size also conveys the susceptibility to removal by populations of actively grazing zooplankton. Only organisms in which the maximum linear dimension (m) is <50 \(\mu\)m are considered liable to elimination by grazers (Burns, 1969). Individual filter feeders can ingest larger particles that are suitably narrow in diameter and suitability orientated for consumption (Nadin-Hurley & Duncan, 1976; Ferguson et al., 1982) thus we have also classed Group-VI diatoms as available to grazers.

The model runs incorporate a daily inoculum of algae, spread evenly between the eight
Groups (which in aggregate is equivalent to a total chlorophyll concentration of 1 mg chl a m\(^{-3}\)), to augment what is presumed to be the existing standing crop. This is intended to prevent any population being exhausted by losses but without unduly biasing the outcome attributable to daily augmentation resulting from the recruitment through population growth.

Table 5.2: The morphological and phylogenetic characteristics of the eight modeled groups. The last three columns in the lower part of the table are simple logic statements (True (T)/False (F)) which, if True, activate the relevant PROTECH sub-routines.

<table>
<thead>
<tr>
<th>Functional groups</th>
<th>Surface area (s) ((\mu m^2))</th>
<th>Volume (v) ((\mu m^3))</th>
<th>Max. dimension (m) ((\mu m))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group I (small with high s v(^{-1}))</td>
<td>108</td>
<td>72</td>
<td>11</td>
</tr>
<tr>
<td>Group II (small siliceous flagellate)</td>
<td>2827</td>
<td>14140</td>
<td>30</td>
</tr>
<tr>
<td>Group III (large gas-vacuolate filaments)</td>
<td>7350</td>
<td>13970</td>
<td>300</td>
</tr>
<tr>
<td>Group IV (small non-flagellate)</td>
<td>50</td>
<td>33</td>
<td>4</td>
</tr>
<tr>
<td>Group V (medium/large unicellular flagellate)</td>
<td>1030</td>
<td>2710</td>
<td>21</td>
</tr>
<tr>
<td>Group VI (siliceous non-flagellate)</td>
<td>6690</td>
<td>5160</td>
<td>130</td>
</tr>
<tr>
<td>Group VII (large mucilaginous colonies)</td>
<td>7850</td>
<td>66500</td>
<td>50</td>
</tr>
<tr>
<td>Group VIII (nitrogen-fixing cyanobacteria)</td>
<td>6200</td>
<td>29000</td>
<td>75</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Functional groups</th>
<th>Diatom?</th>
<th>Grazed?</th>
<th>Nitrogen fixer?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group I (small with high s v(^{-1}))</td>
<td>F</td>
<td>T</td>
<td>F</td>
</tr>
<tr>
<td>Group II (small siliceous flagellate)</td>
<td>F</td>
<td>T</td>
<td>F</td>
</tr>
<tr>
<td>Group III (large gas-vacuolate filaments)</td>
<td>F</td>
<td>F</td>
<td>F</td>
</tr>
<tr>
<td>Group IV (small non-flagellate)</td>
<td>F</td>
<td>T</td>
<td>F</td>
</tr>
<tr>
<td>Group V (medium/large unicellular flagellate)</td>
<td>F</td>
<td>T</td>
<td>F</td>
</tr>
<tr>
<td>Group VI (siliceous non-flagellate)</td>
<td>T</td>
<td>T</td>
<td>F</td>
</tr>
<tr>
<td>Group VII (large mucilaginous colonies)</td>
<td>F</td>
<td>F</td>
<td>F</td>
</tr>
<tr>
<td>Group VIII (nitrogen-fixing cyanobacteria)</td>
<td>F</td>
<td>F</td>
<td>T</td>
</tr>
</tbody>
</table>
Table 5.3: Summary of vertical movement instructions (based on field observations summarized in Reynolds et al. (2001)) for the eight modeled groups. In all cases of either moving up or down, if the top or bottom layer of the water column is encountered the movement is stopped; if it is the bottom layer the phytoplankton is also lost.

<table>
<thead>
<tr>
<th>Phytoplankton</th>
<th>Light condition (µmol photon m(^{-2}) s(^{-1}))</th>
<th>Movement (m d(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group I</td>
<td>&gt;150</td>
<td>Sink 0.5</td>
</tr>
<tr>
<td></td>
<td>≤ 150 but &gt;30</td>
<td>Sink 0.1</td>
</tr>
<tr>
<td></td>
<td>≤ 30</td>
<td>Rise 0.5</td>
</tr>
<tr>
<td>Group II &amp; V</td>
<td>&gt;100</td>
<td>Rise 0.1</td>
</tr>
<tr>
<td></td>
<td>≤ 100</td>
<td>Rise 2.0</td>
</tr>
<tr>
<td>Group III</td>
<td>&gt;30</td>
<td>Sink 0.1</td>
</tr>
<tr>
<td></td>
<td>≤ 30 but &gt;10</td>
<td>No move</td>
</tr>
<tr>
<td></td>
<td>≤ 10</td>
<td>Rise 0.1</td>
</tr>
<tr>
<td>Group IV &amp; VII</td>
<td>All</td>
<td>Sink 0.1</td>
</tr>
<tr>
<td>Group VI</td>
<td>≤ 500</td>
<td>Sink 0.2</td>
</tr>
<tr>
<td></td>
<td>&gt;500</td>
<td>Sink 1.0</td>
</tr>
<tr>
<td>Group VIII</td>
<td>&gt;100</td>
<td>Sink 0.3</td>
</tr>
<tr>
<td></td>
<td>≤ 100 but &gt;30</td>
<td>Sink 0.1</td>
</tr>
<tr>
<td></td>
<td>≤ 30 but &gt;10</td>
<td>No move</td>
</tr>
<tr>
<td></td>
<td>≤ 10</td>
<td>Rise 0.1</td>
</tr>
</tbody>
</table>

5.3 Model runs

5.3.1 Resource abundance

The initial outputs simulate the changing abundance and composition of the phytoplankton during a calendar year in each of the four systems, each commenced with an abundance of nutrient resources (molybdate-reactive phosphorus, MRP; dissolved combined inorganic nitrogen, DIN; soluble reactive silicon, SRSi) and receiving continuing daily inputs of MRP, DIN, SRSi, as summarized in Table 5.1. The physical medium also varies during this period: it is interesting to compare the physical structure of the water column. In each of the four scenarios, the water column becomes segregated, shown, in this instance, by the extent of the mixed layer, effectively, the distance from the surface to the calculated point of a first change in density. Although PROTECH may be used to generate full data for each 0.1-m vertical layer (see for example, Reynolds et al., 2001), the approach we have adopted to present our results mimics an integrated sample of the upper 5 m of the water column, consistent with many sampling protocols. For example, as a consequence of enhanced insolation and air temperature, the mixed layer of the shallow temperate lake (Fig. 5.1a) shrinks over a couple of weeks starting on day 126 (early May) to be 5.2 m above the bottom (i.e. to 4.8 m below the surface).

A further enhancement of stratification is registered on day 223, in mid August, before a general increase in mixing, eventually to complete isothermy on day 300 (end of October). Comparing this plot with the simulation of the 50-m column at temperate latitude (Fig. 5.1c), the vernal shrinkage of mixed depth is similarly timed but proceeds only until the mixed layer...
Figure 5.1: The dynamics of the eight simulated groups (expressed as group specific chlorophyll a, mg m\(^{-3}\)) and mixed depth (m) over a year. a) shallow, temperate lake, b) shallow, Mediterranean lake, c) deep, temperate lake and d) deep, Mediterranean lake. Note that mixed depth (solid black line) is measured relative to the lake bottom and periods where nutrients were limiting in the simulations are represented by solid horizontal lines (Si: red line, N: brown line, P: black line).
hovers at 10-12 m below the water surface and takes longer to break down at the year end (day 340, well into December). In the corresponding plots for the Mediterranean location (Fig. 5.1b & d), the earlier onset of stratification in the shallow lake is evident (Fig. 5.1b), as its persistence in the autumn and the closeness with which it occasionally comes to the water surface. The period of stratification in the deeper Mediterranean lake (Fig. 5.1d) is broadly comparable with that of the shallow Mediterranean lake but is longer than in the deep temperate lake (Fig. 5.1c).

The Group specific biomass (as expressed by its chlorophyll-\(a\) content) is respectively shown for each of the four model systems (Fig. 5.1), by their integrated concentrations in the top 5 m of the water column. It is worth reiterating that the starting concentrations of each algal Group (I–VIII) and the quantity of each inoculated daily are mutually identical; yet the shared growth conditions seem to select strongly in favor of the recruitment of only some Groups rather than others. Moreover, the selection is not constant, with Groups being favored or discounted in turn, thus creating the evident model periodicities. Thus, in the case of the shallow temperate lake during the first half of the year (Fig. 5.1a), Group IV, then Group VI and Group I are recruited preferentially. As growth draws on the resources available, so as the conditions become less favorable because nutrients fall to concentrations that are no longer able to sustain the potential growth that the unmodified model equations predict. Such occasions are marked by the horizontal bars, identifying as appropriate those periods when either Si, or N or P has fallen to a growth-limiting concentration; these do not distinguish relative severity. Biomass lost to sinking or grazing is no longer replaced readily and aggregate standing biomass tends to fall away during the middle part of the year, when other, typically larger, species Groups (III and VIII) begin to figure in the assemblage (Fig. 5.1a).

In the shallower Mediterranean system (Fig. 5.1b), it is apparent that the same species-Groups are selected but in altered proportions and starting earlier in the year than seen in the temperate equivalent and reflecting the different insolation and air temperature pattern. Notably, Group I performs better than Group IV in the early months; Group III is more abundant and more persistent. In the deeper temperate system (Fig. 5.1c), it is striking how weak recruitment is in the first half of the year and that it is only after day 165 (mid June) that the stratification is sufficiently well established for phytoplankton (Groups I, VI and III) to be recruited in strength; the latter Group of filamentous algae eventually ascended to dominance. In the deep Mediterranean scenario (Fig. 5.1d), it is Group VI and, especially, Group III that are most successful. These performances are indicative of tolerance of the light conditions (long periods in the dark part of water columns mixed to depth); they are scarcely conditioned by nutrient limitation.

5.3.2 The effect of biomass removal by grazers

Building on the baseline simulation, we next slightly altered the modeled conditions in order to test deductions about the early growth of small algae (Groups I and IV) in the shallower water columns in the first half of the year, and the likelihood that the summer collapse in
their populations is attributable to seasonally developing grazing pressure, we simply turned off the grazer function in PROTECH, i.e. no alga was removed by grazer consumption. The outputs from runs based on shallow and deep lakes at latitudes 52.8 °N and 32.5 °N (Fig. 5.2) each followed a reasonably similar pattern to that seen in the baseline scenario (Fig. 5.1).

In the shallow temperate lake, the ungrazed vernal biomass (Fig. 5.2a) is scarcely different from the baseline run and is similarly dominated by Groups IV, I and VI. However, there is a widening departure later in the year as the dominance of Group IV is allowed to persist, while Groups VIII and, especially, Group III are reduced relative to the baseline run (Fig. 5.1a). In the lower-latitude shallow lake (Fig. 5.2b), preferential selection of Group I over Group IV is again evident (cf. Fig. 5.1b) but Group III and Group VIII organisms still dominate the summer assemblage in much the same way.

In the deeper lakes, Group III dominates at either latitude (Fig. 5.2c & d) but the evidently enhanced performances of Group VI are attributable to the cessation of consumption by grazers.
5.3.3 The effect of impaired light penetration

The impact on recruitment and succession of a depressed insolation level was tested next by raising the background vertical extinction coefficient ($\varepsilon_w$) from 0.1 to 0.5 m$^{-1}$. This reduces the depth of the photic zone and, thus, the daily photoperiod experienced by algae entrained in all but the shallowest of mixed layers. In both the 10-m temperate and Mediterranean lakes (Fig. 5.3a & b), the poorer light conditions delays the development of the phytoplankton and severely reduces the biomass attained by Groups I and IV, relative to the baseline (Fig. 5.1a & b); in contrast, the recruitment of Group VI is scarcely altered and that of Group III, the filamentous Cyanobacteria, is evidently enhanced. Similarly, the recruitment of the Groups of small algae (I and IV) is depressed in favor of Group III. Lower summer biomass features moderate populations of Group-VIII nitrogen-fixers.

![Graph showing the dynamics of the eight simulated groups over a year with increased background light coefficient.](https://example.com/graph.png)

**Figure 5.3:** The dynamics of the eight simulated groups (expressed as group specific chlorophyll a, mg m$^{-3}$) over a year but with an increased background light coefficient. a) shallow, temperate lake, b) shallow, Mediterranean lake, c) deep, temperate lake and d) deep, Mediterranean lake. Note that periods where nutrients were limiting in the simulations are represented by solid horizontal lines (Si: red line, N: brown line, P: black line).

In the deeper water columns at either latitude, growth of all Groups is severely depressed (Fig. 5.3c & d) except in the case of Group III, which still manages to raise its biomass to about two-thirds of that in the corresponding baseline (Fig. 5.1c & d). Also, it is interesting to note that at no time does nutrient availability interfere with growth.
5.3.4 The effects of nitrogen shortage

PROTECH is readily amenable to testing the effects of adjustments in the supply of each nutrient. Impairment of the MRP available affects the net growth of all species, so any interspecific differentiation of performances would be attributable to spatial differences in sourcing (nutrients gained in deep, unmixed layers) and to rapid vertical migrations of replete populations. Impairment of SRSi availability is likely to have adverse effects upon the growth responses only of species requiring moderate to large amounts for the assembly of exoskeletal structures, i.e., those of Group VI. Impairment of the availability of DIN would have a similar simultaneously depressive effect on the net growth of most of the phytoplankton as phosphorus shortages but for the biological advantage conferred on nitrogen-fixing Cyanobacteria being intensive in its energy use, requiring substantial levels of phosphorus as well as of trace metals (iron, molybdenum, vanadium), nitrogen fixation is not a characteristic activity but confined to periods of external DIN shortages.

In PROTECH, the “opportunistic” resort to nitrogen fixation is simulated by allowing Group VIII organisms to grow and to draw their nutrient requirements from the stocks in solution as do other Groups but to “ignore” (be unaffected by) low environmental levels of DIN. Therefore, PROTECH simulations were conducted for each of the four habitats but with a constraint on DIN availability (the initial concentration and that of the daily additions were halved to 500 and 2500 mg N m$^{-3}$, respectively). Events in the simulated shallow temperate lake (Fig. 5.4a) are, initially, similar to those in the corresponding baseline (Fig. 5.1a), though yields soon became constrained by the earlier onset of nitrogen limitation. Predictably, only Group VIII was able to thrive, pending the onset of phosphorus limitation. In the shallow Mediterranean lake (Fig. 5.4b), Group VIII replaces Group III as the dominant through most of the growing season. In the absence of significant nitrogen limitation, light limitation was still the most important factor which led to Groups VI and III remaining the principal forms in both deep columns (Fig. 5.4c & d).

5.3.5 Effect of excluding high-performance organisms

So far, the simulated conditions have strongly favored representing Group-I, -III, -IV and -VIII organisms, while Group VI (diatoms) is also well represented. Although they are inoculated in all the runs, the remaining Groups are scarcely picked out in the scenario outputs. Clearly, their performances are poor compared with the species that were selected in the earlier runs and are inadequate to establish them when nutrients or light have been reduced to limiting levels. This might have told us something about the distributions and relative competitiveness of flagellates in Groups II and V, and the colonial forms in Group VII species, but we decided to execute PROTECH simulations of assemblages in which some of the high-performance or specialist species were excluded. Thus, simulations were run for the four lakes using baseline conditions but with the exclusion of species ascribed to Groups I, III, IV and VIII. Examining the shallow temperate lake first (Fig. 5.5a), it can be seen that Group-VI diatoms increase smoothly to a greater April peak biomass than that observed in the equivalent baseline (Fig.
Figure 5.4: The dynamics of the eight simulated groups (expressed as group specific chlorophyll $a$, mg m$^{-3}$) over a year but with reduced nitrate inputs. a) shallow, temperate lake, b) shallow, Mediterranean lake, c) deep, temperate lake and d) deep, Mediterranean lake. Note that periods where nutrients were limiting in the simulations are represented by solid horizontal lines (Si: red line, N: brown line, P: black line).

5.1a), even though its timing is scarcely changed. Thus, we are justified in judging the diatoms as being “outperformed” rather than “outcompeted” by smaller organisms in the baseline simulation; the reduced contest for resources nevertheless allowed the diatoms to build a larger biomass. It also seems likely that this diatom biomass wasted slowly, through a combination of silicon exhaustion, sedimentation and grazing. A phase of strong recruitment by Group-V flagellates is signaled in the middle months of the year (including a rather modest growth of Group-II silicoflagellates), after which, the mucilaginous colonies of Group VII develop a dominant biomass.

The successional sequence in the shallow Mediterranean lake (Fig. 5.5b) is very similar to that in the temperate (Fig. 5.5a), although, once again, it commences about a month earlier; however, neither the flagellates (Group V) nor the mucilaginous colonial species (Group VII) achieve biomass levels that are comparable with those attained at the higher latitude. In the deeper temperate lake (Fig. 5.5c), the similar sequence was visibly confined to the summer period, more by temperature and stratification than by nutrients, as only silicon was shown to limiting for any length of time. The sequential differences in the deeper Mediterranean lake (Fig. 5.5d) are mainly ones of timing (note the earlier diatom growth, cf. the deeper temperate
Figure 5.5: The dynamics of only four simulated groups (chlorophyll $a$, mg m$^{-3}$) over a year. a) shallow, temperate lake, b) shallow, Mediterranean lake, c) deep, temperate lake and d) deep, Mediterranean lake. Note that periods where nutrients were limiting in the simulations are represented by solid horizontal lines (Si: red line, N: brown line, P: black line).

Overall, we may deduce that all the devised algal groups were, at some time, able to grow in the simulated environments; given the severity of selective conditions imposed, special features of morphological or physiological adaptation were, undoubtedly, strongly influential in refining the species structure of the resultant assemblage. The outputs may be slightly exaggerated but, qualitatively, are sufficiently realistic to raise confidence in the power of PROTECH to simulate well-known dynamic patterns observable in nature.

5.4 Morphological and physiological traits of phytoplankton and their relevance to assemblage composition

Just as numerous species of freshwater phytoplankton have been recognized and described (about 5000 have been named over the last 150 years: Reynolds, 2006), so as a correspondingly wide diversity of contrasting characteristic behavioral traits has been discerned (Kruk et al., 2010). For instance, it is now well established that the most efficient conversion of assimilated carbon and nutrient resources to reproductive biomass is achieved by organisms characterized
by having a high surface area-to-volume ratio, either through having a small absolute size (typical of nanoplatinktic species) or, among larger-celled species, a convoluted shape, departing far from that of a sphere of identical volume (consider many microplanktic diatoms). Through having the capacity for rapid dynamic response to favorable light- and nutrient-conditions coinciding with seasonally lengthening days and warming waters of shallow or stratifying lakes, such organisms are able to develop substantial populations that sequester a significant amount of the resource available. To predict which species dominates is difficult and often stochastic; but the functional traits of the eventual dominant may be anticipated with consequence. However, the extent of the success of that species (how large a crop will be attained?), and its persistence (for how long will it remain dominant?) depend on the continued adequacy of sustaining resources, as well as the strength of responses consequent upon its abundance. For instance, small organisms (Groups I, IV, V) are vulnerable to respirational exhaustion if they fall out of the illuminated layers and to consumption as food by animals. Sooner or later, the advantage moves towards larger organisms which escape grazing (III, VII, VIII) and, given their abilities to move relative to the medium (e.g. they can swim or control buoyancy), may be able to better defend their biomass against these losses. However, these traits do not necessarily always overcome the inadequacies of the intrinsically slow growth rates associated with large phytoplankton. Lengthening of cells or filaments of many cells is another strategy of size increase that not only preserves high surface-to-volume ratios but also simultaneously helps to maintain optimal interception of underwater light (Kirk, 1976; Reynolds, 2006; Reynolds et al., 2001).

In such ways, specific morphology is, indeed, a reliable predictive guide to the composition of the phytoplankton (Kruk et al., 2011). However, its power benefits from reinforcement by additional information relating to the physiological capabilities of its components. The case of the capability to fix atmospheric nitrogen is one to which we have been able to draw particular attention. The requirement for skeletal silicon seems to be a trait specific to diatoms that can select against them preferentially if not satisfied. How far and how fast the phytoplankton can move are governed by specific morphological and physiological criteria that assist in improving the veracity of predicted responses to the environmental conditions.

While it is true that the largest lake to which PROTECH simulations have so far been applied to is Pyhäjärvi (“only” 154 km²; Pätynen et al., 2014), we believe it to be fundamentally true that the dynamic responses of phytoplankton to the imposed medium of growth are, essentially, the consequence of the properties (traits) of the organisms. These will be scaled according to the lake (or even the ocean) under consideration. Thus, given the desire and potential applications of a scheme for anticipating and predicting the role of these traits in shaping phytoplankton assemblages (Kruk et al., 2011), it is scarcely surprising that there have been several notable attempts to incorporate quantitative measures of such traits into models (Yoshiyama et al., 2009; Segura et al., 2013). We believe that the simulations presented in this paper will demonstrate convincingly how specific algal traits may be invoked to influence the composition of the phytoplankton, in terms of functional types if not actual species. From its initial conception, PROTECH has relied upon the particular
dynamic responses of utilized species, defined by their morphologies (dimension, surface area and volume), by the relative satisfaction of their known environmental needs and through the expression of specific specialist traits governing motility and acquiring resources. This seems not to have been widely appreciated but, accepting the developmental history of PROTECH, we have the confidence of experience in its ability to reconstruct the dynamic responses of trait-separated organisms (Groups) to environmental conditions.

Acknowledgements

We thank the German Meteorological Service (DWD) for providing meteorological data. M.F. was supported by the DFG (German Science Foundation; grant Ri 2040/1-1) and the IMPRS (International Max Planck Research School) for Organismal Biology.
5.4. MORPHOLOGICAL AND PHYSIOLOGICAL TRAITS OF PHYTOPLANKTON
Algal internal nutrient stores feedback on vertical phosphorus distribution in large lakes

Frassl, M.A., Rothhaupt, K.-O., Rinke K.

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Abstract

We applied a coupled hydrodynamic-ecological lake model to Lake Constance and investigated the consequences of luxury uptake of mineral resources (phosphate) by phytoplankton on the distribution of this resource in the environment. We compared two different resource limitation models, a static P model with a fixed cell stoichiometry disabling luxury uptake (the Monod approach) and a dynamic P model with a flexible cell stoichiometry enabling luxury uptake (the Droop approach). Our research was based on the finding that a model simulation using the static P model showed good results for phytoplankton dynamics but was unable to simulate the vertical distribution of the algal resource properly. In this model, the resource was only depleted in the euphotic zone (ca. 0-20 m) while in Lake Constance observed phosphate depletion was about twice as deep (down to ca. 40-50 m).

A simulation using a dynamic P model reproduced the vertical extension of resource depletion. The driving process behind the deeper resource depletion was luxury uptake of phosphate by algae sedimenting out of the productive zone. Even though the spatial extent of phosphate depletion strongly differed, the difference in phytoplankton dynamics between the two resource limitation models was minor.

It is shown that a process acting at the cellular level has wide implications at the ecosystem level. Thereby, the inclusion of a flexible cell stoichiometry of phytoplankton into a complex lake model is important for predicting spatial nutrient gradients within the lake.
6.1 Introduction

Nutrient concentrations in lakes are important determinants of phytoplankton dynamics and trophic state (Vollenweider, 1968). In most lake systems, phosphorus is identified as the primary limiting resource for phytoplankton growth (Dillon & Rigler, 1974) as expressed by highly significant correlations between total phosphorus and chlorophyll concentrations. Accordingly, a reliable prediction of phytoplankton dynamics necessitates a good understanding of the consumer-resource dynamics between phytoplankton and phosphorus.

Different models exist for simulating phosphate uptake and phosphorus-dependent growth. Under equilibrium conditions, for example in a chemostat, the growth rate of algal cells in relation to ambient resource concentration follows a Monod kinetic. Monod (1949) described a saturating relationship between resource concentration and growth rate characterized by a maximum growth rate and a half saturation constant (Fig. 6.1). This simple, empirical relationship is still used in several modelling studies (e.g. Omlin et al., 2001; Petzoldt et al., 2009). A more sophisticated, mechanistic approach to resource-limited growth considers cell growth as a two-step process: first, nutrients are taken up into the cell and stored in an intracellular storage and second, nutrients are taken from this storage for sustaining growth. The amount of nutrient in the intracellular storage becomes a dynamic variable and is expressed as a specific nutrient content (nutrient per biomass) termed the cell quota $Q$. Droop (1968) formulated a dynamic model that includes an internal cell quota, affected by the rate of nutrient uptake and cell growth rate. The cell growth rate itself is formulated to be a saturating function of the internal cell quota (Fig. 6.1). This leads to a decoupling of nutrient uptake and growth and the potential decoupling of these two processes in space and time, i.e. cell growth is not directly linked to the external nutrient concentration as in the Monod model.

The utilisation of the Droop approach is widely applied by theoretical ecologists (e.g. Grover, 2011; Jäger et al., 2010; Klausmeier et al., 2004). However, lake ecosystem models surprisingly often stick to the Monod approach (e.g. Omlin et al., 2001; Riley & Stefan, 1988; Rinke et al., 2010). Both, Droop and Monod models converge in their predictions under equilibrium conditions (e.g. in chemostats). Based on the different formulations of nutrient-dependent growth, however, it appears obvious that both models produce different dynamics of algal populations at non-equilibrium conditions (Sunda et al., 2009). Empirical studies of algal dynamics in the field revealed that the Droop model provides more accurate predictions for nutrient-dependent growth rates than the Monod model (Sommer, 1991). In addition, the decoupling of nutrient uptake and cell growth in the Droop model allows accounting for luxury uptake: a phenomenon described by algal physiologists referring to the fact that nutrient uptake by algal cells can be much faster than cell growth (Tilman & Kilham, 1976). Luxury uptake, in turn, is associated with an increasing cell quota of that nutrient. Due to luxury uptake, algal cells can proceed to grow over several cell cycles after transfer from a nutrient-rich to a nutrient-free medium by utilising the internally stored nutrient depot.

The better predictive power for algal dynamics in the field by the Droop model leads to the question to which extent luxury uptake may affect the vertical resource distribution in
CHAPTER 6. INTERNAL NUTRIENT STORES

Figure 6.1: Schematic representation of a static P model (A) and a dynamic P model (B); $K_P$: Half-saturation constant in the static P model (Monod model); $Q_{\text{min}}$: minimal internal cell quota in the dynamic P model (Droop model).

the habitat. Some evidence for this is provided by Benndorf (1968) pointing to the fact that internal storage may also affect spatial distribution of the resource. Using empirical data, this study revealed high fluxes of phosphorus into sedimenting algal cells during a sinking bloom of pennate diatoms. As sinking algal cells got progressively limited by light, the cell growth ceased completely during the sinking. These non-growing cells, however, were still alive and able to take up nutrients. Similar observations were obtained in Lake Constance where lower C:P ratios within sedimentation traps towards larger depths indicated luxury uptake of phosphate by sedimenting algal cells (Güde & Gries, 1998).

Further support for the importance of the process described by Benndorf (1968) arose in a modelling study in Lake Constance using the coupled hydrodynamic-ecological model DYRESM-CAEDYM (Rinke et al., 2010). In that model, which used a Monod approach for nutrient-dependent growth of algae, phosphate depletion occurred only in the euphotic layer, i.e. the depth layers where enough light is available for positive net growth. Yet field observations indicated phosphate was depleted down to almost twice the euphotic depth. In the current study, we hypothesize that the luxury uptake of phosphate by sedimenting algae explains the spatial extent of phosphate depletion into greater depths where no positive net growth is possible.

The main objective of this study is to analyze the effects of internal nutrient storage of algal cells on spatial distribution of the nutrient in the environment. By bridging over several levels of biological organization, our research question aims at resolving the consequences of a cellular process (internal nutrient storage) on (i) plankton dynamics at the population level and (ii) the spatial resource distribution at the ecosystem level. We based our approach on a coupled hydrodynamic-ecological lake model and focused on phytoplankton and phosphorus dynamics. This model is run by using either a static internal cellular nutrient content, as implemented in the Monod model, or a dynamic internal cellular nutrient content as given in Droop’s formulation.
6.2 Materials and Methods

6.2.1 Study Site

Lake Constance is a large, monomictic lake located along the northern edge of the central European Alps. Basic limnological characteristics of Lake Constance are given in Table 6.1 and more detailed information is available in the literature (Bäuerle et al., 1998; Güde & Gries, 1998; Wessels, 1998). Phosphorus is the limiting nutrient for phytoplankton growth in the lake. Lake Constance suffered from eutrophication reaching a eutrophic state around 1980 with phosphorus concentrations up to 90 µg L\(^{-1}\). The lake has undergone a continuous reoligotrophication since then and has now reached an almost natural state with phosphorus concentrations of < 10 µg L\(^{-1}\). The change in phosphorus concentration over this time span is mirrored by the development of phytoplankton biomass with high biomass levels in the 1980s and declining concentrations since then.

<table>
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<td>Wessels (1998)</td>
</tr>
<tr>
<td>Catchment area</td>
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<td>Wessels (1998)</td>
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<td>Outflow (Seerhein, mean 1961-1991)</td>
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<td>Bäuerle et al. (1998)</td>
</tr>
<tr>
<td>Drinking water abstraction</td>
<td>0.139 km(^3) yr(^{-1})</td>
<td>Bäuerle et al. (1998)</td>
</tr>
</tbody>
</table>

6.2.2 Model

For examining the phytoplankton and nutrient dynamics in the lake, the dynamically coupled ecological-hydrodynamic model DYRESM-CAEDYM was used (V5.0.0; DYRESM 3.1.0-04; CAEDYM 3.3.0-02; Centre for Water Research, Australia). DYRESM-CAEDYM is a well-established lake ecosystem model that has been applied to a wide range of different lakes and reservoirs (Mooij et al., 2010; Trolle et al., 2012). The model has been applied to Lake Constance previously (Rinke et al., 2010). With the one-dimensional Dynamic Reservoir Simulation Model (DYRESM, Imberger & Patterson, 1981), stratification and mixing dynamics are simulated. The lake is vertically divided into Lagrangian layers that split and merge depending on the water volume and density changes. By means of these layers, the vertical distribution of heat and salinity is represented. Its change over time is modelled in response to meteorological forcing (i.e. air temperature, shortwave radiation, incident longwave radiation, vapour pressure, wind speed and rain) and inflow data (water volume, temperature, salinity and nutrient concentrations). In a comparative study between different one-dimensional lake models, DYRESM has proven to give good results for lake stratification and mixing without the need for an extensive calibration (Perroud et al., 2009).
The information calculated by DYRESM is passed to the Computational Aquatic Ecosystem Dynamics Model (CAEDYM, Hipsey et al., 2010), which simulates biogeochemical processes in lakes including nutrient and plankton dynamics. CAEDYM equations are solved for every DYRESM layer resulting in a spatial resolution of the ecological processes. CAEDYM allows for different complexity of the food web. The user chooses which functional groups are included in the simulations. In this study, two functional phytoplankton groups (summer and spring phytoplankton) and one zooplankton group are simulated. A detailed description of the parameterization of the model for an application to Lake Constance is given in Rinke et al. (2010). Further information on model structure was given in detail previously (e.g. Bruce et al., 2006; Gal et al., 2009; Romero et al., 2004). In our study, the focus is on evaluating alternative model formulations for phosphate limited growth with respect to population dynamics and resource distribution. In this regard, CAEDYM is advantageous as it offers the possibility to test different nutrient limitation models embedded in a spatially resolved ecosystem model.

For mathematically describing nutrient limitation of phytoplankton growth, two alternative models are compared: 1) the static P model, which equals the Monod model, is based on a static specific nutrient content in algal biomass, and 2) the dynamic P model, which is based on the Droop model, assumes a dynamic internal nutrient content per algal biomass (the cell quota). In the first model, phytoplankton growth is directly coupled to the nutrient concentration in the habitat (Monod, 1949). In the latter model (Droop, 1968) an internal store is introduced that allows a temporal (and spatial) decoupling between nutrient uptake and cell growth. Both approaches are implemented in CAEDYM as alternative procedures.

Within CAEDYM, phytoplankton growth rate is a product of a maximal growth rate $\mu_{\text{max}}$, the minimum of a number of limiting terms $f()$ describing dependency on light $I$, nutrient concentrations $N$ (nitrogen) and $P$ (phosphorus), and a term for temperature limitation $f(T)$.

$$\mu = \mu_{\text{max}} \min[f(I), f(N), f(P)] f(T)$$

(6.1)

According to this equation, temperature always has an effect on the overall growth while for the other factors Liebig’s Law of the minimum takes effect. As Lake Constance represents a phosphorus limited system, we focused on phosphorus as the limiting nutrient.

In the static P model, the phosphorus limitation term $f_{\text{static}}(P)$ only depends on the phosphate concentration $P$ and a half-saturation constant $K_P$:

$$f_{\text{static}}(P) = \frac{P}{P + K_P}$$

(6.2)

The uptake rate of phosphate $U_P$ in the static P model scales linearly with growth rate $\mu$ and phytoplankton biomass $A$ multiplied by a fixed internal phosphorus content of algal biomass $k_{1P}$:

$$U_{P,\text{static}} = k_{1P} \mu A$$

(6.3)

In this approach, nutrient-dependent algal growth is spatio-temporally confined to loca-
tions and periods where resources are above a critical minimum level allowing population growth to compensate for all loss terms (i.e. positive net growth). Periods with critically low resource levels are associated with losses of biomass (e.g. by respiration, sedimentation, grazing) and release of nutrients. As within this model formulation nutrient uptake occurs only where positive growth is possible, it is necessarily restricted to the euphotic layer where enough light is available for primary production.

The Droop model is based on scaling the actual growth rate $\mu_D$ to the ratio between the internal cell quota $Q$ and a minimal internal cell quota $Q_{\text{min}}$ by means of a maximal theoretical growth rate $\mu'_{\text{max}}$.

$$\mu_D = \mu'_{\text{max}} \left(1 - \frac{Q_{\text{min}}}{Q}\right) \quad (6.4)$$

By introducing cell quotas, assimilated nutrients can be stored within the cell and utilised for growth at a later stage. Hence, nutrient uptake and cell growth are decoupled in time. For sinking cells this fact leads also to a decoupling in space along the vertical axis. The parameter of a minimum quota leads to a critical internal nutrient concentration that has to be surpassed before growth can take place. In the Droop equation as given in Eq. 6.4, the parameter $\mu'_{\text{max}}$ is called the maximal theoretical growth rate because it can only be reached if the cell quota becomes infinite. In order to avoid the use of this maximal theoretical growth rate, a normalised form of the Droop model is implemented in CAEDYM as a growth limitation term $f_{\text{dynamic}}(P)$. That is, a realized maximum growth rate $\mu_{\text{max}}$ (see Eq. 6.1) is achieved, when the cell quota reaches the maximum cell quota $Q_{\text{max}}$:

$$f_{\text{dynamic}}(P) = \frac{Q_{\text{max}}}{Q_{\text{max}} - Q_{\text{min}}} \left(1 - \frac{Q_{\text{min}}}{Q}\right) \quad (6.5)$$

The phosphate uptake function $U_{P,\text{dynamic}}$ scales with phytoplankton biomass $A$ and depends on a maximal uptake rate $U_{P,\text{max}}$, a temperature $(T)$ scale, the cell quota $Q$, and the external nutrient concentration via a Michaelis-Menten kinetic:

$$U_{P,\text{dynamic}} = U_{P,\text{max}} \left(f(T) \frac{Q_{\text{max}} - Q}{Q_{\text{max}} - Q_{\text{min}}} + \frac{P}{K_{P,\text{uptake}}} \right) A \quad (6.6)$$

Uptake becomes zero with $Q = Q_{\text{max}}$, setting an upper boundary to the cell quota.

Contrary to the static $P$ model, uptake in the dynamic $P$ model is not directly coupled to cell growth. This has two consequences. First, the decoupling of cell growth and nutrient uptake allows the cell to store nutrients and later use them for growth. Second, phytoplankton are able to assimilate phosphate, whenever the phosphate concentration is sufficiently high and the cell quota is below maximum. Accordingly, within this model formulation nutrient uptake can also occur at times or locations where no positive net growth is possible. Uptake can, for example, occur beneath the euphotic depth, where light is limiting and no positive net growth is possible. Owing to technical reasons, CAEDYM is not directly calculating the quota as a state variable, but the absolute concentration of internally stored phosphorus $P_{\text{internal}}$ (i.e. given in mg P L$^{-1}$), which is affected by uptake $U_{P,\text{dynamic}}$ and losses $L$ (excretion and
mortality), \( G \) (grazing) and \( S \) (settling):

\[
\frac{dP_{\text{internal}}}{dt} = U_{P, \text{dynamic}} - L_P P_{\text{internal}} - GA - S
\]  

(6.7)

From this internal phosphate concentration the cell quota \( Q \) is calculated by:

\[
Q = \frac{P_{\text{internal}}}{A}
\]

(6.8)

Note the difference in phosphorus contents between the static and the dynamic P model. While the internal phosphorus content \( k_{IP} \) in the static P model represents an average phosphorus content, P:Chla within the dynamic P model is varying from \( Q_{\text{min}} \) to \( Q_{\text{max}} \) (i.e. \( Q_{\text{min}} < k_{IP} < Q_{\text{max}} \)).

In the case of sufficient phosphate supply, either light or nitrogen can have a limiting effect. The light limitation function is described by an exponential response to incoming irradiance \( I \) with \( I_k \) determining the slope of the light response curve (Webb et al., 1974):

\[
f(I) = 1 - \exp \left( -\frac{I}{I_k} \right)
\]

(6.9)

Nitrogen limitation is modelled by using a static N model (cf. Eq. 6.2 and Eq. 6.3). As nitrogen is available in excess in Lake Constance we did not evaluate the simulation results for nitrogen. Settling of phytoplankton is calculated from a constant settling velocity (Hipsey et al., 2010).

### 6.2.3 Scenarios

A simulation using the static P model for nutrient-dependent growth was compared to a simulation using the dynamic P model. We explicitly studied the spatio-temporal occurrence of phytoplankton biomass and phosphate depletion and evaluated how observed patterns in vertical phosphate distribution in the lake were reproduced by the models. The relation between external phosphate \( P \) in the water column and phosphate that was taken up from the water column by phytoplankton and stored internally \( (P_A) \), was described by the index \( i_P \):

\[
i_P = \frac{P}{P + \sum_{j=1}^{n} P_A}
\]

(6.10)

For the static P model \( P_A \) is calculated by multiplying phytoplankton biomass \( A \) of algal group \( j \) with the constant internal phosphorus constant \( k_{IP} \) of group \( j \) (cf. Eq. 6.3). Within the dynamic P model \( P_A \) equals \( P_{\text{internal}} \) (cf. Eq. 6.7). The smaller the index, the more phosphate is bound within phytoplankton biomass relative to total phosphate pool existent within the water column.
6.2.4 Parameterization

We applied a slightly simplified version of the model configuration developed in Rinke et al. (2010). That is, we generalized the algal groups and constrained the number to two major groups, spring and summer algal groups. We chose these two groups based on the plankton succession patterns of Lake Constance characterized by an algal spring bloom of small, fast growing phytoplankton and a summer bloom of larger and slower growing and largely inedible phytoplankton (Sommer et al., 1986). Thus, summer algae are characterized by low growth rate, higher settling velocity, and low susceptibility to zooplankton grazing (e.g. large pennate diatoms like Asterionella, Fragillaria, Tabellaria). The spring group has a higher maximum growth rate and a slower settling velocity as well as a higher grazing pressure from zooplankton (e.g. small centric diatoms like Cyclotella, Stephanodiscus and flagellates like Cryptomonas).

We based our parameterization for both the static and the dynamic model on the controlled experimental data gathered from Tilman & Kilham (1976). They conducted growth experiments with two algal species Asterionella formosa (Hass.) and Cyclotella meneghiniana (Kutz.) and compared the different parameters for the growth models with three different experimental designs using continuous and batch cultures. We chose to parameterize the generalized algal groups based on these two diatom species as (i) they are common in Lake Constance, (ii) represent the opposing characteristics for spring and summer algal groups (high vs. low growth rate, etc.), and (iii) experimentally derived parameterizations for static and dynamic P-models are available. Values in the study of Tilman & Kilham (1976) were stated in $\mu$mol cell$^{-1}$ and converted to $\mu$g P $\mu$g C$^{-1}$ based on the assumption that 10% of the wet mass consists of carbon. Since we ran CAEDYM with chlorophyll units as a measure of algal biomass, we multiplied the carbon-based values with a stoichiometric factor $Y_{C:chla}$ (the average carbon to chlorophyll ratio in the respective functional group, see Table 6.2).

A maximum cell quota was only indirectly determined in the experiments as it is not included in the original Droop equation. If organisms are limited by more than one resource maximum cell quotas are required, however, in order to avoid unlimited uptake of the non-limiting resource. For instance, if growth is limited by light, an algal cell in a phosphate-rich environment would constantly take up and store phosphorus at unrealistically high quantities. Therefore, we estimated the maximum cell quota based on the luxury uptake factor provided by Tilman & Kilham (1976). Maximum nutrient uptake $U_{P,max}$ and half saturation constant $K_{P,uptake}$ were also estimated following measurements by Tilman & Kilham (1976). The parameters used for simulating phytoplankton growth within CAEDYM are summarized in Table 6.2.

6.2.5 Data

We simulated four years (1994–1997) and compared the model outputs with field data. This comparison was done just for the last three years. We intentionally skipped 1994 from the analysis in order to achieve independence from the initial conditions. Water temperature data were collected by the monitoring programme of the Internationale Gewässerschutzkomission
Table 6.2: Parameters of the phytoplankton module of CAEDYM

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_s$</td>
<td>Settling velocity</td>
<td>m d$^{-1}$</td>
<td>0.52 1.04</td>
</tr>
<tr>
<td>$p_z$</td>
<td>Grazing preference</td>
<td>-</td>
<td>1 0.1</td>
</tr>
<tr>
<td>$Y_{C,chl}$</td>
<td>Average ratio of C to chlorophyll a</td>
<td>mg C mg$^{-1}$ Chla</td>
<td>40 40</td>
</tr>
<tr>
<td>$I_k$</td>
<td>Shape parameter in P-I-curve</td>
<td>day$^{-1}$</td>
<td>45 30</td>
</tr>
<tr>
<td>$\vartheta_A$</td>
<td>Temperature scaling</td>
<td>-</td>
<td>1.05 1.10</td>
</tr>
<tr>
<td>$T_{std}$</td>
<td>Standard temperature</td>
<td>$^\circ$C</td>
<td>20 20</td>
</tr>
<tr>
<td>$T_{opt}$</td>
<td>Optimum temperature</td>
<td>$^\circ$C</td>
<td>23 25</td>
</tr>
<tr>
<td>$T_{max}$</td>
<td>Maximum temperature</td>
<td>$^\circ$C</td>
<td>30 30</td>
</tr>
<tr>
<td>$K_N$</td>
<td>Half-saturation constant for N</td>
<td>mg L$^{-1}$</td>
<td>0.1 0.1</td>
</tr>
<tr>
<td>$k_{IN}$</td>
<td>Constant internal N ratio</td>
<td>mg N mg$^{-1}$ Chla</td>
<td>2.45 5.45</td>
</tr>
<tr>
<td>$\mu_{max}$</td>
<td>Maximum growth rate</td>
<td>day$^{-1}$</td>
<td>2.5 1.8</td>
</tr>
<tr>
<td>$K_P$</td>
<td>Half-saturation constant for P</td>
<td>$\mu$g L$^{-1}$</td>
<td>7.0 0.5</td>
</tr>
<tr>
<td>$k_{IP}$</td>
<td>Constant internal P ratio</td>
<td>mg P mg$^{-1}$ Chla</td>
<td>0.5 0.4</td>
</tr>
<tr>
<td>$Q_{min}$</td>
<td>Minimum internal P concentration</td>
<td>mg P mg$^{-1}$ Chla</td>
<td>0.19 0.07</td>
</tr>
<tr>
<td>$Q_{max}$</td>
<td>Maximum internal P concentration</td>
<td>mg P mg$^{-1}$ Chla</td>
<td>0.95 2.89</td>
</tr>
<tr>
<td>$U_{P,max}$</td>
<td>Maximum P uptake rate</td>
<td>mg P mg$^{-1}$ Chla day$^{-1}$</td>
<td>1.70 5.95</td>
</tr>
<tr>
<td>$K_{P,uptake}$</td>
<td>Half-saturation constant for P</td>
<td>$\mu$g L$^{-1}$</td>
<td>18.6 31.0</td>
</tr>
</tbody>
</table>

Für den Bodensee (IGKB) and kindly provided by the Institute of Lake Research of the State Baden-Württemberg (Institut für Seenforschung, Landesanstalt für Umwelt, Messungen und Naturschutz Baden-Württemberg). The data were collected biweekly at the deepest point of the lake (station Fischbach-Uttwil at 47$^\circ$ 37.440’N, 9$^\circ$ 22.528’E, Fig. 6.2), at 15 different water depths: 0, 1, 2.5, 5, 7.5, 10, 15, 20, 30, 50, 100, 150, 200, 230 and 250 m (Güde et al., 1998). Chlorophyll concentrations and soluble reactive phosphorus data were measured by the Limnological Institute of the University of Konstanz in the western part of the lake (Überlinger See, 47$^\circ$ 45.453’N, 9$^\circ$ 7.743’E, Fig. 6.2) (Häse et al., 1998). The data from the University of Konstanz are available at a higher temporal resolution, i.e. weekly during summer and biweekly during winter at 19 different water depths, and allow a better characterization of the ecological dynamics. Using temperature data from another sampling point in Lake Constance is unproblematic as stratification dynamics between both stations were found to be comparable (Straile et al., 2010). Details on field methods and sampling procedures are given in Stich & Brinker (2010) and in Häse et al. (1998).

Meteorological data with an hourly resolution were provided by the German meteorological
service (DWD) and the Central Institute for Meteorology and Geodynamics (ZAMG).

Analysis and processing of the data was done with the statistical software R (R Core Team, 2012).

6.3 Results

We evaluated the physical model by comparing measured water temperatures from 15 depths with the model output for water temperatures over a period of three years (Fig. 6.3). Deviations between simulated and measured temperatures remained small. The model reproduced about 97% of the variability in measured temperatures ($T_{meas} = 1.05 \times T_{sim} - 0.05$, $r^2 = 0.97$, $p < 0.001$). A regression analysis of simulated versus measured temperatures showed little divergence from the bisecting line indicating a high accuracy of the physical model (Fig. 6.4). Note that small differences to the simulation shown in Rinke et al. (2010) result from different DYRESM-CAEDYM model versions.

Similar to the physical model, the ecological model was able to simulate phytoplankton dynamics in good agreement with observations. By calculating vertically averaged chlorophyll concentrations over the upper 20 m, which is considered to be the euphotic layer, we found standing stock and dominant patterns in algal dynamics (e.g. spring bloom) to be well reproduced by the model (Fig. 6.5; static P model: $A_{meas} = 0.57 \times A_{sim} + 1.09$, $r^2 = 0.40$, $p < 0.001$; dynamic P model: $A_{meas} = 0.90 \times A_{sim} + 0.36$, $r^2 = 0.47$, $p < 0.001$). Interestingly, differences in algal dynamics between simulations using either a static or dynamic P model for nutrient dependent growth were minor (Fig. 6.5 & 6.6). The dynamic P model, however, created systematically higher chlorophyll concentrations during the spring bloom (Fig. 6.6). Also the slope in the regression analysis of measured versus simulated chlorophyll concentrations was much closer to unity for the dynamic P model compared to the static P
Figure 6.3: Comparison between water temperature [°C] of the upper 100 m from 1995–1997, obtained from (A) simulation results and (B) field measurements.

Figure 6.4: Comparison of measured and simulated water temperatures from 1995–1997 over the whole water column (0-250 m). The dotted line represents the bisecting line with a slope of one and an intercept of zero, indicating a perfect fit \( r^2 = 0.96 \).
6.3. RESULTS

**Figure 6.5:** Average total chlorophyll concentrations in 0-20 m depth (grey = measured concentrations, blue = static P model, red = dynamic P model).

**Figure 6.6:** Difference of average total chlorophyll concentrations in 0-20 m depth between static P model and dynamic P model (Chla\textsubscript{stat} - Chla\textsubscript{dyn}).

model (see above). Higher chlorophyll concentrations in the dynamic P model were expected because the minimal P-content per chlorophyll is lower in the dynamic P model in comparison to the static P model with its fixed C:P ratio. The maximal difference in total chlorophyll between static and dynamic P model was 7.5 µg L\textsuperscript{-1}. Differences in total chlorophyll at later times during the growing season remained small in all three simulated years (Fig. 6.6). The duration of the growing season, however, is slightly shorter in both models than in the observations. Simulated and observed vertical distribution of chlorophyll showed similar patterns (Fig. 6.7). At water depths deeper than 20 m hardly any chlorophyll can be found except during times of fast sedimentation of algal populations. That is, the only difference in algal dynamics between static and dynamic P model occurred in the spring bloom maximum, while other phenomenological patterns (e.g. timing of the spring bloom, occurrence of clear water phase) remained similar.
**Figure 6.7:** Comparison between phosphorus concentrations within the upper 100 m (A-C) and total chlorophyll a within the upper 50 m (D-F). Results are shown from the static P model (A, D), the dynamic P model (B, E) and field measurements (C, F).
Phosphate distribution patterns over the same period and depth range indicated clear differences between static and dynamic P model (Fig. 6.7). Phosphate concentrations in the lake showed an intense phosphate depletion down to 50 m depth during the growing season. When using the static P model, the phosphate depletion occurred only in the upper 15 m, i.e. the static P model simulated a markedly shallower layer of phosphate-depletion than observed in the lake. Obviously, the static P model restricted the spatial extent of phosphorus depletion to the euphotic layer where positive net growth of algae is taking place and light is not limiting. Deviations between model and data in depths between 15 and 50 m were very high and lead to a low $r^2$ of 0.35 when comparing observed and simulated phosphate concentrations over the upper 50 m ($SRP_{\text{meas}} = 0.68 \times SRP_{\text{sim}} + 9.42$, $r^2 = 0.35$, $p < 0.001$). The beginning of phosphate depletion was also slightly delayed in the model and of shorter duration. Deep water phosphate enrichment (ca. 30 m depth) is predicted by the static P model at the end of the growing season, which does not exist in the observations.

Phosphate depletion simulated with the dynamic P model reached down to greater depths, persisted over longer times and complied with the observed phosphate depletion in Lake Constance. As a result, the dynamic P model improved the simulation of phosphate concentration markedly ($SRP_{\text{meas}} = 0.86 \times SRP_{\text{sim}} + 2.48$, $r^2 = 0.61$, $p < 0.001$) in comparison to the static P model. Phosphate enrichment below the layers with phosphate depletion also occurred in the simulation of the dynamic P model at a depth of about 45 m and at lower concentration. To test the effect of internal wave activity on the vertical excursions of the phosphate depletion, we tested the correlation between phosphate concentration and water temperature at 50 m depth at station FU: $SRP_{\text{meas}} = -3.60 \times T_{\text{meas}} + 33.47$, $r^2 = 0.30$, $p < 0.001$.

The amount of phosphate that has not been taken up by phytoplankton, as given by the index $i_P$, confirmed the dynamics described above (Fig. 6.8). With the start of phytoplankton growth $i_P$ approaches zero in the surface layers due to phosphate uptake by the algae. In the dynamic P model algal phosphate uptake during spring occurred down to depths larger than 30 m while in the static P model phosphate uptake was restricted to the upper 15 m.

In the dynamic P model, most of the phosphate from the top 30 m of the water column is taken up by the spring phytoplankton, as they produce high biomasses during the spring mass development (Fig. 6.9). Nevertheless, concerning the vertical distribution, summer phytoplankton play a major role. They dominate the algal community after the clear water phase and are characterized by higher settling velocity. The phosphate uptake of these sinking phytoplankton cells – having a higher capacity for internal storage of phosphorus and a faster settling – are mainly responsible for the phosphate depletion below 30 m as mirrored by the depth distribution of the internal P store (Fig. 6.9). In order to test the effect of settling velocity on the vertical extent of phosphate depletion we ran a simulation where settling of phytoplankton was switched off. This simulation showed much shallower phosphate depletion (Fig. 6.10) indicating that high settling velocities are an important prerequisite for a deep phosphate depletion through luxury uptake.
Figure 6.8: Phosphate index $i_P$, describing the amount of phosphate relative to the sum of free phosphate and phosphate bound by phytoplankton. Results are shown for the static P model (A) and the dynamic P model (B).

Figure 6.9: Comparison between simulated concentrations of chlorophyll a (A, B) and internal stored phosphorus concentration (C, D) of both spring (A, C) and summer (B, D) phytoplankton, simulated by the dynamic P model.
6.4 Discussion

Our study aimed at analyzing the effects of internal nutrient storage by algae on the vertical distribution of algal resources in their habitat by applying a coupled hydrodynamic-ecological lake model. We compared algal dynamics and spatial distribution of phosphate in the water column between two model scenarios using either a static (Monod model) or a dynamic (Droop model) submodel for phosphorus-dependent growth. Our approach bridges over several levels of biological organization as we analyzed the consequences of luxury resource uptake, i.e. a process acting at the cellular level, at the population and ecosystem level. Our approach allows modelling of cellular processes (e.g. nutrient uptake), population dynamics of different algal groups, and resource distribution dynamics in the ecosystem in one coherent, spatially explicit, framework. We show that the capability of phytoplankton to internally store nutrients has a strong effect on the spatial distribution of their resource leading to deeper phosphate depletion in the lake.

The lake model successfully reproduced key patterns in temperature stratification and phytoplankton dynamics observed in the field. Interestingly, the qualitative agreement between simulated and observed phytoplankton dynamics occurred independently of the choice of the submodel for nutrient dependent growth (i.e. static vs. dynamic). The differences in mean total chlorophyll of the upper 20 m between static and dynamic P model remained small. Yet, the choice of the P model strongly affected the simulated vertical phosphate depletion within the lake. The static P model predicts phosphate depletion only within the euphotic layers. In contrast, phosphate depletion simulated by the dynamic P model reached down to much greater depths; approximately twice as deep as the euphotic depth. In this model, nutrient uptake and phytoplankton growth are decoupled in space and time and thus allow

Figure 6.10: The isolines show the depth at which simulated phosphorus concentration equals 5 µg L$^{-1}$. Simulation results are depicted for the year 1997 with standard settling rates for phytoplankton ($v_s = 0.52$ m d$^{-1}$ and 1.04 m d$^{-1}$, for small and large phytoplankter, respectively, black) or without settling of phytoplankton ($v_s = 0$ m d$^{-1}$, grey).
for nutrient uptake in deep layers where light limitation inhibits phytoplankton growth. This spatial decoupling explains why major phenological patterns in total chlorophyll dynamics (apart from the spring bloom maximum) remained similar between the two simulations. The higher uptake of nutrients in the simulation using a dynamic P model was not associated with higher growth rates as it occurs at depths where positive net growth is hardly possible due to light limitation. Empirical evidence of the predicted uptake of phosphate by sinking, non-growing algae was found by Benndorf (1968).

The depth of the euphotic zone is an important characteristic for the vertical phosphate depletion - irrespective of the chosen nutrient limitation model. Simulations allowing for a better light utilisation for growth, i.e. with a steeper $P-I$-curve (cf. Eq. 6.9) and a corresponding larger light compensation depth resulted in a deeper depletion. Such a parameter change, however, goes along with an unrealistically long growing season. In this respect it has to be kept in mind, too, that parameters used in this study have been independently derived from experiments and not calibrated.

We found a strong contrast between the spring and summer algal group with respect to their contribution to algal and nutrient dynamics. While the spring phytoplankton reached a higher standing stock and was responsible for high chlorophyll concentrations in spring, the summer phytoplankton had a stronger effect on the vertical phosphate flux and phosphate depletion (Fig. 6.8 & 6.9). This can be explained by the much higher phosphorus storage capacities of the summer phytoplankton group and their higher settling velocity. The combined effects of settling and nutrient uptake of the summer phytoplankton group caused a continuous deepening of the phosphate depleted surface layer. We identified high settling velocity as a key trait for algae that deplete phosphate down to great depths by running a simulation where settling was switched off. In this simulation much shallower phosphate depletion occurred. The higher biomass of the spring phytoplankton can be explained by their higher growth rate and an advantage in temperature-dependency of growth that allows them to start growing earlier and take up large amounts of phosphate available at the start of the growing season. Large parts of this assimilated phosphate, however, are incorporated into zooplankton biomass by grazing. This phosphate is therefore not exported, but kept within the upper water layers. It gets partly released during the clear water phase and is available for summer phytoplankton growth.

The identification of a high settling velocity as a prerequisite for deep phosphate depletion suggests a systematic influence of lake size on the depletion. High settling velocities are associated with high sinking losses at the population level. Hence, those algae having high settling velocities (e.g. large diatoms) can only survive in epilimnia with sufficient vertical mixing. We therefore hypothesize that lakes with a large surface area, long wind fetch, or high average wind speeds show systematically deeper phosphate depletion because they offer an optimal habitat for algae having high settling velocities.

The more intense phosphate depletion in the dynamic P model indicates a weaker potential influence of upwelling events in this configuration. Wind events can cause upwelling and an upward flux of nutrients from lower depths. In case of deep phosphate depletion, however,
this effect will be lower because water from comparatively deeper layers has to be affected in order to effectively transport phosphate upward.

6.4.1 Static vs. dynamic approaches of nutrient-limited growth of algae

The two model formulations of phosphorus-dependent growth used within this study imply different assumptions about cell stoichiometry. The static P model has a fixed C:P ratio, neglecting the effect of a variable stoichiometry within the cell. The dynamic P model takes variable nutrient stores within the cell into account and thus includes a flexible stoichiometry. Other dynamic resource models of uptake and growth have been formulated in the past, e.g. flexible nutrient uptake sites (e.g. Bonachela et al., 2011) or reserve and structure components in the Dynamic Energy Budget theory (DEB theory, Kooijman, 2001). We made use of the classical Droop equation as it constitutes a widely spread approach among phytoplankton ecologists being frequently applied in theoretical and empirical studies (e.g. Diehl et al., 2005; Sommer, 1991).

The difficulty of parameterizing a Droop approach might have led to the frequent usage of Monod’s equation within many lake models (e.g Benndorf & Recknagel, 1982; Omlin et al., 2001; Vilhena et al., 2010). Comprehensive and work-intense growth experiments are required to determine the various growth parameters that are needed to fully describe the Droop equation. Unfortunately, field measurements of internal stores within the field are scarce (Sommer, 1991). Nevertheless, our results show that parameters derived from experiments satisfactorily describe growth dynamics in the field. This may point towards a general applicability of these parameters to different lakes.

Also other studies indicated that the Monod equation is the poorer approach in describing cell growth under dynamic conditions (Flynn, 2010; Sommer, 1991; Sunda et al., 2009). Beyond that, our results show that the choice of nutrient limitation model has a large effect on the vertical nutrient distribution within the system. The static P model does not predict the spatial pattern of phosphate depletion caused by sedimenting phytoplankton. That is, phosphate uptake alone, i.e. without storage within the cell, cannot explain the observed deep depletion. This spatial effect will be higher for deeper, stably stratified lakes, compared to shallower lakes. The deeper the lake, the larger is the aphotic layer where luxury uptake takes place and the stronger is the effect of exported nutrients that cannot be re-introduced into the epilimnion by short mixing events. In deep lakes, the right description of nutrient distribution is important, for example, when it comes to growth of metalimnetic algae. Deep chlorophyll maxima (e.g. of Planktothrix rubescens) cannot develop in a system with very deep nutrient depletion due to nutrient limitation. Algal luxury uptake and settling is obviously also an important component in phosphorus sedimentation in deep lakes, which effectively reduces the trophic state (Vollenweider, 1982).

The dynamic P model, however, did not fully explain the vertical phosphate distribution in Lake Constance as approximately one quarter of the observed variability remained unexplained by the model. To some extent, this unexplained variability arose from vertical excursions of the phosphate gradient due to internal wave activities. A regression between
phosphate concentrations and water temperature at 50 m depth at station FU showed a negative correlation (also compare Fig. 6.3 & 6.7 and see Boehrer et al., 2000). Such dynamics, of course, cannot be reproduced by a one-dimensional model. Nevertheless, a prominent difference in phosphate concentrations between observations and both model formulations is still visible in larger depths, below the layers of phosphate depletion. Here, an increase in phosphate concentration is predicted by the model outputs, presumably caused by decaying algal populations that release their internally stored phosphorus. Such a peak in phosphorus concentration cannot be identified in the data. In fact, all phosphorus taken up by algal cells have to be released back in the water, when sinking cells decay within the water column. We hypothesize that the algal-borne phosphate is consumed by processes currently not included in the model.

A potential process consuming phosphate in greater depths within lakes may be bacterial activity. Rothhaupt & Güde (1992) have shown that bacteria can incorporate large quantities of the total phosphorus pool. As they have a low half saturation constant for phosphorus uptake bacteria can deplete phosphate in the water to very low levels. Unlike for phytoplankton, bacterial production is not dependent on light and bacterial production may profit from decaying algae at greater depths. Macrophytes may also play a role in phosphate uptake from the water column. However, they are likely to have a negligible effect on net phosphate depletion (Angelstein & Schubert, 2008; Rooney & Kalf, 2003), particularly in large lakes with a large pelagic component. In Lake Constance, macrophytes are rarely found below 10 m depth (Schmieder, 1997) and are unlikely to induce phosphate depletion at greater depths. Another factor may be grazing activity by diurnally migrating zooplankton (Petzoldt et al., 2009; Rinke & Petzoldt, 2008). In Lake Constance, diel vertical migration of Daphnia extends down to 30–50 m depth (Stich & Lampert, 1981) and grazing by migrating daphnids at these depths during the day could be a sink for algal-bound phosphorus.

Dynamic nutrient uptake models have been studied extensively in theoretical biology with regards to the description of competition between different phytoplankton species (e.g. Grover, 2011; Revilla & Weissing, 2008). Nutrient storage capabilities of phytoplankton species influence the competitive outcome in spatiotemporally variable environments (e.g. Grover, 2011; Kerimoglu et al., 2012a) and thus affect species composition. These results also support the need to include dynamic P models in ecosystem models in the future. The uptake of phosphate by settling algae might also have the potential to support oligotrophication by exporting phosphorus from the upper layers. In that case, dynamic resource limitation models will provide more accurate estimates about the anticipated nutrient uptake by sedimenting algae.

### 6.4.2 Accounting for stoichiometric constraints in ecosystem models

We have shown that luxury uptake by phytoplankton cells combined with sedimentation can explain deep phosphate depletion within large lakes. Our results furthermore point to the fact that the different pathways of phosphate depletion, that is, sedimentation on the one hand and grazing and remineralization on the other hand, are linked. Through the ability of luxury uptake, phytoplankton respond to shifting intensities of energy (e.g. light) and
mineral resource (e.g. phosphorus) limitations with a shift in C:P stoichiometry (Urabe & Sterner, 1996). This response has an effect on the energy and mass balance of herbivores. High C:P ratios are considered as low food quality for zooplankton resulting in negative effects on fecundity and somatic growth as was, for example, shown for Daphnia (DeMott et al., 1998, 2001). A decrease of phytoplankton C:P ratios and an associated increase in food quality with depth provides an advantage to migrating zooplankton (see above). This effect could be analyzed by lake ecosystem models with more than one zooplankton group. The propagation of nutrient stoichiometry along the food web and the corresponding effects on trophic interactions play an important role in food web dynamics (Sterner & Elser, 2002).

6.4.3 Phosphate sedimentation under transient state

Previous studies have shown the necessity of revisiting phosphate-dependent turnover processes in lakes (Ramin et al., 2012) for assessing the relative importance of the different underlying mechanisms in gradually changing ecosystems (e.g. due to climate change). One part of this is to fully understand the mechanisms behind phosphate sedimentation. Warmer water temperatures for example will intensify and prolong stratification (Livingstone, 2003). As species with high sedimentation rates will be incapable of maintaining positive net growth under less turbulent conditions (Huisman et al., 2002), this temperature effect will indirectly affect species composition of phytoplankton. In fact, experiments have indicated a shift towards smaller phytoplankton species in warmer climates (Daufresne et al., 2009). This, in turn, can interfere with phosphate sedimentation by phytoplankton.

With the Droop equation embedded into a hydrodynamic-ecological lake model, we were able to show that the elemental stoichiometry of algae exhibits a systematic seasonal change and alters along the vertical axis. We showed that the changing stoichiometry at the cellular level has a strong feedback on nutrient distribution at the ecosystem level. Thus, we conclude that the uptake of phosphate by sedimenting algae is a key process for understanding phosphate depletion into greater, aphotic depths. Lake ecosystem models should make use of dynamic internal nutrient models like the Droop model, not only to account for stoichiometric effects in the food web but also for correctly reproducing spatial resource distribution in the habitat.

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Yohannes. We thank the anonymous reviewers and Ram Yerubandi for their constructive comments to improve the quality of the manuscript. For funding and supporting our work, we thank the DFG (Deutsche Forschungsgemeinschaft, grant Ri 2040/1-1) and the IMPRS (International Max Planck Research School) for Organismal Biology as well as the Zukunftskolleg at the University of Konstanz.
General discussion

In the previous chapters, the effects of internal and external factors on monomictic lake ecosystem dynamics were investigated through the application of two complex aquatic ecosystem models. The investigation put different scales of variability in phytoplankton dynamics into focus: the variability in phytoplankton spring bloom onset through inter- and intra-annually varying meteorology, the variability in phytoplankton succession and community composition through different environmental settings and finally the spatial variability of nutrients that result from the different capabilities of phytoplankton groups to store nutrients.

The following paragraphs will connect the findings of the individual chapters and discuss the implications of the results for phytoplankton modelling.

7.1 Meteorological drivers of phytoplankton dynamics

In the first part of my thesis I considered how climate and meteorological conditions influence phytoplankton dynamics. A new methodology for simulating the impact of climate change and meteorological variability on large monomictic lakes was introduced and applied. The method coupled a complex lake model DYRESM-CAEDYM with a stochastic weather generator (VG). This coupled modelling system provided the basis for a detailed analysis of meteorological effects on phytoplankton dynamics in spring. By simulating several hundred years, changes in the distributions of cardinal dates could be identified (chapter 3 & 4). Moreover, the relative importance of the different meteorological variables was studied. It was shown that overall weather conditions, that is the interplay of different meteorological variables, drive phytoplankton phenology. In fact, there was not a particular meteorological variable that tended to be the main trigger of the onset of a bloom. That is, positive effects in one variable, such as an episode of warm air temperatures, can be counterbalanced by the others, e.g. strong winds. In addition, the simulation experiment was used to determine effective time scales at which these meteorological variables act on PSB timing. The results showed that the relative importance of wind speed and shortwave radiation on the PSB onset is larger than
that of air temperature.

### 7.1.1 The impact of climate change and meteorological variability

Many limnological studies have reported changes in lake ecosystems due to climate change (Adrian et al., 2009; Shimoda et al., 2011). Mathematical models are often used to understand these changes, since in modelling studies confounding factors can be excluded from the analysis. For example, by keeping nutrient loads constant between years, the simulated variability in the lake’s response is caused exclusively by the variation in meteorological input data. However, several different approaches exist to model climate change effects on ecosystems and depending on the research question one approach is superior to the other.

Weather generators allow to produce a large number of annually varying years as input data to ecosystem models. Thereby, weather generator studies enable probabilistic analyses of simulation results and thus indicate the stochasticity within a system, and within its dynamics. The large number of generated years also allows for an explicit analysis of rare events. For example, extreme meteorological conditions, like hot spells or cold spells can be compared with each other, or years with a large number of strong wind events in a specific season can be analysed in detail. Furthermore, simulations with weather generators facilitate the mechanistic understanding of meteorological effects on lake ecosystems. For example, the effects of a warmer climate, expressed as a higher average air temperature, can be compared to changes in meteorological variability, expressed as a change in duration and/or amplitude of weather episodes.

Another approach that has been applied in many different impact studies due to its simplicity, is to vary single meteorological variables by a fixed percentage (e.g. Bueche & Vetter, 2014) or by increasing temperatures by e.g. 1...6 Kelvin (e.g. Trolle et al., 2011; Kupisch et al., 2012). This approach provides a first impression of how an ecosystem will respond to changing conditions. However, the results can be misleading, as meteorological variables co-vary and climate change will not only affect one variable. Furthermore, changing a single time series neglects inter- and intra-annual differences in warming. Overall, large uncertainties and potential biases are inherent to this approach.

A third approach, which has also been used in lake ecosystem modelling is to force a model with the output of global or regional climate models (e.g. Elliott et al., 2005; Weinberger & Vetter, 2012). This approach is often chosen when the aim of the study is to obtain predictive results for the future state of the system being modelled. The difficulty inherent in this approach is that the global and regional climate model results must be downscaled and bias-corrected before being applied to the local site (Maraun et al., 2010; Themeßl et al., 2011). And while climate models are improving in their predictive power, there are still large uncertainties connected with the results of global and regional simulations (IPCC, 2013).

Comparing these three approaches, weather generators have several benefits when the aim of a study is to analyse effects of meteorological forcing on ecosystems. They include dependency structures between meteorological variables and allow ‘what-if’ scenarios. However, the largest advantage is the probabilistic approach of weather generators and their capability to
reflect inter- and intra-annual variability in climate and weather conditions. For this reason, I have chosen to apply the weather generator approach in this thesis.

In the first weather generator study (chapter 3), an increase in the mean air temperature generally reproduced conditions that were observed in previous studies on climate change. With a warmer climate, the date of both the onset of stratification and the phytoplankton spring bloom was earlier. While this has been shown and discussed before (Winder & Schindler, 2004b; Thackeray et al., 2008), the application of VG gave new insights into this shift in dates. Keeping the correlations between the different meteorological variables and not changing them independently from each other resulted in an enhanced warming of the water column in winter compared to the warming observed in summer. This was explained by the seasonally varying cooling effect of evaporation, which is strongest in summer. A similar, strong interaction between evaporation and heat storage has been observed in Lake Superior, a large North American lake (Spence et al., 2013). In Lake Superior, evaporation in spring and autumn strongly affected the seasonal energy budget through the interaction with ice cover duration.

The ability of VG to generate a multitude of realisations allowed the analysis of distributions of cardinal dates in phytoplankton development. While the mean in phytoplankton spring bloom onset was shifted to earlier dates in the year with an increased mean air temperature, the distribution of the PSB onset widened. This result showed that a shift of PSB timing to earlier days in a warmer climate can be counterbalanced to some degree by other meteorological variables in individual years. For example, earlier in the year, it is more likely that strong wind events destroy developing stratification and thereby delay PSB onset. Additionally, incoming shortwave radiation has lower light levels and lower energy input earlier in the year, which slows down phytoplankton growth. Effects of individual factors such as mixing (Gaedke et al., 1998a; Berger et al., 2007) and light intensities (Talling, 1971; Sommer & Lengfellner, 2008) on phytoplankton growth have been noted before. However, the changes that I observed in the probability distribution of the timing of the bloom resulted from interactions between meteorological variables and due to interannual variability. This interaction and variability are difficult to analyse in the field or through experiments and would be impossible to analyse using the common climate impact studies that utilise single time series simulations.

It is important to note that VG was not developed for making predictions about future climatic states, but to analyse outcomes of potential states of the climate system (Schlabing, in preparation). The aim of developing VG was to improve our understanding of the different components that constitute climate (the different meteorological variables and changes in mean, in variability and extremes) and to identify decisive weather episodes that affect phytoplankton phenology. With the weather generator used in this thesis, the mean and the variability of a climatic state can be changed independently from each other. At the same time, VG preserves the correlation structure between the different meteorological variables. This latter point is important when studying climate effects on phytoplankton dynamics, since stratification and mixing, which affect the light climate and thus phytoplankton growth,
are strongly driven by weather patterns (see chapter 4). However, keeping the correlations between variables in a future climate like those observed in the past was an assumption that we made during data generation. To validate this assumption, we generated weather data for a time period in the 1990s based on observed data from the 1980s. We then showed that the generated data fit the observations and thus showed the ability of VG to extrapolate over a short period of time (see chapter 3). However, whether dependency structures between generated variables remain the same or change in a future climate is not entirely ruled out by our test, and should be tested when more data become available for future years.

Beside having the opportunity to choose from different approaches to generate the meteorological input for climate simulations, different approaches exist for the lake models themselves, too. For example, for the hydrodynamical simulation the user has to decide on how to represent the spatial dimension. In this thesis, all simulations were done with a one-dimensional lake model, neglecting horizontal variability within lakes. Nevertheless, large lakes show processes that are caused by spatial heterogeneity (e.g. internal waves or differential cooling, Wahl & Peeters, 2014). With a warming climate, some of these processes may become important for deep water and oxygen renewal (Eder, 2013) due to changes in the lakes’ mixing pattern (Straile et al., 2010). Therefore, when studying these processes, a three-dimensional model representation will be more appropriate (see e.g. Eder, 2013). In other cases, when horizontal gradients are negligible, a one-dimensional model may suffice and even be more appropriate for the study, for example when a high number of simulation runs is required (chapter 4). This shows that the choice of the model representation is strongly dependent on the research question.

As every approach has its benefits and drawbacks, the safest path to follow is to apply different methods during the analysis (compare results from this thesis and Eder, 2013). This combination of approaches will ensure an in-depth understanding of the lake being studied. It will help managers at the local level, who require clear statements about the future state of a system, to counteract negative effects of climate change. Based on the results of comparing different approaches, ‘no-regret’ measures can be taken, while acknowledging the uncertainty inherent in predictions of future conditions.

7.2 Phytoplankton traits

In the second part of my thesis, I focused on phytoplankton traits and how they are interlinked with their environment. The trait-based model PROTECH was applied to simulate phytoplankton succession under different environmental conditions. We found that the dynamic responses of phytoplankton to different environmental conditions depended on the properties (traits) of the organisms. These specific traits also influenced the composition of the phytoplankton community. The study showed that PROTECH was able to describe this dynamic response of trait-separated organisms.

DYRESM-CAEDYM (DYCD) was used for a closer analysis of the feedback of nutrient-related traits on the lake (chapter 6). The model study with DYCD showed that phyto-
plankton has the potential to affect whole lake ecosystems, by modifying the spatial extent of phosphate depletion in the lake. This spatial variability results from the variability in phytoplankton’s capability to store nutrients. Algae that were capable of storing large amounts of phosphate, exported nutrients from the productive zone through sedimentation, showing the potential to significantly reduce nutrient concentrations in the epilimnion over a longer time scale. Therefore, when drawing conclusions about ecosystem functioning, phytoplankton traits must be considered.

7.2.1 Trait-based modelling of phytoplankton succession

Variability in phytoplankton trait composition in four alternative lake settings was analysed in chapter 5. The four simulated lakes varied in lake depth and climate, leading to different thermal structures. The two main differences between the lakes were the surface mixed layer depths and the duration of stratification. Phytoplankton trait diversity was larger in the shallow lakes, but did not differ between climates. The main difference between climates was the succession and standing stock of simulated groups. By testing different limitation functions (grazing, light, nitrogen), the role of various phytoplankton traits became apparent.

The simulated lower trait diversity in the deep lakes may be a result of two factors. Simulated chlorophyll concentrations were analysed over the upper 5 m of the water column to mimic common sampling techniques. However, in another simulation study Elliott et al. (2002) showed that sampling depth altered conclusions about species dominance. Therefore, limiting our analysis to the upper 5 m may have meant that species occurring at larger depths were overlooked. The more probable explanation for the lower trait diversity is light limitation, which would allow only a few phytoplankton groups to sustain a positive net growth. This latter assumption was strengthened by several observations: (i) a peak in chlorophyll concentrations appeared as soon as the surface mixed layer became shallow enough to allow some groups the maintenance of positive net growth. (ii) The phytoplankton groups present in the deeper lakes had the highest maximum cell dimension and largest surface to volume ratios. These two morphological traits would allow them to persist under poorer light conditions. Furthermore, Group III, the dominant group in the deep lakes can adjust its position in the water column depending on the light condition. This trait allows Group III to move upwards to depths with higher light intensities. (iii) Phosphorus and nitrogen limitation in the deep lakes did practically not occur showing that the system was light limited and not nutrient limited.

Observation (i) is in line with chapter 4, in which the strong dependence of phytoplankton dynamics on the surface mixed layer depth in deep lakes was shown. Physical processes of mixing and stratification are represented in a simple manner in PROTECH compared to fully hydrodynamic one-dimensional models as DYRESM (Reynolds et al., 2001). This simplification therefore limits the applicability of PROTECH. However, the depths of mixed layers in our simulations are within the range of mixed layer depths in similarly deep lakes (Talling, 1971; Elliott & Thackeray, 2004). Compared to the depths of the mixed layer, the amount and frequency of mixing, which results in spatial heterogeneity within the water
column, may be of larger importance. Pomati et al. (2012) found spatial heterogeneity to enhance phytoplankton diversity. A lack of spatial heterogeneity (in the vertical) might be another reason for the lower group diversity in the deep lakes. Meteorological forcing of simulations was artificial in chapter 5. Due to that reason, meteorological variability and extremes are not present in the time series used to drive PROTECH. I assume that the application of real meteorological data will result in a more heterogeneous thermal structure due to the higher amount of disturbances. As a result, a larger number of species is expected to coexist (Reynolds et al., 1993; Hambright & Zohary, 2000).

Spatial heterogeneity (e.g. nutrient distribution) in the water column can also be caused by phytoplankton itself through the capability to internally store nutrients (see chapter 6). The process of internal nutrient storage is not implemented in PROTECH. While this will have little effect on vertical nutrient distribution in shallow lakes, the difference in nutrient depletion might be significant in deep lakes over a long time period. However, phytoplankton dynamics in chapter 6 were not found to differ largely between the static and the dynamic P model. Thus, the effect of a deeper nutrient depletion should not play a role on total phytoplankton dynamics in the simulations of chapter 5, too. The larger effect of an internal nutrient storage in these simulations is expected to be on competitive advantages of one phytoplankton group over the other.

In chapter 5, the aim was to test how phytoplankton traits determine phytoplankton composition in different lake ecosystems. Comparing phytoplankton dynamics in different lake environments is challenging in respect to effort, cost and comparability (e.g. Schindler & Fee, 1974). Chapter 5 showed an experimental set-up to easily test effects of different limitation functions in various environments. Although, such a ‘modelling lab’ is artificial and e.g. meteorological time series need to be closer to reality in future applications, it is still useful to test our understanding of natural systems and to compare different models with each other. Continued development of the virtual lake ecosystems and the model input data will gradually bring the results closer to reality. Outcomes can then be compared to results from meta-analyses (e.g. Jeppesen et al., 2005; Blenchner et al., 2007; Rigosi et al., 2014) and collaborative multi-lake comparisons, which are conducted by research networks like NELAKE, AEMON or GLEON (Weathers et al., 2013).

PROTECH was successful in simulating changes in communities under different environmental conditions. Although the model was always initiated with the same community conditions, results showed that the community composition and succession varied between simulation runs. The major benefit of PROTECH compared to other complex aquatic ecological models is its unique approach to simulating phytoplankton dynamics. Specifically, in the model phytoplankton dynamics are based on algal traits, and laboratory studies and field measurements are used for parameterisation. Calibration of phytoplankton related parameters is therefore not necessary. The ease of applicability together with a strong focus on the ecology of the phytoplankton facilitates to focus on biological interaction and succession.
7.2.2 Phytoplankton traits and the spatial distributions of nutrients

In chapter 6, the impact of cellular nutrient storage on nutrient distribution within lakes was studied. Field studies suggested an influence of phosphate storage on the vertical distribution of that resource in lake ecosystems (Benndorf, 1968). Similar theoretical studies are lacking, as most of them have mainly considered the effect of nutrient storage on competitive exclusion (Revilla & Weissing, 2008; Grover, 2011). Recently, the spatial aspect of nutrient gradients in lakes and its interaction with internal stores attracted larger notice in theoretical ecology (Jäger et al., 2010; Kerimoglu et al., 2012a). In chapter 6, it was shown, that luxury uptake does have the potential to shape the resource distribution within the whole ecosystem. This became clear through the application of a model formulation that did not allow for nutrient storage. This model formulation was not able to reproduce the deep phosphate depletion that had been observed in Lake Constance. Looking at cellular nutrient storage in an ecosystem context revealed the importance of the spatial and temporal decoupling of nutrient uptake.

For deep systems, nutrient storage and settling rates of different phytoplankton showed to be an important trait for the phosphate flux. In the model setup the resolution of trait diversity was low with just two functional groups. However, those two functional groups comprised important features of phytoplankton succession in Lake Constance (Sommer, 1986). Spring phytoplankton had high growth rates and high palatability. Compared to that the summer phytoplankton possessed a larger phosphate storage capacity, which allowed them to persist under nutrient limited conditions during summer. The summer phytoplankton also had a higher settling rate and was mainly responsible for the downward nutrient flux.

A deep phosphate depletion caused by nutrient storing and sedimenting phytoplankton had implications for eutrophication/oligotrophication processes in deep lakes. By storing nutrients in epi- and metalimnion and transporting it downwards, phytoplankton does strengthen nutrient export from the productive layers and thereby promotes re-oligotrophication of the system. The extent depends on the species composition, as phytoplankton with a large storage capacity and settling rate are needed for an efficient export of phosphate. Simulations in chapter 6 were conducted for the years 1994–1997. Quantifying phosphate fluxes in Lake Constance during more eutrophic years (1980ies) compared to oligotrophic years (2000s) would give insight on the export efficiency. During the 1980s, phosphate depletion in Lake Constance did not reach as deep as in the 1990s and later (data from Institute for Lake Research, ISF, Langenargen, Germany, not shown). This observation is in line with the hypothesis of uptake by phytoplankton. In a more eutrophic system, algal cells could fill their P stores within the euphotic depth and would not have the capacity to take up more phosphate while sedimenting down the water column.

Other causes for the deep phosphate depletion in Lake Constance have to be considered, too. While coprecipitation of calcite crystals with phosphate has been regarded as a possible mechanism (Murphy et al., 1983; Kleiner, 1988), field studies estimated its overall effect in Lake Constance as of minor importance (Stabel, 1986). Küchler-Krischun & Kleiner (1990) argued for a combination of calcite precipitation and P-uptake by phytoplankton. They showed that calcite crystals encapsulate algal cells and sink down the water column. This
process would not necessarily stop the algae from still taking up phosphate from the water column. At the same time, it increases their sedimentation rate, thus allowing for a deep phosphate depletion before decomposition of the algal cells.

Another process not to be neglected is uptake by bacteria. Rothhaupt & Güde (1992) experimentally showed the high phosphate uptake capability of bacteria, especially at low phosphate concentrations. Gächter & Mares (1985) found settling seston in lakes to be a sink of phosphate and explained this observation through bacterial activity. This theory was corroborated by Hupfer et al. (1995), who explained P-uptake through iron and manganese oxidising bacteria.

A final conclusion about the true mechanism behind the deep phosphate depletion cannot be drawn based on my simulation results, as alternative processes were not tested. To deduce the importance of each single mechanism behind the depletion pattern, further field measurements are needed. Biomass samples at different depth intervals, down to larger depths together with the C:P ratio of algae and bacteria at those depths would allow the estimation of phosphate stored within the cells. The observations could be compared with a modelling experiment, within which all potential mechanisms could be quantified and tested against each other.

As discussed above, a depth-specific sampling C:P ratios is needed for the parameterisation of the dynamic P model (chapter 6). The chapter therefore touches on the application of ecological stoichiometric theory within aquatic ecosystem models. Phytoplankton show a different C:P stoichiometry, depending on energy (e.g. light) and mineral (e.g. phosphorus) resources (Urabe & Sterner, 1996). Accordingly, cell stoichiometry will vary over depths, but also in dependence of the nutrient-related traits (e.g. storage, uptake). By allowing algae to have a flexible C:P ratio, food quality effects can be included into the lake model. This allows a more realistic quantification of energy and matter flows through the food web, since e.g. zooplankton growth was shown to depend on phytoplankton C:P ratios (DeMott et al., 1998).

Another issue concerning the parameterisation, which is of large importance to the ecological modelling community, was highlighted in this thesis. Immense effort is put into calibration and optimisation of model parameters. However, when it comes to model structure, often the ‘convenient’ path is followed (Robson, 2014a) and a thorough testing of different functional forms is neglected. This lack was brought forward by Flynn (2005), who stated that experimentally working limnologists and aquatic modellers are not working collaboratively enough. He argued that modellers too easily choose the simplified, but maybe wrong approach. My results underscore Flynn’s statement that the decision which of the different formulations of a process will be applied within the model has to be made carefully.

Theoretical and field studies help to decide which formulation may be best. For example, in theoretical studies, the inability of the Monod model to describe growth under fluctuating conditions has been stated several times (e.g. Sunda et al., 2009; Flynn, 2010). Further evidence was given by field studies (Sommer, 1991). However, some lake models still make use of the Monod equation to simulate nutrient-limited growth of phytoplankton (Omlin et al., 2001; Vilhena et al., 2010; Schlabing et al., 2014). This might be sufficient in some instances.
Our results showed that the qualitative agreement between phytoplankton measurements and simulation results were similar for both nutrient models (Fig. 6.5 & 6.7, chapter 6). Also, the timing of PSB onset did not differ between the static and dynamic P model, suggesting that results in chapter 3 & 4 would not differ when run with the dynamic P parametrisation.

In general, the structural set up of models has to be discussed critically (‘conceptual model evaluation’ Augusiak et al., 2013) and simulation results should be tested at different levels of aggregation (‘pattern oriented modelling’, e.g. Topping et al., 2012). For example, instead of comparing state variables, transfer rates could be used for model validation or in a stoichiometric approach mass balances can be calculated easily. The following papers and citations on good modelling practise go into detail on this issue: Bennett et al. (2013); Grimm et al. (2014).

### 7.3 Implications for phytoplankton modelling

By coupling a statistical weather generator to a dynamic lake ecosystem model, we introduced a new method into climate impact studies on lake ecosystems. Moreover, instead of analysing effects of an average climate, the application allows studying the effect of weather conditions on phytoplankton dynamics. Based on the methods and results presented in the previous chapters, it is straightforward to conduct further analyses on specific questions as discussed below.

#### 7.3.1 Moving up the trophic cascade: consumer-resource interactions

Changing variability of weather episodes led to a higher probability of very early and very late bloom onsets potentially entailing temporal mismatches between phytoplankton and its grazers or fish reproduction. Temporal mismatch between phytoplankton and zooplankton is a controversial topic in climate impact research. PSB onset and zooplankton dynamics were found to be sensitive to different drivers, that is stratification (Berger et al., 2007) and temperature (Schalau et al., 2008). Long term data analyses showed an increasing mismatch (e.g. Winder & Schindler, 2004a), while other (experimental) studies found no mismatch with increasing temperatures (Berger et al., 2014) or even a reduction of time-lags between phytoplankton and microzooplankton phenological events (e.g. Aberle et al., 2012). A recent simulation study argued that temporal mismatch arises from seasonally different warming (Straile et al., 2015). Our simulations of the current climate (Chapter 4) showed a large spread of PSB timing simply caused by inter- and intra-annual variability in meteorology. Increasing the meteorological variability (Chapter 3) showed that the maximum of PSB standing stock was probably nutrient limited whereas the minimum could be zooplankton controlled. Years being detrimental for zooplankton growth would lead to a higher phytoplankton maximum and vice versa, years being beneficial for zooplankton development would lead to a lower phytoplankton maximum. Analysing these dependencies between meteorology, phytoplankton and zooplankton in more detail can be done in the VG simulations by analysing joint frequency distributions of phytoplankton and zooplankton timing. However, phytoplankton -
zooplankton interactions were kept simple in DYRESM-CAEDYM (one zooplankton group, Rinke et al., 2010) and PROTECH (static temperature-dependent grazing rate Reynolds et al., 2001). Since microzooplankton was found to affect the phytoplankton spring bloom in both the ocean (Irigoien et al., 2005) and in lakes (Tirok & Gaedke, 2006), too, it might prove more important to refine zooplankton representations in both models before going into detail on the meteorological effects on consumer resource interactions (e.g. Rinke, 2006; Kerimoglu et al., 2014).

7.3.2 Seasonality in internal and external factors

The PEG model (Sommer, 1986) conceptually describes the seasonal course of phytoplankton and zooplankton dynamics in lakes. Most analyses of the coupled simulations with VG focused on the spring season (chapter 3 & 4). In a further step, the full seasonal cycle could be looked at. It would be interesting to find out relevant meteorological variables and effective time scales for other cardinal dates in phytoplankton phenology. Exemplarily, phytoplankton dynamics in autumn shall be discussed briefly. The increasing probability of strong wind events in autumn in combination with an eroding stratification due to cooling air temperatures increase the potential of nutrient upwelling. Since the epilimnion becomes nutrient depleted during summer, these upwelling events are important for phytoplankton to fulfil their nutrient requirement and especially metalimnetic algae can benefit from this mechanism (Pannard et al., 2011). Theoretically, a deeper phosphate depletion will lead to a lower impact of these strong wind events causing nutrient upwelling. Therefore, it would be attractive to use the internal stores parameterisation to investigate the importance of nutrient upwelling events. The occurrence of nutrient upwelling could be studied along a range of different lake depths, using the model set-up from chapter 5 in combination with meteorological time series generated with the weather generator.

This combination of the different modelling approaches implemented in this thesis could also be used for quantifying the relative importances of internal and external factors during the course of the year. This is a scientifically interesting step, since the seasonality in environmental forcing was discussed in the PEG model (see Fig.6, Sommer, 1986), which is a conceptual model and thus neglects quantification. Physical forcing could be tested through the application of the weather generator, whereas biotic interactions require a highly resolved phytoplankton model as was demonstrated with the PROTECH application.

7.3.3 The catchment

External factors like nutrient input and climate or meteorology are well integrated into aquatic ecosystem models. With the weather generator, it is now possible to analyse effects of weather events on lakes covering interannual variability. However, in the climate change application (chapter 3), we neglected the important point of changes in the catchment of the lake.

For the alpine region, intensified snow-melt and a change of precipitation towards larger rainfalls in winter is predicted to strongly affect the flow regime of alpine rivers (Middelkoop
et al., 2001). Together with lower summer discharge this will change the inflow regime of the Alpine Rhine, the largest inflow into Lake Constance. Additionally, changes in precipitation intensity and frequency in the catchment affect not only the water budget, but also nutrient washout from agricultural land, changing the availability of nutrients throughout the year. To include these changes into climate change studies, a simple first step would be to simulate scenarios with increased or decreased nutrient loading, initial nutrient concentrations in the lake or changed water inflow. A more advanced and much more intriguing extension would be the coupling of weather generator, lake model and a catchment model. Through such an application, climate effects but also land use changes in the catchment are integrated in a dynamic way.

7.3.4 Long-term changes in phytoplankton dynamics

Some changes in lake ecosystems occur on a decadal or even larger time scale (e.g. climate change, Smol & Cumming, 2000 or nutrient change, Jochimsen et al., 2013). During these time scales, the lake ecosystem has to respond to perturbations caused by changing external and internal factors. The ability of a lake to respond to these perturbations is referred to as its resilience. The resilience of a lake, also considered as its structural stability, largely depends on its biodiversity (Gunderson, 2000); the greater the biodiversity, the more resilient the lake. However, ecological models cannot easily simulate a large species diversity. Most phytoplankton models are limited in the number of modelled phytoplankton groups and do not allow for new species to enter the system (Mooij et al., 2010). Furthermore, organism characteristics are often parameterised for a specific species. Describing species in a generalised way and aggregating them into functional groups or based on traits can counteract this problem (McGill et al., 2006; Litchman & Klausmeier, 2008). If the modelled species are chosen in a way that they represent a most diverse range of possible traits, results can be analysed in a generalised way. This parameterisation problem was addressed for the DYRESM-CAEDYM model runs in chapter 3 & 4 by defining four functional groups with some central traits: small vs. large algae and silica-dependent (diatoms) vs. non-silica dependent algae. In contrast, the model applied in chapter 5 generally calculates phytoplankton dynamics based on traits that can be easily measured. PROTECH therefore does not need to be parameterised by the model user. However, in both models, the problem still remains that the amount of groups simulated is limited (e.g. a maximum of 8 groups can be chosen in PROTECH, Reynolds et al., 2001).

A promising approach to tackle the dynamics inherent in biodiversity change are adaptive models, in which traits are allowed to vary in time (e.g. Wirtz & Eckhardt, 1996; Brugge- man & Kooijman, 2007; Smith et al., 2011). These can be combined with new monitoring technologies (e.g. flow cytometer) that allow high-frequency measurements of traits in the field (Pomati et al., 2013). This combination may allow for the calibration and validation of adaptive models. However, the incorporation of adaptive models into complex aquatic ecosystem models is just now being realised (Pahlow et al., 2008) and many challenges remain for aquatic ecosystem modellers.
In conclusion, this thesis succeeded in implementing methods that allow both the analysis of specific lakes as well as generalised simulations that cover a wide range of reservoirs and lake ecosystems. The coupled modelling system of a weather generator and an aquatic ecosystem model opens new avenues in lake ecosystem research. Moreover, it provides a tool for lake and reservoir managers to develop an integrated management plan that optimises water balance and water quality management. The coupled system could assess how a system will respond to changes in management policy, providing an in depth risk assessment of the probability of, for example, the occurrence of anoxia under different withdrawal scenarios or under different levels of nutrient loading. The hypothetical model systems developed here can be utilised to improve our understanding of global scale problems occurring across a wide range of aquatic systems. This could be the occurrence of cyanobacteria blooms, which cause major water quality problems worldwide. It is often a specific trait of the cyanobacteria that gives them an advantage over the other phytoplankton species in a lake or reservoir. Therefore, the application of trait based models like PROTECH can be used to deepen our understanding on the occurrence of cyanobacteria. Further development of the hypothetical lake set-up would allow the evaluation of the potential success of different traits over a wide range of environmental conditions. However, a more generalised set-up like those of adaptive trait-based models would be beneficial to counteract the limited choice of simulated algal groups. Finally, the application of a more realistic meteorological input produced with the weather generator can easily be achieved. At the same time it would significantly improve transferability of the results from the hypothetical lake systems to real-world systems.
Summary

Lakes are dynamic systems that are permanently altered by external influences and internal feedbacks. Phytoplankton is an integral part of lake systems and to explain its phenology and succession is a crucial step in understanding the complexity of lakes ecosystems. Mathematical models help to grasp this complexity and expand our knowledge of how lake ecosystems react to altered boundary conditions. In this thesis, two complex lake ecosystem models (DYRESM-CAEDYM & PROTECH) were applied to investigate the effects of internal and external factors on lake ecosystems. In both cases, the investigations focused on either the variability in phytoplankton phenology or the succession of phytoplankton.

In the first part of this thesis, effects of climate change and meteorological variability on phytoplankton spring bloom (PSB) timing were studied. To accomplish this, a new method was introduced, which coupled a statistical weather generator (VG) with a complex lake model. The weather generator has three important features. First, the co-variation between different meteorological variables is accounted for. Changes in one meteorological variable will thus produce changes in other related meteorological variables. Second, the generation of multiple time series for each meteorological variable accounts for the variability inherent in the system and allows for a probabilistic analysis of simulation results including rare events. Third, the flexibility of VG enables the generation of sets of time series, each with different statistical properties. A simulation study with a fully-crossed design gave insight into the effects of increased mean air temperature and altered meteorological variability on the water temperature and chlorophyll concentration in a lake. An increase in mean air temperature on average shifted the onset of the spring phytoplankton bloom to an earlier date in the year, and a higher meteorological variability increased the probability of an extremely early and an extremely late onset of the bloom. Analysis of the modelled cardinal dates (stratification onset and bloom onset) showed an increase in the width of the distributions. This result could only be explained by the interplay between different meteorological drivers. For example, while an increase in air temperatures shifts the PSB onset to an earlier date, high wind speeds and low irradiance earlier in the year may counteract this shift and delay phytoplankton growth. This finding showed that a more in-depth analysis of the effect of different meteorological variables on phytoplankton spring bloom timing was needed. In this subsequent analysis increasing air temperature and shortwave radiation and decreasing wind separately from each other all led
to an earlier onset. However, the variability in the onset of stratification and timing of the PSB within a set of 500 simulations could not be explained by one meteorological variable alone. Instead, the interplay between the meteorological variables is crucial, with wind speed having the largest relative importance for PSB timing. Furthermore, wind speed was effective over shorter time scales than air temperature and shortwave radiation. In summary, the application of a weather generator to a lake ecosystem emphasised the need to study climate change effects on lakes in the context of meteorological situations and not with a uni-variate approach, such as a simple increase in air temperature.

The second part of this thesis placed the focus on phytoplankton traits and how they interact with the lake ecosystem. Phytoplankton traits (e.g. cell morphology, nutrient uptake and storage) are used to aggregate information on the large species diversity observed in phytoplankton communities. Therefore, one model study considered how trait composition varies under different lake morphometries, climates and environmental scenarios and how this affects phytoplankton succession. Furthermore, another model study assessed whether a particular trait, such as intercellular nutrient storage, can drive a change in an ecosystem property, such as a lake’s spatial nutrient distribution.

A trait-based modelling approach was performed using the ecological model PROTECH (Phytoplankton RespOnses To Environmental CHange). This model describes phytoplankton growth based on morphological traits such as cell size, surface and volume. The model’s ability to describe phytoplankton succession in lakes of different size and different climatic regions was tested. It was found that the model predicted the expected success of different traits under various environmental conditions. For example, cells with high surface-to-volume ratios were successful during periods of light limitation. Despite the same initial conditions for all model set-ups, different phytoplankton groups soon started to dominate the community due to advantages given by their traits. The model experiment showed that PROTECH can be used to analyse differences in phytoplankton succession in various lake ecosystems based on phytoplankton traits.

In the last chapter, the feedback of phytoplankton traits on the lake ecosystem was assessed. For this purpose, I conducted a structural testing of two different resource limitation models embedded in an aquatic ecosystem model. The first model was a static P model, which disabled nutrient storage, while the second model, a dynamic P model, enabled cells to store phosphate in the phytoplankton cells. For the latter, the ability to store nutrients allowed the phytoplankton to take up nutrients while settling out of the water column. Allowing luxury uptake resulted in a phosphate depletion into larger depths of the water column, relative to the static P model case. This depletion even occurred below the euphotic zone where net growth of phytoplankton is not possible. However, phytoplankton dynamics in the upper 20 m of the water column did not differ largely between the two model realisations. These simulation results complied with findings in the large monomictic Lake Constance, where phosphate depletion occurs through to the deeper water (40–50 m depth). By testing the two different physiological models it was shown that a mechanism acting at the cell level can have an effect at the ecosystem scale. However, the precise impact of nutrient relocation through
cellular storage will depend on the trait composition within the phytoplankton community.

In conclusion, this thesis succeeded in implementing methods that allow both the analysis of specific lake ecosystems as well as generalised simulations of a wide range of reservoirs and lake ecosystems. The joint application of a weather generator and a complex lake ecosystem model introduced a new approach to studying the effects of climate change and meteorological variability on lake ecosystems. This coupling provides practitioners with a better understanding of the variability inherent in their system and the effect of meteorological variables on phytoplankton dynamics, which is difficult to analyse in the field. A comparative modelling study showed that when using models for applied questions, it is important to include phytoplankton traits, since they were found to have a feedback at the ecosystem scale. Additionally, trait based modelling helps to aggregate phytoplankton observations and thereby generalise model outcomes. This was successfully applied in a model set-up with generalised hypothetical lakes making the interpretation of model results possible over a wide range of lake ecosystems.
Zusammenfassung


Im letzten Kapitel wurde das Feedback von funktionellen Eigenschaften des Phytoplanktons auf ein Seenökosystem eingeschätzt. Dafür führte ich Simulationen durch, in denen ich die Struktur eines aquatischen Ökosystems leicht veränderte, indem ich zwei unterschiedliche

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**Chapter 3:** The research question was jointly developed by the authors. The weather generator was developed by Dirk Schlabing with help of Magdalena Eder. They prepared the meteorological input data. I conducted the simulations with the lake model and analysed the simulation results. Dirk Schlabing and I wrote the main body of the text. Magdalena Eder contributed in writing and preparation of tables. Karsten Rinke, and András Bárdossy made suggestions for improvement of the manuscript.

**Chapter 4:** The idea for this chapter emerged from discussions with the co-authors of chapter 3 and Karl-Otto Rothhaupt. I developed the research question and modelling design in discussion with Karsten Rinke. The weather generator was developed by Dirk Schlabing. Preparation of input data, simulations and analyses were done by myself. I wrote the main part of the manuscript with contributions of Dirk Schlabing and Karsten Rinke. All co-authors commented on the study design and made suggestions for improvement of the manuscript.

**Chapter 5:** The concept for this chapter was developed by Collin Reynolds and Alex Elliott. Both prepared the largest part of the manuscript. I contributed to the design of the numerical simulations and prepared input data. I wrote parts of the methods section and provided suggestions for improving the manuscript.

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