Adapting the water management to mitigate the impact of multiple stressors on an urban lake: Case study Lake Tegel, Germany

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Lochiel, Lochiel, beware of the day!
For, dark and despairing, my sight I may seal,
But man cannot cover what God would reveal:
'Tis the sunset of life gives me mystical lore,
And coming events cast their shadow before.

Thomas Campbell, *Lochiel's Warning (1802)*

Preface

I am very grateful for having had the chance to develop and adapt this PhD project over these last three years. A lot of small scientific studies I conducted during this time did not make it into this final thesis. Still, I am very happy to have had the chance to learn how to do independent research and having the freedom to think outside of the box. In the end, I became fascinated with the principles behind physical limnology and the magic hidden in environmental fluid dynamics.

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An overview of all supplementary scientific work is given in chapter 7.

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Abstract

Urban lakes are aquatic ecosystems that are influenced by a water management system and by a possibly strongly sealed urban catchment. The water management aims to fulfill multiple objectives: providing drinking water, sanitation and recreation for the people as well as keeping the ecosystem in a sustainable and resilient state. Urban lakes are facing several stressors. For instance, climate change will affect thermal characteristics of lakes, frequency and duration of rainfall events, inflow discharges as well as atmospheric circulation patterns (especially wind speed and wind direction). Urbanization will cause further morphological degradation and an increasing pressure to utilize urban freshwater resources. Consequences of these stressors could be eutrophication of the urban lake ecosystem causing the formation of harmful algal blooms, the settling of invasive species or the development of a legacy contamination in the sediment. An adaptive and sophisticated urban lake management system has the potential to mitigate the impacts of these stressors on the urban lake ecosystem to keep them in a sustainable and resilient state.

The aim of this thesis is to explore the feedback mechanisms between Lake Tegel in Berlin, Germany, and its respective water management system. Lake Tegel's water management consists of a phosphorus elimination plant (PEP), which reduces the inflow's phosphate concentrations, a lake pipeline, which bypasses additional discharges to the PEP, and groundwater abstraction wells for bank filtration. This thesis covers a spectrum from past, present to future management measures by (1) analyzing the impact of past management measures by investigating the sediment composition, (2) current management measures by monitoring the lake water quality, and (3) future management measures by using numerical models. The sediment composition of Lake Tegel was examined by taking sediment cores at different sites and by comparing them with sediment cores from reference lakes. The cores were analyzed using X-ray fluorescence spectroscopy with high spatial resolution. Data were statistically evaluated by using principal component analysis (PCA), k-means clustering and self-organizing maps. To get frequent field data, a logger chain monitoring electrical conductivity, water temperature and dissolved oxygen was deployed at Lake Tegel's deepest site. Monitored data were used to explore limnophysical conditions of the stratification periods from 2017 until 2018. To project the impact of climate change on the lake system and to analyze alternative management measures, numerical models were calibrated and validated to Lake Tegel. A vertical 1D model (GLM-AED2) was used to explore the impact of climate change under different management setups on Lake Tegel's stratification stability, onset and offset as well as on the dynamics of dissolved oxygen and phosphate concentrations. A depth-averaged 2D model (open TELEMAC-MASCARET with EUTRO for water quality) was applied to compute water exchange times in dependence of the wind and to project the formation of phytoplankton blooms after short-duration heavy rainfall events under different management setups and wind directions.

The results confirmed that Lake Tegel's sediment composition was spatially heterogeneous probably due to the management system and the flow dynamics. The strong impact of flow dynamics on potential sedimentation processes was also confirmed by the application of the depth-averaged 2D model. The past management measures were successful in reducing the abundance of heavy metals making Lake Tegel's recent sediment layers similar to the ones of a reference lake with low urban impact. The recent monitoring of Lake Tegel revealed the existence of vertical seiches in the periods 12 and 8 h, a weak stratification period in winter 2017/2018 and the existence of a proposed density current that originated from the PEP during the winter season and affected the bottom water heat and dissolved oxygen budget. The vertical 1D model projected that future water temperatures will increase and that the summer stratification will extend with earlier onset and later offset. Further, the

additional water discharges by the PEP with low phosphorus loadings can buffer high nutrient loadings from the River Havel inflow and weaken the summer stratification stability, which could otherwise benefit the formation of harmful cyanobacteria blooms. Therefore, the PEP discharges and the corresponding low nutrient loadings are a positive factor to mitigate the impact of climate change on the Lake Tegel ecosystem. Computing the influence time distributions in dependence of wind direction using the depth-averaged 2D model clarified that under east-wind conditions, which intensify river intrusion into Lake Tegel, the influence times were the shortest. From the evaluation of the short-duration heavy rainfall scenarios it was recommended to reduce external nutrient loadings and to increase external discharges to mitigate the formation of phytoplankton blooms.

The water quality of Lake Tegel is controlled by the wind stress and external inflows. Therefore, the hydrodynamics are quite complicated and result in heterogeneity regarding the sediment composition. Such 'run-of-the-river' systems can be managed by modifying external discharges even further to reduce the lake hydraulic residence time, to weaken summer stratification stability as well as to mitigate the formation of phytoplankton blooms. Nonetheless, an elimination of external nutrient loadings in the PEP is the most important management measure to keep Lake Tegel in a clear-water state. The existing management system structure at Lake Tegel seems to be crucial in sustaining the lake's good ecological state and water quality especially regarding the projected impact of climate change. The numerical simulations showed that deactivating the management measures would affect Lake Tegel in manifold ways. Without the nutrient-low PEP loadings and additional discharges by the lake pipeline phytoplankton blooms will occur more often during the summer period, which will affect turbidity and water temperatures. Eventually, the thermal stratification is modified promoting the formation of cyanobacteria blooms. Also, short-duration heavy rainfall events will promote phytoplankton growth when nutrient-low PEP discharges were absent. An active and adaptive lake management that utilizes the PEP as well as the lake pipeline can keep the Lake Tegel ecosystem in a good and sustainable state and prevent a regime shift towards a turbid phytoplankton-dominated state.

Urban lakes are vulnerable aquatic ecosystems that have to be analyzed more thoroughly in the future to keep them in a sustainable and resilient state. Available and additional water quality and sediment quality data should be used to set up a sophisticated urban lake model solving the 3D Navier-Stokes equations coupled to a sediment diagenesis model. This will benefit the formulation of water management scenarios with focus on external nutrient loadings and their (potentially short) retention time in the lake system. Such a sophisticated urban lake model could then be used as part of an urban catchment model, which further incorporates river, wastewater treatment plant, groundwater, soil and urban runoff sub-models and can investigate future applied research questions regarding the urban 'Integrated Water Resources Management'.

Zusammenfassung

Urbane Seen sind aquatische Ökosysteme, welche durch ein Wasserbewirtschaftungssystem und ein möglicherweise stark versiegeltes, urbanes Einzugsgebiet beeinflusst werden. Mit der Wasserbewirtschaftung werden meist folgende Ziele verfolgt: die Bereitstellung von Trinkwasser, sanitäre Versorgung, die Nutzung der Seen als Erholungsgebiete für die Stadtbevölkerung und den Erhalt des Seenökosystems in einem nachhaltigen und belastbaren Zustand. Urbane Seen sind verschiedenen Belastungen ausgesetzt. Der Klimawandel zum Beispiel wird die thermischen Eigenschaften der Seen, die Häufigkeit und Dauer von Niederschlagsereignissen, Zuflüsse und atmosphärische Zirkulationsmuster (insbesondere Windrichtung und -geschwindigkeit) beeinflussen. Urbanisierung kann eine weitere morphologische Beeinträchtigung der Seen und einen steigenden Nutzungsdruck bewirken. Konsequenzen dieser Stressfaktoren können die Eutrophierung des Seenökosystems mit Massenentwicklungen zum Teil toxischer Cyanobakterien, die Ansiedlung invasiver Arten oder die Anreicherung von Schadstoffen in den Sedimenten sein. Eine, an die jeweilige Situation angepasste, Bewirtschaftungsstrategie für urbane Seen kann den Einfluss dieser Stressfaktoren abschwächen und nachhaltig eine gute Wasserqualität sichern.

Das Ziel dieser Arbeit ist es, die jeweiligen Wechselwirkungen zwischen dem Tegeler See in Berlin, Deutschland, und seinem Wasserbewirtschaftungssystem zu untersuchen. Die Wasserbewirtschaftung am Tegeler See besteht im Wesentlichen aus einer Oberflächenwasseraufbereitungsanlage (OWA), welche die Phosphorkonzentrationen im Zufluss reduziert, einer Seenleitung, welche zusätzliche Wassermengen dem Zufluss zuführen kann, und Grundwasserbrunnen, welche ein Gemisch aus See- und Grundwasser zur Trinkwassergewinnung fördern. Die vorgelegte Arbeit spannt dabei einen Bogen von der Vergangenheit über die Gegenwart bis hin in die Zukunft. Die Vorgehensweise bestand darin, (1) die Wirkung von früheren Maßnahmen durch Sedimentkernuntersuchungen zu rekonstruieren, (2) den Einfluss aktueller Maßnahmen mittels eines erweiterten Monitorings zu erfassen und (3) mittels numerischer Modelle geeignete Maßnahmen unter zukünftigen Klima- und Belastungsszenarien in ihrer Wirkung zu beschreiben. Um aktuelle und frühere stoffliche Belastungen anhand von Sedimentprofilen zu erkenne, wurden Sedimentkerne an verschiedenen Stellen des Tegeler Sees entnommen und diese mit Sedimentkernen von Referenzseen verglichen. Die Sedimentkerne wurden dazu räumlich mittels hochaufgelöster Röntgenfluoreszenzspektroskopie analysiert. Zur statistischen Auswertung wurden die Hauptkomponentenanalyse (PCA), k-means Clusteranalyse und selbstorganisierende Karten verwendet. Um zeitlich hochaufgelöste Freilanddaten zu erhalten, wurde eine Datenloggerkette an der tiefsten Stelle des Tegeler Sees installiert, welche die elektrischen Leitfähigkeiten, Wassertemperaturen und gelösten Sauerstoffkonzentrationen misst. Die aufgezeichneten Daten wurden zur Analyse limnophysikalischer Bedingungen während der Schichtungsperioden 2017 bis 2018 verwendet. Für Prognosen zu den Auswirkungen verschiedener Bewirtschaftungsmaßnahmen unter zukünftigen Klimabedingungen wurden numerische Modelle am Tegeler See kalibriert und validiert. Ein vertikales 1D-Modell (GLM-AED2) wurde zur Untersuchung des Einflusses des Klimawandels unter verschiedenen Bewirtschaftungsansätzen auf das Schichtungsverhalten sowie die jahreszeitlichen Dynamiken von Sauerstoff- und Phosphatkonzentrationen des Tegeler Sees eingesetzt. Ein tiefengemitteltes 2D-Modell (open TELEMAC-MASCARET gekoppelt mit EUTRO für die Wasserqualität) wurde verwendet, um Wasseraustauschzeiten in Abhängigkeit des Windes zu berechnen und um die Entwicklung des Phytoplanktons nach kurzzeitigen Starkregenereignissen unter verschiedenen Bewirtschaftungsansätzen und Windrichtungen zu simulieren.

Die Ergebnisse zeigten, dass die Sedimentzusammensetzung am Tegeler See aufgrund der Wasserbewirtschaftung und der Fließdynamik räumlich stark heterogen ist. Der star-

ke Einfluss der Fließdynamik auf mögliche Sedimentationsprozesse wurde auch von dem tiefengemittelten 2D-Modell bestätigt. Der Erfolg von früheren Bewirtschaftungsmaßnahmen war in einer Verringerung der Schwermetallgehalte im Sediment erkennbar, sodass die rezenten Sedimentschichten des Tegeler Sees ähnlich zu denen eines wenig beeinflussten Referenzsees sind. Die Datenaufzeichnung am Tegeler See hat die Existenz von vertikalen Seiches mit Perioden von 12 und 8 h, eine schwach ausgeprägte Schichtung im Winter 2017/2018 und das Vorhandensein eines vermuteten Dichtestroms belegt, welcher durch den Betrieb der OWA während des Winters entsteht und die Tiefenbilanz von Wärme und Sauerstoff beeinflussen kann. Das vertikale 1D-Modell zeigte, dass zukünftige Wassertemperaturen ansteigen werden und die Sommerschichtungsperiode sich verlängern wird. Ebenfalls wird die zukünftige Sommerschichtung früher beginnen und später enden. Die zusätzlichen Abflüsse der OWA sowie die Phosphoreliminierung sind in der Lage, die hohe Nährstoffzufuhr über die Havel zu vermindern. Außerdem wird die Stabilität der Sommerschichtung verringert, sodass die Gefahr der Bildung von Cyanobakterienblüten abnimmt. Daher stellen die OWA-Zuflüsse einen positiven Faktor zur Abschwächung der Folgen des Klimawandels auf das Seenökosystem des Tegeler Sees dar. Die Berechnung der räumlichen Verteilung von Wasseraustauschzeiten in Abhängigkeit der Windrichtung mittels des tiefengemittelten 2D-Modells belegte, dass bei Ostwind die Einmischung von Flusswasser in den Tegeler See am stärksten, dafür aber auch die Einflusszeiten am kürzesten sind. Des Weiteren waren die Reduktion externer Nährstoffe sowie eine Erhöhung der Zuflussmengen geeignete Bewirtschaftungsstrategien, um die Bildung von Phytoplanktonblüten nach Starkregenereignissen zu vermeiden.

Der Wasserqualität des Tegeler Sees wird durch den Wind und externe Zuflüsse stark beeinflusst. Daraus ergibt sich eine komplizierte hydrodynamische Situation am Tegeler See, welche auch an der heterogenen Sedimentverteilung erkennbar ist. Diese durch überwiegend externe Zuflüsse kontrollierten Seensysteme können durch die Bewirtschaftung der Zuflüsse weiter gesteuert werden, zum Beispiel durch die Verringerung der hydraulischen Wasseraufenthaltszeit sowie der Abschwächung der Sommerschichtung und der daraus folgenden Verhinderung von Phytoplanktonblüten. Dennoch bleibt die wichtigste Bewirtschaftungsmaßnahme die externe Nährstoffreduktion in der OWA, um den Tegeler See in einem Klarwasserzustand zu erhalten. Das bestehende Wasserbewirtschaftungssystem am Tegeler See erscheint geeignet zu sein, um das Seenökosystem in einem guten ökologischen Zustand mit guter Wasserqualität, insbesondere in Hinsicht auf bevorstehende Konsequenzen des Klimawandels, zu erhalten. Die Modellierungen zeigten, dass ein Wegfallen der Bewirtschaftungsmaßnahmen den Tegeler See vielfältig beeinflussen kann. Ohne die nährstoffarmen OWA-Zuflüsse und zusätzlichen Abflüsse durch die Seenleitung bildeten sich auf lange Sicht im Sommer vermehrt Phytoplanktonblüten, welche die Trübung sowie die Wassertemperaturen beeinflussen und die thermische Schichtung verstärken, was wiederum Cyanobakterienblüten begünstigen würde. Ebenso würden die kurzfristigen Auswirkungen von Starkregenereignissen ohne die nährstoffarmen OWA-Zuflüsse die Bildung von Phytoplanktonblüten begünstigen. Eine aktive und an die jeweilige Situation angepasste Seenbewirtschaftung, insbesondere durch Nutzung der OWA und der Seenleitung, kann den Tegeler See und die Wasserqualität in einem guten und nachhaltigen Zustand belassen und einen erneuten Regimewechsel hin zur Phytoplanktondominanz mit geringer Sichttiefe vermeiden.

Urbane Seen sind besonders gefährdete aquatische Ökosysteme, welche in der Zukunft detaillierter und sorgfältiger analysiert werden sollten, um sie in einem nachhaltigen und belastbaren Zustand zu erhalten. Vorhandene und zu erhebende Daten zur Wasser- und Sedimentqualität sollten für die Formulierung eines urbanen Seenmodells genutzt werden, welches die dreidimensionalen Navier-Stokes Gleichungen mit einem Sedimentdiagenese-

modell koppelt. Dieses gekoppelte Modell sollte zur Simulation von Bewirtschaftungsszenarien mit Fokus auf der externen Nährstoffzufuhr und der (meist kurzen) Aufenthaltszeit verwendet werden. Ein solches Modell für urbane Seen kann dann als Teil eines Gesamtmodells für das gesamte urbane Einzugsgebiet einschließlich Fluss-, Kläranlagen, Grundwasser-, Boden- und Abflussmodellen genutzt werden, welches in der Lage ist, angewandte Fragen hinsichtlich des urbanen 'Integrierten Wasserressourcenmanagements' zu beantworten.

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Chapter 1

Introduction

1.1 The urban water cycle

Cities worldwide were built near rivers, lakes or next to the ocean for numerous reasons. Probably the most important ones were to get access to freshwater, to discharge wastes and for traffic. Due to the growth of cities and the increasing migration of the rural population to the cities, their neighboring aquatic systems were strongly modified over time. With technological advances, those aquatic systems were connected to technical systems like sewer pipelines, the canalization and wastewater treatment plants. To achieve steady shipping traffic, rivers were straightened and artificial canals were built. Lakes were modified to become reservoir-like systems to use them, for example for drinking water abstraction or for flood protection. Thus, there are several differences between the biogeochemical cycling in a non-anthropogenic affected natural lake and in an urban one. Urban lakes can be influenced by multiple interfaces between natural and technical systems, which are of interest for an efficient and adaptive water management (Gessner et al., 2014). Schueler and Simpson (2001) defined urban lakes as aquatic ecosystems with a small surface area, a shallow average depth, a high ratio of the catchment to the surface area, a catchment area which is partially sealed and having an interacting management system. Therefore, urban lakes can be characterized as small, shallow surface water systems that are strongly influenced by matter and energy fluxes between different interfaces (Gessner et al., 2014) as well as by the respective urban catchment and the management system.

Due to the global on-going and increasing urbanisation, the importance of urban surface water systems will rise. The sustainable and sophisticated management and protection of the water quality of these systems will be crucial for drinking water abstraction, biodiversity, fishery and/or recreational uses (Naselli-Flores, 2008). Global climate change will provide additional challenges to the water management in the form of water scarcity, reduced discharges and changes of the stratification (Adrian et al., 2009). Still, main stressors for the water quality are diffuse pollution and hydromorphological degradation (Hering et al., 2015). Especially urban lakes are severely affected by the urban 'semi-closed' water cycle. Wastewater treatment plants serve to minimize the pollution of aquatic systems aiming for an efficient elimination of nutrients and harmful substances. However, treated wastewaters often contain dissolved substances that are not eliminated during the process, for instance micropollutants. Discharging these residual substances into urban lakes will strongly interact with their interfaces. Aquatic ecosystems that are either limited by phosphorus, nitrogen or both can experience dramatic changes when receiving increased loadings of these nutrients. Especially in the context of global warming the need for a dual management of phosphate as well as nitrate will increase due to longer vegetation periods in summer, stronger

stability of the water column, ideal conditions for the development of toxic cyanobacteria blooms and an increased depletion of oxygen in deeper water layers. Furthermore, sporadic and intense heavy rainfall events can become more frequent due to climate change. Such extreme events can cause the runoff of heavy stormwater flows into urban surface waters further acting as a stressor to the ecosystem. Process understanding of possible feedback mechanisms and interactions is crucial for the success and efficiency of the management of urban lakes. Due to the awareness of this pollution in Europe, the Water Framework Directive was set up to achieve a good ecological status (or at least potential good status) for water bodies. There are gaps of knowledge, for example about the different time scales between feedback processes (between external environmental and technical factors as well as between biogeochemical processes and fluid processes of the respective urban lake (Britton et al., 1975)), about the transport kinetics of contaminants in surface waters and about gas exchange processes between surface waters and the atmosphere (Gessner et al., 2014).

1.2 Scientific background

1.2.1 Physical limnology

The bathymetry, morphometry and occurrence of lakes are subjected to external factors, be it geological events over long time scales (the ice ages as one of the main factors forcing the formation of lakes in Germany), climate, catchment events and (morphological) degradation by anthropogenic water management. In the scope of this thesis, the aim was to investigate urban lakes. These managed surface water systems usually exhibit a much longer lateral than vertical dimension, but are still small enough to neglect the effect of the Coriolis force, and are still deep enough to display stratification periods in dependence of seasonal meteorological forcings and patterns. The climate, landscape and flows define one of the most important management criteria for lakes, the residence time τ, which is classically defined as:

$$\tau = \frac{V}{Q} \tag{1.1}$$

where V is the lake volume; and Q is the mean outflow rate. A short residence time indicates a lake system that is dominated by external processes (inflows), whereas a long residence time indicates a lake system strongly influenced by internal fluxes either from the atmosphere, biological activity or the sediment (diagenesis) (Fischer et al., 1979). In general, these flows can be described by the continuity and the momentum equations. For incompressible flow, the continuity (conservation of mass) can be expressed as:

$$\sum_i \frac{\partial U_i}{\partial x_i} = 0 \tag{1.2}$$

where i symbolizes the respective dimension, ranging from 1-3; U is a velocity component; and x is a spatial component. The momentum can be expressed in Eulerian form with the Navier-Stokes equations for viscous, incompressible flows while neglecting the Coriolis term:

$$\frac{\partial U_i}{\partial t} + \sum_j U_j \frac{\partial U_i}{\partial x_j} = -\delta_{i3} g - \frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \sum_j \frac{\partial^2 U_i}{\partial x_j^2} \tag{1.3}$$

where $\delta_{i3} = 1$ for $i = 3$ and 0 otherwise; g is gravity vector; ρ is density; p is pressure and ν is the kinematic viscosity, which includes physical as well as turbulent viscosity (all symbols without their respective units) (Lerman et al., 1995). In a nutshell, equation 1.3 shows the

change of the velocity over time plus convective acceleration which equals gravity (only along a vertical axis), a pressure gradient and viscous terms.

As the momentum equation showed, water flow is dependent on water density, which depends on temperature and, especially for saltwater, on the respective chemical composition. Density of fresh water, ρ_0, can be approximated by a fifth-order polynomial:

$$\rho_0(T) = 999.842594 + 6.793952 \times 10^{-2}T - 9.095290 \times 10^{-3}T^2 + 1.001685 \times 10^{-4}T^3 - 1.120083 \times 10^{-6}T^4 + 6.536332 \times 10^{-9}T^5 \quad (1.4)$$

where T is the temperature (Millero and Poisson, 1981).

For transport processes, equation Eq. 1.3 can be modified to include a source/sink term:

$$\frac{\partial C}{\partial t} + \sum_j U_j \frac{\partial C}{\partial x_j} = D^C \sum_j \frac{\partial^2 C}{\partial x_j^2} + S_C \quad (1.5)$$

where C is a concentration; D^C is molecular diffusivity, which also includes turbulent diffusivity; and S_C is a source/sink term that also includes reactive transport and interactions between substances (Lerman et al., 1995). The transport of heat can in a similar way be expressed for the water temperature T by substituting the source/sink term S_C with $\frac{S_T}{c_p \rho}$ where S_T is source/sink term for heat and c_p is specific heat of water (Lerman et al., 1995). Further, the diffusivity of a concentration is substituted by the heat conductivity. Therefore, heat energy fluxes are affecting the fluid dynamics of the system.

The main energy fluxes affecting the dynamics of fluids in lakes are external ones and either originate from the atmosphere or from the catchment. These energy fluxes drive mixing and transport processes in lakes. The thermal energy budget, which mainly affects water density, can be described as:

$$H_{net} = H_S + H_A + H_W + H_E + H_C + H_P + H_I \quad (1.6)$$

where the net heat exchange H_{net} equals the sum of the solar radiation, H_S, the scattered infrared radiation emitted from the sky, H_A, the scattered infrared radiation emitted from the water surface, H_W, the evaporation heat flux, H_E, the convection heat flux, H_C, the heat flux from precipitation, H_P and the heat flux from in- and outflows, H_I (Lerman et al., 1995). Changes of mechanical energy directly result in mixing processes in lakes. The change in potential energy, P_{pot}, can be described as

$$P_{pot} = \frac{\partial E_{pot}}{\partial t} = -\frac{1}{2} g h_{mix}^2 \frac{\partial \rho}{\partial t} \quad (1.7)$$

where E_{pot} is the potential energy; and h_{mix} is the mixed surface layer depth (Lerman et al., 1995). A direct quantity to describe energy exchanges between turbulent mixing processes and the potential energy of the water column is the buoyancy flux J_b:

$$J_b = K_z^\rho \frac{g}{\rho} \frac{\partial \rho}{\partial z} \quad (1.8)$$

where K_z^ρ is the vertical turbulent diffusion coefficient for energy (Lerman et al., 1995). The buoyancy flux quantifies the production of potential energy from turbulent kinetic energy sources. A negative bouyancy flux increases potential energy, whereas a positive one creates kinetic energy for additional mixing (Lerman et al., 1995). To numerically solve such systems of equations, initial and boundary conditions are needed, for which the buoyancy flux is an

example for an upper boundary condition. The resulting density differences in a water column can be described by the buoyancy frequency N:

$$N = \sqrt{-\frac{g}{\rho_0}\frac{\partial \rho}{\partial z}} \tag{1.9}$$

where ρ_0 is a reference water density. The buoyancy frequency is an indicator for the amount of potential energy in the water column and therefore the stability of the stratification. The kinetic energy fluxes, which have to surpass the potential energy of the water column for mixing, are mainly caused by wind stress, shear stresses, entrainments of inflows, density currents, convective cooling and heating (Lerman et al., 1995). These exchanges of thermal and kinetic energy as well as the specific characteristics of water are responsible for the most profound feature of lakes - thermal stratification. Water has its highest density of $1000\,\mathrm{kg\,m^{-3}}$ at $4\,^{\circ}\mathrm{C}$. In winter, this causes the denser water to be in the bottom layer with lighter water above it. Many lakes are also covered by a layer of ice at the surface, which blocks the generation of turbulence by wind. With increasing air temperatures, water in the surface layer is heating up and temperature gradients are dissolved by mixing. In summer, this causes the formation of a stratification in the lake column. Therefore in summer, a warmer surface mixed water layer, the epilimnion, is usually separated by a layer with a high vertical temperature gradient, the thermocline, from a stagnant and colder bottom water layer, the hypolimnion (Maniak, 2010). The thermocline acts as a transport barrier for dissolved substances due to its high density and temperature gradient. Many German lakes have two annual mixing events, one in spring and one in autumn, and, therefore, are called dimictic. Fig. 1.1 shows the idealized annual course of vertical water temperature profiles in an example lake.

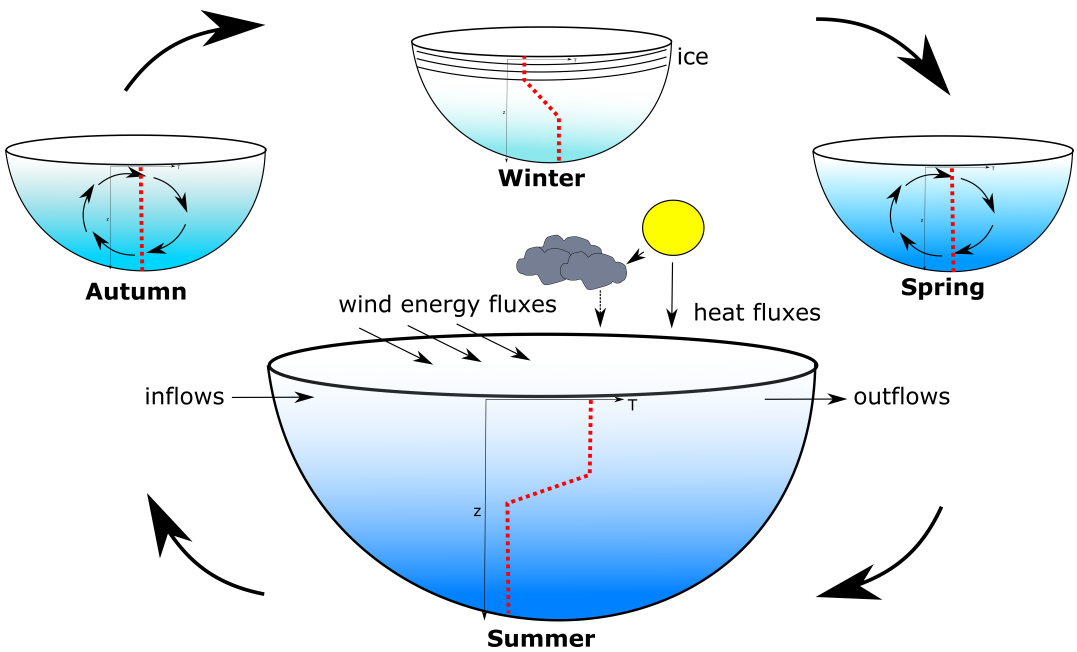

Figure 1.1: Many German temperate lakes depict periods of stratification (summer, winter) and mixing (spring, autumn). Schematic vertical profiles of water temperature are visualized for each season.

Several additional mixing processes are created by either convection (locally intense cooling and heating), density differences (Kelvin-Helmholtz-billowings), wind (Stokes drifts,

seiches), inflows (density currents) or the sediment (mineralization) (Lerman et al., 1995). These mixing processes can act on different spatial and temporal scales. Seiches, as an example, are basin-scale standing waves in lakes either at the surface or internally, which are caused by wind stress and the deflection of the wave at the shore. The propagation speed of internal seiches is hereby limited by the previously stated buoyancy frequency N. The occurrence of internal seiches in lakes can intensify transport processes over the thermocline and therefore affect the lake ecosystem by transporting nutrients or dissolved oxygen from the surface to the bottom layer (Ostrovsky et al., 1996, Boegman, 2009). Further, the impact of such seiche-induced transports of heat and oxygen can even affect the sediment layer and therefore diagenetic reactions, for instance the binding and release of phosphate in the sediment (Bernhardt et al., 2014). Density or gravity currents entraining into lakes are also important factors that can affect stratification and the lake ecosystem. The depth at which these currents entrain into the lake water column depends on the currents respective density, temperature and entrainment rate (which is mainly a function of the inflow slope and the discharge (Lerman et al., 1995)). Both types of currents are entraining from the inflow into the lake at a depth which equals a neutral point of buoyancy. During summer stratification, denser currents either entrain at the thermocline depth or below, forming an underflow (Fischer et al., 1979). The intrusion depth of such inflows can cause increased local concentrations of nutrients, micropollutants and biological communities (Wells and Nadarajah, 2009).

1.2.2 Lake ecology and nutrient cycles

A lake ecosystem is typically visualized as a hierarchy ranging from primary producers (autotrophs) to herbivores and carnivores (Scheffer, 2004). Most lake systems are inhabited by bacteria, periphyton and phytoplankton, aquatic plants, invertebrates as well as vertebrates (zooplankton) and fish. Important environmental factors for the establishment of species are the photic environment below the water surface (for primary producers), the water temperature and the availability of nutrients as well as dissolved oxygen. Light intensity is a prerequisite for photosynthesis and is attenuated in water according to Lambert-Beer's law:

$$I_z = I_0 e^{-kz} \tag{1.10}$$

where I_z and I_0 are the respective light intensities at the depth z or at the water surface; and k is the light attenuation coefficient, which can be approximated as $k \sim \frac{1.7}{d_{secchi}}$; where d_{secchi} is the measured Secchi depth.

Heat and nutrients as well as dissolved oxygen are transported vertically in a lake by mixing processes and turbulent fluxes. Especially dissolved oxygen is consumed by bacterial respiration as well as redox reactions and produced by photosynthetically active organisms. During stratification periods, dissolved oxygen is replenished in the mixed surface water layer but its vertical transport is blocked by the thermocline. Therefore, most lakes experience a period of oxygen depletion during stratification periods in bottom water layer, which affects the ecosystem structure as well as redox reactions at the sediment-water interface. In these deep layers, photosynthesis is also limited due to the scarce availability of light.

The availability of nutrients is the other main limiting factor for aquatic species. A textbook example for this limitation by nutrients is the Redfield ratio for maritime phytoplankton. It states that the molar ratio of $C : N : P$ is $106 : 16 : 1$ (Redfield, 1934), therefore limiting the growth of phytoplankton to the abundance of phosphorus and to nitrogen. It should be noted that the Redfield ratio can have a wide range for specific phytoplankton communities (Martiny et al., 2014). For most lake environments, the elements nitrogen (N) and phosphorus (P) are the main nutrients that determine the trophic state of the lake. The trophic state

relates the nutrient loadings from the catchment to the lake volume and acts as a criteria for the distinction between low-productivity oligotrophic lakes to high-productivity eutrophic lakes (Schlesinger and Bernhardt, 2013). The ratio of $N : P$ is a frequently used proxy to determine the growth of cyanobacteria and the consequential management strategy. In contrast to phosphorus, certain phytoplankton can fixate nitrogen from the atmosphere and deliver it into the lake ecosystem. Therefore, the water management is mostly focused on phosphorus limitation (Schindler, 1977). Further, in contrast to nitrogen, phosphorus can be stored internally in the lake sediments and can be released under certain redox conditions. Therefore, past phosphorus loadings can become a problem even years after the lake restoration has happened. Nonetheless, the past management strategy mainly focusing on phosphorus reductions (Schindler et al., 2008) is slowly changing to a dual management strategy focusing on controlling phosphorus and nitrogen (Paerl et al., 2016).

In general, nutrients can enter the lake system either as inorganic or organic nutrients and in a dissolved or particulate state. Particulate forms can be mineralized to dissolved forms by bacteria. Nitrogen is mostly discharged into lakes in its inorganic forms ammonium, NH_4, or nitrate, NO_3. Phytoplankton assimilate these inorganic forms. In the lake, certain phytoplankton can also fixate nitrogen from the atmosphere. Further, bacteria can either cause nitrification (transformation of ammonium to nitrate) or denitrification (transformation of nitrate to gaseous nitrogen, N_2) (Ikeda and Adachi, 1976).

Phosphorus mostly enters a lake as inorganic orthophosphate, $o - PO_4$. This phosphate form is then assimilated by organisms becoming organic phosphate. After death, organic phosphate is mineralized/decomposed to inorganic phosphate. Phosphate can be easily bound by clay minerals especially in iron-rich environments in the simple schematic form of $Fe(III) \sim P$ (or $Fe_3(PO_4)_2$) or be mineralized into vivianite (Rothe et al., 2014). A subsequent release of phosphate from the sediment depends on pH as well as the redox conditions at the sediment-water-interface.

Two prominent freshwater phytoplankton groups are diatoms and cyanobacteria (Fig. 1.2). The former is often characterized as an r strategist (fast growth, high metabolism) and the latter as K strategist (slower growth, certain traits that favor during competitive times) (Shimoda and Arhonditsis, 2016). Certain cyanobacteria can also produce toxins like cyanotoxin and are therefore of high concern for water managers (Paerl et al., 2011). Especially during stratification events, cyanobacteria have the advantage to actively mitigate upwards due to their vacuole movement whereas diatoms just sink down (Visser et al., 2016).

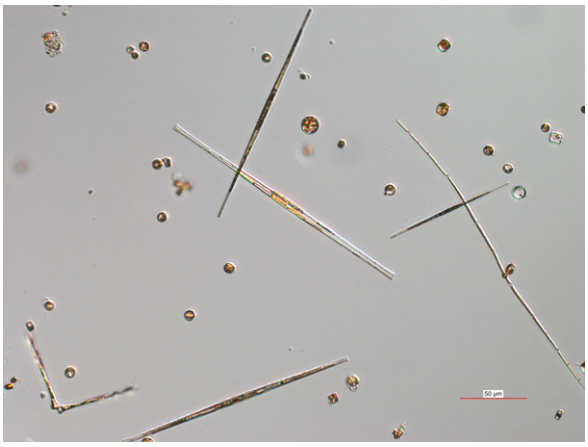

Figure 1.2: Microscope photograph of a sample taken in Lake Tegel on 16.02.2017: centric- and bar-shaped figures are diatoms (*Fragilaria ulna angustissima*), whereas the filaments refer to cyanobacteria (*Limnothrix redekei*).

1.2.3 Numerical lake modeling

The classical 'ancestor' of most lake models is the Vollenweider model (Vollenweider, 1976), which focuses on the steady-state phosphorus concentrations in a lake:

$$TP = \frac{L}{z(\sigma + \rho)} \tag{1.11}$$

where TP is the phosphorus concentration in the lake; L is the annual phosphorus loading into the lake; z is the mean lake depth; σ is the phosphorus net sedimentation rate; and ρ is the hydraulic flushing rate. This model is easy to use and expandable to also include the dynamics of other nutrients. Further, it incorporates the main decision making criteria of lake managers: the hydraulic retention time of the lake. Variations and more advanced versions of the Vollenweider model are still used nowadays (e.g. Hupfer et al. (2015)). Shortcomings of the Vollenweider model are the zero-dimensional approach, lacking a vertical resolution, and the statistical model assumption, which does not explicitly has a time reference and is therefore only valid for a long time period. Therefore, for a better physical representation of lakes, numerical lake models that also incorporate a spatial as well as temporal dimension are needed.

In the 1960s and 1970s, scientific progress regarding environmental fluid dynamics and physical processes in lakes were achieved (Imberger and Hamblin, 1982, Fischer et al., 1979, Spigel and Imberger, 1980, Csanady, 1975, Mortimer, 1971, Imboden, 1973). A main reason for this scientific progress was the aim of the scientific community to tackle lake eutrophication problems using mechanistic models (Rinke et al., 2014). These scientific advancements resulted in the formulation of modeling frameworks for numerical lake models with a vertical dimension and most equations can still be considered as the fundamentals for modern numerical lake models. The simulated spatial dimensions depend on the morphometry of the lake as well as the model purpose (and the available computational power):

- zero-dimensional models (also called one-box models) for shallow lakes (assuming complete mixing of the water column)
  - a special variety of the zero-dimensional models are two-box models, which assume a differentiation between an epilimnion and a hypolimnion with different characteristics but completely mixed
- vertical 1D models (z) for stratified lakes with a profound vertical density structure as well as a homogeneous horizontal density structure and a small till moderate size (no effect of earth's rotation)
- longitudinal-vertical 2D models (z-x) for stratified lakes to investigate vertical changes of variables (e.g. inflow dynamics)
- depth-averaged 2D models (x-y) for shallow lakes to investigate horizontal changes of variables
- 3D models (x-y-z) for moderate till large and deep lakes to investigate lateral and longitudinal changes of variables

Due to their application to practical management cases, most hydraulic lake models are already either simulating water quality as an essential part of the model or can be coupled to a water quality model. These coupled models (hydrodynamic simulations coupled to biogeochemical reactions and ecological mechanisms) can range from simple (for instance

just incorporating aggregated biotic compartments or state variables) to very complex models (for instance prey-predator feedback mechanisms and functional phytoplankton groups) and are the state-of-the-art. An interesting note is the strife of the lake ecosystem community for community-frameworks and open-access (Trolle et al., 2012). In the following, some commonly used lake modeling suites are shortly described and analyzed focusing on the hydrodynamic calculations as well as nutrient and phytoplankton dynamics. The small overview only includes physically-based lakes models (where empirical field and expert knowledge determines simplified interactions between the different modeled compartments), therefore excluding statistical models and approaches using, for example, machine learning algorithms.

PCLake (zero-dimensional model)

PCLake is an integrated zero-dimensional ecological model developed by the Netherlands National Institute for Public Health and the Environment in the early 1990s for the simulation of shallow lakes (Aldenberg et al., 1995, Janse, 2005). The model was calibrated on over 40 European lakes and its model sensitivity was extensively studied, enabling simulations with PCLake to have a wide acceptance (Janse et al., 2010). It is written in C++. Its focus lies on the dynamic shift between alternate stable states in shallow lakes: from a macrophyte-dominated clear water state to a phytoplankton-dominated turbid state (Scheffer et al., 1993). To address these stable states, PCLake calculates mass balances of nutrients (phosphorus, nitrogen, silica), underwater light environment, phytoplankton as well as (submerged) macrophyte dynamics and a simplified shallow lake food web (zooplankton, zoobenthos, fish, etc.). In the default version, the model includes simulations of the water column and the top layer of the sediment, but can be extended to also simulate an adjacent wetland with marsh vegetation. For input variables, PCLake needs water inflow, an infiltration rate, loadings of nutrients and particulate substances, temperature, light, the lake's morphometry (size and depth) and sediment features. Phytoplankton dynamics depend on a maximum growth rate, an optimum temperature function, the depth-integrated Steele's function for photoinhibition (as default) and a minimum function of nutrients based on Liebig's law. The phytoplankton growth is further controlled by respiration stress, mortality, settling and grazing.

PCLake was used to simulate the impact of climate change on a Danish lake with high internal phosphorus fluxes (Rolighed et al., 2016). Here the authors showed that the ecosystem was limited by nitrogen and that cyanobacteria benefited by an increase of water temperatures. Gillefalk et al. (2018) simulated the effects of bank filtration on shallow lake ecosystems using PCLake.

DYRESM-CAEDYM (vertical 1D model)

DYRESM (DYnamic REServoir Simulation Model) is a 1D hydrodynamic lake model explicitly simulating the vertical distribution of water temperature, salinity and density with a daily time step. It was developed by the Centre for Water Research, University of Western Australia, in 1994 (Imerito, 2015). The hydrodynamic model was highly influential and is still used in lake modeling studies. It is written in Fortran95. DYRESM uses a Lagrangian layer structure to simulate in-lake mixing processes by adjusting the thickness of individual layers and by combining adjacent layers. To avoid numerical diffusion, the user has to set a minimum layer thickness. The primary drivers of the model are surface heat, mass and momentum fluxes between the atmosphere and the surface mixed water layer and are calculated using bulk aerodynamic formulae. Dynamics in the surface mixed layer are determined by comparing the available turbulent kinetic energy (which consists of kinetic energy for convective overturn and wind stirring, $TKE_{avail} = KE_{convection} + KE_{stirring}$)

with the needed amount of potential energy for mixing (PE_{mixing}). The surface mixed layer deepens when sufficient energy is available (Hamilton and Schladow, 1997). Afterwards the amount of needed potential energy is subtracted form the available TKE_{avail}. When not sufficient energy is available, the TKE_{avail} is augmented with turbulent energy by shear stress (KE_{shear}) and deepening can continue until the available energy is not sufficient for mixing anymore. Deep mixing is calculated using a parameterization approach: from bottom to top internal mixing between adjacent layers is happening and kinetic energy at the bottom is created by bottom shear stress. Inflow dynamics are calculated by determining the depth of neutral buoyancy for the inflow, whereas the entrainment depends on a drag coefficient, the inflow shape, slope and angle as well as the bulk Richardson number.

DYRESM can be used as a driver for the ecosystem model CAEDYM (Computational Aquatic Ecosystem Dynamics Model), which was also developed by the Centre for Water Research, University of Western Australia (Hipsey, 2008). CAEDYM incorporates a flexible setup, which allows the user to generate a custom ecological and biogeochemical setup based on previous hydrodynamic calculations. The dynamics of carbon, nitrogen, phosphorus, silica and dissolved oxygen are stated using mass balances. Also, CAEDYM incorporates the movement and settling of inorganic particles. Phytoplankton species can be simulated as functional groups depending on a maximum potential growth rate, a temperature function, a minimum function between light (non- or photoinhibition) and nutrient availability, and grazing. The nutrient dynamics for phytoplankton growth are either calculated via a constant assumption using Michaelis-Menten equation (half-saturation constants for each nutrient determine the uptake) or dynamically by incorporating intracellular storage. CAEDYM can also calculate mineral respiration of organic matter by bacteria, zooplankton growth and grazing pressure as well as geochemical and diagenetic reactions (redox reactions and sediment fluxes, either static with empirical relationships or dynamic by numerically resolving the sediment conditions).

Rigosi et al. (2011) used DYRESM-CAEDYM to successfully simulate peak sequences and timings of functional phytoplankton groups in a Spanish reservoir.

GLM-AED2 (vertical 1D model)

GLM (General Lake Model) is a community-driven lake modeling suite developed by the Aquatic EcoDynamics Research Group at University of Western Australia in collaboration with the 'Global Lake Ecological Observatory Network' (GLEON) (Hipsey et al., 2014). It is open-access and freely configurable. GLM depicts a modernized code structure, written in C (and some subscripts in Fortran), and can be considered as kind of state-of-the-art vertical 1D model for lake hydrodynamics. The hydrodynamic calculations of GLM are performed on a Lagrangian flexible grid structure and many of the atmospheric fluxes, mixing and flow algorithms are based on previous models developed at the University of Western Australia, e.g. DYRESM (see paragraph above for more information). The user-specific customizations of the model code and its active maintenance and community make GLM appealing for modern lake simulations.

GLM acts as a driver for the ecosystem model AED (Aquatic Ecodynamics Model Library), with which it is internally coupled (Hipsey et al., 2013) and which was also developed by the Aquatic EcoDynamics Research Group at University of Western Australia. AED consists of two core libraries with several modules, from which the user can develop a specific ecosystem model. The basic library is just called AED2 and includes modules to calculate the dynamics of dissolved oxygen, phosphorus, nitrogen, silica, carbon, organic matter, phytoplankton, zooplankton and tracers as well as geochemical and diagenetic reactions. The advanced library is AED2+ and includes more advanced processes like dynamics of bivalves, pathogens, isotopes and sediment biogeochemsitry. In its recent and advanced

state and coupled to higher dimensional hydrodynamic models (e.g. 2D or 3D), AED2+ can also include the simulation of terrestrial processes. AED can simulate several functional phytoplankton groups based on a maximum growth rate, a temperature scaling and a minimum function consisting of light and nutrient availability. The user can choose from several light functions and can simulate internal nutrient dynamics either statically or dynamically.

GLM was used to optimize the water withdrawal management in a German reservoir while keeping sustainable oxygen conditions in the hypolimnion (Weber et al., 2017).

CE-QUAL-W2 (longitudinal-vertical 2D model)

CE-QUAL-W2 is a hydrodynamic model (Cole and Wells, 2017), written in Fortran90, continuously developed since 1975 when it was created as LARM (Laterally Averaged Reservoir Model). It assumes lateral homogeneity and is suitable for the simulation of long and narrow waterbodies (like reservoirs with a dendritic morphometry) with profound longitudinal and vertical gradients. CE-QUAL-W2 is maintained by the Water Quality Research Group of Portland State University. CE-QUAL-W2 solves the continuity and momentum equation assuming incompressible fluids, Boussinesq approximation for density changes as well as that velocities and pressures are turbulent time averages (Wells and Cole, 2000). The model can predict water elevation, velocities and water temperatures. Several water quality parameters, like tracers, inorganic substances, phytoplankton, periphyton, epiphyton, chemical and biological oxygen demand, nitrogen, phosphorus and organic matter, can be simulated internally. The spatial dimensions are expressed in a fixed grid spacing. For turbulence, several closure schemes can be activated by the user, e.g. k-ε. Phytoplankton can be simulated as functional groups, in which the growth depends on the maximum growth rate, a temperature function and a minimum function of light (expressed by Steele's equation) and nutrients (expressed using half-saturation coefficients). Further, respiration, excretion, mortality, settling and grazing affect the simulated phytoplankton biomass.

The sensitivity of reservoir management measures and calibration fits were investigated using CE-QUAL-W2 for a US reservoir by Brett et al. (2016).

open TELEMAC-MASCARET (depth-averaged 2D/3D model)

The open TELEMAC-MASCARET modeling system (abbreviated as TELEMAC in this thesis) was developed by the LNHE of EDF R&D (National Hydraulics and Environment Laboratory of the Research and Development Directorate of the French Electricity Board). TELEMAC is open-source and the user can easily modify the code in subroutines, which are written in Fortran90. For hydrodynamic simulations of flow and transport, TELEMAC has the options to either solve the depth-averaged two-dimensional Saint-Venant equations (TELEMAC-2D) or the three-dimensional Navier-Stokes equations (TELEMAC-3D). For the 3D case, TELEMAC assumes the hydrostatic pressure hypothesis and the Boussinesq approximation for the momentum. For turbulence, several options are available (for instance k-ε). Spatial discretization of the model domain is done using a unstructured grid made of triangular elements and in the 3D case additionally of prisms using sigma transformation. For the two-dimensional setup (which was subsequently used in this thesis), TELEMAC-2D solves the shallow water equations (continuity, momentum and transport) simultaneously (Hervouet and Ata, 2017b); here now given explicitly for the two dimensions x and y:

$$\frac{\partial h}{\partial t} + \frac{\partial uh}{\partial x} + \frac{\partial vh}{\partial y} = r_f \tag{1.12}$$

$$\frac{\partial uh}{\partial t} + \frac{\partial u^2 h}{\partial x} + \frac{\partial uvh}{\partial y} - \frac{\partial}{\partial x}(\nu_t \frac{\partial u}{\partial x} h) - \frac{\partial}{\partial y}(\nu_t \frac{\partial u}{\partial y} h) = h(\frac{f_x}{\rho} - g\frac{\partial(h + z_b)}{\partial x}) \tag{1.13}$$

$$\frac{\partial vh}{\partial t} + \frac{\partial v^2 h}{\partial y} + \frac{\partial uvh}{\partial x} - \frac{\partial}{\partial x}(\nu_t \frac{\partial v}{\partial x} h) - \frac{\partial}{\partial y}(\nu_t \frac{\partial v}{\partial y} h) = h(\frac{f_y}{\rho} - g\frac{\partial(h + z_b)}{\partial y}) \tag{1.14}$$

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial x} + v\frac{\partial C_i}{\partial y} - \frac{\partial}{\partial x}(\nu_{t,t}\frac{\partial C_i}{\partial x}) - \frac{\partial}{\partial y}(\nu_{t,t}\frac{\partial C_i}{\partial y}) = r_t \tag{1.15}$$

where u and v are the velocity vectors in x and y, respectively; r_f is a fluid source or sink term; ν_t is the turbulent viscosity; f_x and f_y are shear stresses; z_b is the bottom elevation; C_i is the respective tracer i; $\nu_{t,t}$ is the turbulent diffusivity; and r_t is a tracer source or sink accounting for reactive transport.

Shear stresses can, for instance, consist of bottom friction and wind (as well as Coriolis force and air-pressure gradient), both terms are acting in the same way and are added to the right side of the momentum equation. Bottom friction shear stress in x direction can be expressed by the Manning-Strickler law:

$$f_{bottom,x} = -\frac{g}{k_{St}^2 h^{1/3}} \frac{\rho}{h} u \sqrt{u^2 + v^2} \tag{1.16}$$

where k_{St} is the Strickler coefficient. The wind shear stress for the x direction is given by:

$$f_{wind,x} = \frac{1}{h} \frac{\rho_{air}}{\rho_{water}} a_{wind} U_{wind} \sqrt{U_{wind}^2 + V_{wind}^2} \tag{1.17}$$

where a_{wind} is the wind stress coefficient; and U_{wind} and V_{Wind} are wind velocities in x and y, respectively.

Matta et al. (2017) applied TELEMAC-3D to simulate the impact of wind stress on the thermal characteristics of a drinking water reservoir and gave management recommendations regarding the drinking water abstraction during and after a storm event.

For water quality simulations, TELEMAC enables the user to choose from five different modules:

- "O2" for oxygen dynamics in dependence of photosynthesis, organic loadings and ammonium, making it slightly more complex than the Streeter-Phelps model
- "BIOMASS" for the simulation of phytoplankton dynamics (no functional groups) as a function of light, temperature and nutrients (phosphorus and nitrogen)
- "EUTRO" is a combination of "O2" and "BIOMASS", therefore also explicitly simulating vegetal photosynthesis
- "MICROPOL" simulates transport and reaction dynamics of micropollutants, especially their particulate transport and interactions with the sediment
- "THERMIC" simulates water temperature dynamics in dependence of atmosphere-water interactions
- In the most recent version of TELEMAC-3D (v7p3r0), it is also possible to couple the hydrodynamic simulations with AED2

Each water quality module uses a different amount of simulated tracers that are solved as sink or source terms, r, on the right hand side of Eq. 1.15. Regarding phytoplankton growth dynamics, the TELEMAC water quality modules determine these dynamics by computing temperature forcing, light forcing (depth-integrated Smith function), nutrient limitation function of phosphorus as well as nitrogen and a toxicity factor. The growth is

balanced by mortality and respiration, which are multiplied by a factor for temperature forcing. The water quality formulations of the "EUTRO" module are given in Chapter 5.

For the simulations in this thesis, the models GLM-AED2 and TELEMAC-2D were applied to Lake Tegel. The first one can be considered as the state-of-the-art for vertical 1D modeling of lake ecosystems and was chosen to analyze the projected impact of climate change on stratification at Lake Tegel over several decades. For this research study, long-term changes of the vertical composition of water temperatures, density, dissolved oxygen and nutrients are of greater importance for the evaluation and therefore a computationally faster 1D model fits the study aim better. TELEMAC was chosen to simulate the impact of short-duration heavy rainfall events on Lake Tegel's ecosystem. The effects of such heavy rainfall events can be horizontally diverse and are mostly restricted to the surface mixed water layer. Therefore a depth-averaged 2D model can be applied. Further, the Chair of Water Resources Management and Modeling of Hydrosystems, TU Berlin, has a profound experience and knowledge in simulating surface water systems with TELEMAC. Both models are open-source and the codes can be modified to include specific aspects of the individual lake system.

1.3 Lake management

1.3.1 Management strategies

Lake management aims to preserve water quantity and quality in a sustainable and good state aimed at human preferences for recreation, sports, drinking water, ecological services and visual as well as olfactory criteria. Therefore, a main stressor for managed lakes and reservoirs is eutrophication, the enrichment of a water body with nutrients causing high primary production. Another burden for lakes are contaminants originating from agricultural or industrial businesses, for instance micropollutants and heavy metals, which can accumulate in lakes and their sediments and can have toxic effects. In general, the management strategy depends on the hydraulic retention time of the lake, τ. When τ is short, the lake system is dominated by external processes (mainly inflows) and a sophisticated management strategy should focus on controlling these factors, for instance nutrient reduction at the inflow sites. When τ is long, the management should focus on regulating internal factors, e.g. nutrient release processes from the sediment or entrainment of hypolimnetic nutrients into the epilimnion, which can be achieved by a chemical precipiation of, for example, phosphorus. Nonetheless, a sustainable and long-term lake management should focus on the elimination of external nutrient loadings. There is a wide range of lake management strategies applied and verified over the last decades. The success of each management strategy depends on the characteristics of the lake, for instance sediment features, lake depth, retention time, ecosystem structure and catchment. Table 1.1 gives a short overview of examplary management measures. An extended overview of management measures is given in Hupfer and Hilt (2008).

Table 1.1: Example overview of lake management measures, a special focus is given on measures applied to Lake Tegel

Measure	Description	Example
External		
Nutrient loadings reduction	Reduction of nutrient sources in the catchment	Phosphorus elimination plant at Lake Tegel achieved a reduction of 90 % of TP loadings (Heinzmann and Chorus, 1994)
Stormwater retention	Construction of wetlands to store stormwater runoffs	Walker and Hurl (2002) quantified the heavy metal retention of stormwater ponds
Sewage treatment	Connecting industries and households to canalization and wastewater treatment plants	In the 1970s/1980s about 90 % of all settlements at Lake Tegel were connected to the sewage system (Heinzmann and Chorus, 1994)
Flow diversion	Bypassing flows to avoid high contaminant loadings or to modify retention time	Lake pipeline at Lake Tegel, which can increase discharge or bypass inflows (Heinzmann and Chorus, 1994)
Internal		
Phosphorus inactivation	Chemical treatment to precipitate phosphorus and to prevent release from the sediment into the water column	Precipitation of phosphorus by adding poly-aluminium chloride at Feldberger Haussee (Kasprzak et al., 2018)
Sediment removal	Dredging of sediment layers rich in nutrients	Zhang et al. (2010) applied dredging with the intention to improve the water quality at Lake Yuehu, China
Hypolimnetic withdrawal	Withdrawal of bottom water masses to remove nutrients	Overview of applications is given in Nürnberg (2007)
Artificial mixing	Artificial mixing to limit light availability of phytoplankton	An overview with theory and applications is given in Visser et al. (2016)
Aeration	Hypolimnetic aeration or oxygenation to counter bottom oxygen depletion	An overview of applications is given in Beutel and Horne (1999)
Biomanipulation	Manipulating the lake trophic structure to decrease phytoplankton and to shift lakes from a phytoplankton-dominated turbid state to a macrophyte-dominated clear water state	For instance by fish restocking (Olin et al., 2006) and by resettling of macrophytes (Zeng et al., 2018, Hilt et al., 2018)

1.3.2 Challenges for urban lake water management

Although urban lakes and natural lakes share a lot of common stressors, there are certain challenges, which will have a more profound effect on lakes in cities. In the following a

short overview of future challenges for urban lake management mainly in Europe, North America and Oceania is given, neglecting general stressors like eutrophication.

Strong mingling of processes

Urban lakes are heavily connected to other components of the urban hydrological cycle (streams, groundwater, surface runoff) as well as intertwined with technical components (treatments plant, canalization, water supply). Due to the intensive pressure to use surface water systems for diverse aims (recreational activities, ecosystem functions), the interactions between the surface water system and its urban management are fuzzy with steep physical and biogeochemical gradients (Gessner et al., 2014). This causes the combination of different stressors and pressures at different times, for instance the overflow of technical treatments plants as well as the mixing of rivers into a lake during heavy precipitation events. Due to the unsteady and heterogeneous nature of these interfaces, urban lakes tend to be more complex than their more natural counterparts and ecosystem shifts are harder to predict. Therefore, future research has to deal with the sensitivity of urban lakes and the associated uncertainties regarding their dynamics.

Emerging pollutants

Due to technological advancements, trace concentrations of potentially toxic substances like pharmaceuticals (e.g. Gabapentin, Carbamazepine, Sulfamethaxol) and pesticides can be detected and quantified in the aquatic environment. In most cases theses micropollutants originate from the urban catchment specifically the wastewater treatment plants. Advanced wastewater treatment, e.g. activated carbon powder adsorption, ozonation or membrane filtering, can remove the substances before they enter the surface water systems (Luo et al., 2014, Margot et al., 2013). Nonetheless, when accumulating in the aquatic environment, the compound-specific impact of theses substances is partly unknown and requires further studies (Berger et al., 2017). Recent studies conducted experiments and field measurements to quantify compound-specific transport kinetics, which will help in evaluating the potential risk of theses substances on the ecosystem (Schaper et al., 2018, Schimmelpfennig et al., 2016). Here, also unknown degradation products are a potentially dangerous stressor. Another emerging pollutant are microplastics, which are widespread in the water and sediment phase (Eerkes-Medrano et al., 2015) with potentially ecotoxicological effects.

Sediment contamination legacy

Due to past heavy contamination periods, mainly due to rapid industrialization, urban lakes were the sinks of different contaminants, most prominently heavy metals, which are still a threat for lots of surface water systems worldwide (Chen et al., 2015a). Especially for restored urban lakes, the potential release of pollutants from the sediment into the water column, after effluent loadings were reduced, has to be analyzed and monitored.

Sanitation

Improvements in urban sanitation systems as well as the reuse of effluent waters are important tasks especially when considering a 'semi-closed' urban water cycle (Berger et al., 2017). It will be crucial to improve and adapt wastewater treatment plants and to connect urban settlements to the canalization. Also water reuse will become crucial in times of climate change (droughts, decreased flows) and intensified urbanization (higher demand), for instance by using bank filtration at urban lakes to create 'semi-closed' systems.

Climate change and stormwater runoff

Like most freshwater lakes, urban lakes will also be affected by climate change (Adrian et al., 2009). Certain effects of climate change on urban lakes (increased water temperatures,

earlier and longer summer stratification, more stable stratification, intense short-duration rainfall events) will be analyzed with numerical modeling and discussed in this thesis. Certainly, urban stormwater management has to adapt to heavy rainfall events to avoid potentially dangerous combined sewer overflows. Further, also our understanding about rainfall-runoff processes in urban environments has to be improved (Gessner et al., 2014).

Integrated water resources management

An integrated watershed management considering external as well as internal factors to the urban water cycle is an important concept for a future sustainable water management in cities (Wang et al., 2016). These holistic management approaches have to tackle several close-coupled branches, for example social and ecological stressors in the form of ecosystem services (Berger et al., 2017). Future research has to quantify positive feedbacks between human happiness and biodiversity to allow urban planners to optimize the water management of the urban catchment. Also potential interactions between agricultural landuse, groundwater fluxes, urban surface waters and canalization have to be quantified.

Bottom-up citizen science approach

The increased availability of data (e.g. open-access) will certainly shape the involvement of the public with future urban water management measures. Transparent management measures in combination with meeting the demands of local residents will improve the information flow and help establishing trust with the stakeholders (Berger et al., 2017). Also the cooperation of citizens with scientists will help in improving scientific studies and identifying potential threats. A recent example of citizen science is the 'Urban Algae Project', which combines field sampling and a citizen survey to study the ecosystem services of urban ponds (Herrero Ortega et al., 2018).

1.4 Lake Tegel

The main focus of this thesis is the evaluation of the impact of lake management measures on Lake Tegel, Germany. Therefore, the lake itself is described several times in the following chapters (each study focusing on a different aspect of Lake Tegel). The next paragraph gives a first, short description of the main features of Lake Tegel as well as the past contamination history and recent developments.

Lake Tegel is a North German lowland lake formed during the glacial period (Pachur, 1989). It is the second largest lake in Berlin, Germany, with an area of about 3.9 km^2 and a volume of 26.1 Mio. m^3. With a mean depth of about 6.6 m, Lake Tegel can be considered shallow and qualifies as a typical example of an urban lake (see definition in Section 1.1). The lake system has a dendritic morphometry with a deeper basin in the north-east and a shallow area bordered by several islands in the south-west (Fig. 1.3). Lake Tegel depicts a mostly unstable stratification during the summer months and either complete mixing during winter or also a weak winter stratification (see Chapter 3). Depending on the prevailing wind direction and speed, the adjacent River Havel can mix into the main lake basin causing an increased inflow of nutrients into Lake Tegel (Schimmelpfennig et al., 2012a). These wind-induced mixing events have a profound impact on the nutrient composition in the surface mixed layer. The main direct inflow is located in the north-east and consists of the combined discharges of the streams Nordgraben and Tegeler Fließ. The former consists of treated effluents from an upstream wastewater treatment plant. These combined inflows are treated in a phosphorus elimination plant (PEP Tegel), which eliminates up to 90 % of the total phosphorus inflow concentrations (max. plant capacity 6 $m^3\,s^{-1}$ (Heinzmann and Chorus, 1994)). Further components of the lake management are:

- Lake pipeline: bypasses water from the south-west to the PEP or vice versa with a discharge of up to 2.4 $m^3 s^{-1}$ (Heinzmann and Chorus, 1994).
- Hypolimnetic aerators to prevent summer oxygen depletion in the hypolimnion (Heinzmann and Chorus, 1994, Lindenschmidt and Hamblin, 1997)
- Bank filtration abstraction galleries: a mix of lake and groundwater is abstracted for drinking water production

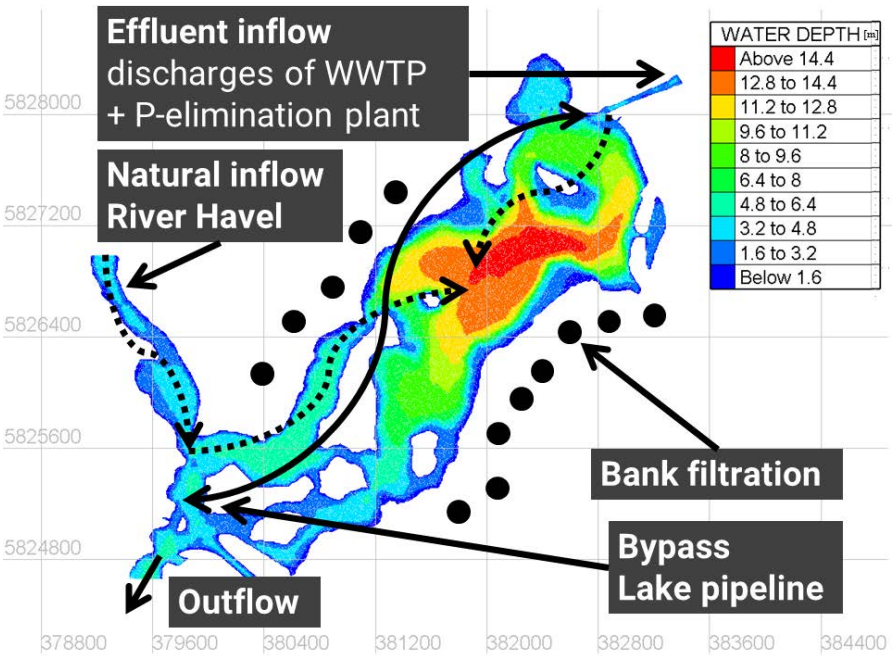

Figure 1.3: Bathymetric map of Lake Tegel including the main inflow conditions (taken from Ladwig et al. (2018)). WWTP - wastewater treatment plant

In the 1930s, Lake Tegel was connected to the Nordgraben and thereby with parts of the catchment of the River Panke. In this catchment area (situated in the north of Berlin), sewage farms were operated. Wastewaters were treated by soil filtration causing high leachings of nutrients and heavy metals into the groundwater and adjacent streams (Wolter, 1992). With increased discharges of the Nordgraben into Lake Tegel in the 1950s, eutrophication of Lake Tegel was intensified and caused excessive periods of phytoplankton growth. In the 1970s, Lake Tegel was experiencing severe periods of hypolimnetic oxygen depletion and cyanobacteria blooms (Schauser and Chorus, 2007a). To improve sewage treatment and to restore the area of the former sewage farms as well as Lake Tegel, the wastewater treatment plant Schönerlinde was constructed in the area of the former sewage farms. Further, also the PEP Tegel, the lake pipeline and the hypolimnetic aerators were constructed in the 1980s. These combined measures helped to restore the lake system into a good ecological state (Schauser and Chorus, 2007a, Chorus and Schauser, 2011). Due to the occurrence of micropollutants in Lake Tegel as well as in abstracted bank filtrate (Schimmelpfennig et al., 2016, Jekel et al., 2013a), the discharges of the Nordgraben into Lake Tegel were partly diverted, resulting in a decrease of the PEP inflow. Further, activated carbon powder was integrated into the treatment process of the PEP to adsorb micropollutants. Recently, toxic non-bloom forming cyanobacteria were detected by chance at Lake Tegel after water moss

floated close to the shorelines (Fastner et al., 2018). These cyanobacteria occurrences have to be monitored in the future and the mechanisms behind their formation have to be explored.

1.5 Scope of this thesis

Due to its water management system and morphometry, the Lake Tegel surface water system is complex and heavily intertwined with feedback mechanisms between multiple factors. In this thesis, the Lake Tegel ecosystem is first explored in *the past* (using a paleolimnological approach), then in *the present* (using a monitoring study) and, finally, in *the future* (using numerical modeling). This approach will offer new insights into the adaption of management measures to keep the Lake Tegel ecosystem in a sustainable state.

Former studies explored the successful shift of the lake from a state of eutrophication to a good ecological state with decreased nutrient concentrations, but did not further explore the spatial sediment composition. Therefore, in this thesis, **(1) an updated survey of the spatial abundance of lithogenic elements and heavy metals at different sediment sites of Lake Tegel is provided**. This will support the evaluation of the impact of past management measures on the sediment composition and in reducing the heavy metal sediment contamination as well as mitigating eutrophication. Also, the sediment survey will identify critical sediment hot-spots, which are hard to manage due to complex flow dynamics (e.g. strong influence by River Havel).

Further, frequent water temperature, electrical conductivity and dissolved oxygen data were monitored at Lake Tegel's deepest site for over a year. These data provide **(2) new updates and further insights into Lake Tegel's stratification dynamics, the appearance of seiches and a density current originating from the PEP during the winter season**. These data can be valuable for future model calibration studies and/or data science evaluations.

Although past studies have investigated the hydrodynamics of Lake Tegel using numerical models, none of these models have employed sophisticated water quality calculations, which are crucial for management applications. In this thesis, **(3) coupled hydrodynamic-ecological models are set up to investigate physical and ecological dynamics of Lake Tegel in future scenarios. There will be a logical progress from a vertical 1D model to a depth-averaged 2D model to simulate the impact of climate change and PEP management alterations on the lake system.** Especially the consideration of climate change effects on the lake will support future management decisions and strategies. Further, the depth-averaged 2D model provides new insights into the water exchange times of the Lake Tegel system, which are valuable diagnostic estimators to quantify the potential impact of contaminants and nutrients on the lake ecosystem.

This thesis is structured into six chapters consisting of the introduction (the current **Chapter 1**), three peer-reviewed journal articles (two published, one submitted), a monitoring study report and a synthesis (Fig. 1.4 shows the spatial and temporal dimensions of each study, e.g. if one-dimensional or two-dimensional, as well as the main study compartment, e.g. sediment or water column).

Chapter 2 presents the sediment survey of Lake Tegel and the comparison with two reference lakes (Lake Großer Wannsee and Lake Userin) to evaluate the success of the past management measures. In total ten sediment cores were analyzed and evaluated using multivariate statistical methods. Main gradients of sediment composition were identified, which were either dominated by lithogenic elements or by heavy metals. The spatial differences in the abundance of heavy metals showed that the management measures were successful in the reduction of heavy metals at Lake Tegel. Further, a strong spatial heterogeneity of sediments in Lake Tegel was identified and gave information about the interactions be-

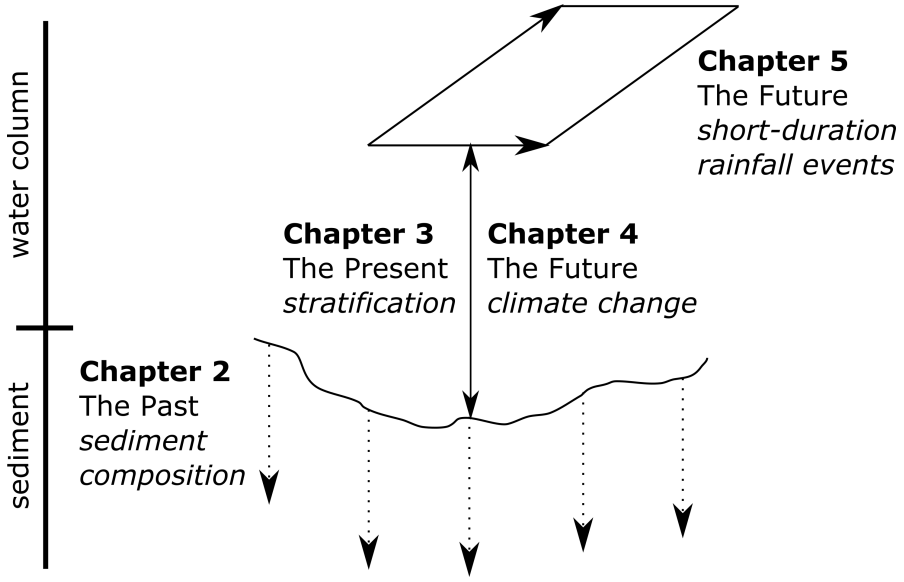

Figure 1.4: Structure of thesis showing the spatial (and temporal) dimensions of each study

tween water management and lake hydrodynamics. The results of this study support the success of the management strategy and provide the location of potential future hot-spots of sediment contamination.

Chapter 3 shows results of a monitoring study conducted at Lake Tegel to get additional physicochemical data. Long-term data of water temperature, dissolved oxygen and electrical conductivity were measured with a high temporal resolution by deploying a logger chain at the deepest site. The data supports an evaluation of the stratification periods from 2017-2018. Further, the vertical modes of potential seiches were calculated and a proposed density current, originating from PEP discharges during winter, was detected. These results provide the basis for future field and modeling studies.

Chapter 4 deals with the calibration, validation and application of a vertical 1D lake model to the Lake Tegel system to quantify the impact of future climate change and PEP management alterations on water temperatures, lake stratification and concentrations of dissolved oxygen as well as phosphate. By coupling an automatic evolutionary algorithm to the lake model, the model was successfully calibrated and validated to replicate water temperatures, dissolved oxygen, phosphate and nitrate dynamics. The scenarios demonstrate that an active lake management can mitigate effects of climate change on the lake ecosystem. Nonetheless, water temperatures will increase and future summer stratification periods will begin earlier and last longer.

Chapter 5 analyzes the impact of short-duration heavy rainfall events on the ecosystem of Lake Tegel. A depth-averaged 2D hydrodynamic model is applied to Lake Tegel using a time series of 15 years. The bottom friction coefficient was calibrated by comparing the concentrations of a simulated tracer with measured field data at Lake Tegel's deepest site. Further, this study is one of the first studies that modified and applied the water quality module EUTRO using field data. Water exchange times, like the hydraulic residence time and the influence time distribution, were computed and evaluated. The study shows that under east-wind conditions the River Havel intrusion into the lake basin was amplified but the influence times were low. Further, by applying principal component analysis it was visualized that the Lake Tegel system is mainly influenced by wind dynamics, inflows and, at long last, by biogeochemical reactions. To mitigate the impact of future short-duration

heavy rainfalls events on the lake ecosystem, a reduction of external nutrient loadings and an increase of external discharges were recommended.

Chapter 6 synthesizes the outcomes of this thesis and gives an outlook for future research.

Chapter 7 gives an overview of supplementary scientific work.

Chapter 2

In the Past: Assessment of the spatial and temporal composition of Lake Tegel's sediments

This study[1] was published as:

Ladwig, R., Heinrich, L., Singer, G., and Hupfer, M.: Sediment core data reconstruct the management history and usage of a heavily modified urban lake in Berlin, Germany, Environ Sci Pollut Res, 24, 25166-25178, DOI https://doi.org/10.1007/s11356-017-0191-z, URL https://link.springer.com/article/10.1007/s11356-017-0191-z, 2017

This is the postprint version of the article. The online version of this article contains supplementary material, which is available to authorized users.

2.1 Abstract

Urban surface waters face several stressors associated with industry and urban water management. Over much of the past century, the wastewater treatment in Berlin, Germany, relied on inefficient sewage farms, which resulted in severe eutrophication and sediment contamination in the recipient surface waterbodies. A prominent example is Lake Tegel, where a multitude of management measures were applied in the last decades for the purpose of ecosystem restoration. In this study, we analyzed sediment cores of three lakes with X-ray fluorescence spectroscopy: Lake Tegel, Lake Großer Wannsee, which is environmentally similar but has a different management history, and Lake Userin, which serves as a reference located in a nature protection area. Multivariate statistical methods (principal component analysis, k-means clustering, and self-organizing maps) were used to assess the sediment quality and to reconstruct the management history of Lake Tegel. Principal component analysis established two main gradients of sediment composition: heavy metals and lithogenic elements. The impact of the management measures was visualized in the lake sediment composition changing from high abundance of heavy metals and reducing redox conditions to less impacted sediments in recent layers. The clustering techniques suggested heterogeneity among sites within Lake Tegel that probably reflect urban water management measures. The abundance of heavy metals in recent lake sediments of Lake Tegel is similar to a lake with low urban impact and is lower than in Lake Großer Wannsee suggesting that the management measures were successful in the reduction of heavy metals, which are still a threat for surface waters worldwide.

[1] Reprinted by permission from Springer Nature Customer Service GmbH: Springer, Environmental Science and Pollution Research, 'Sediment core data reconstruct the management history and usage of a heavily modified urban lake in Berlin, Germany' by Ladwig, R., Heinrich, L., Singer, G., and Hupfer, M., 2017.

2.2 Introduction

Until the twentieth century, German surface water pollution was dominated by industrially derived organic contaminants, heavy metals, saline effluents, acid rain, sewage as well as agriculture-derived nutrients. Nowadays, micropollutants like pharmaceuticals and their derivatives represent an additional pressure, especially in urban areas (Nützmann et al., 2011). The water cycle of Berlin, Germany, is "semi-closed" and relies on discharging treated wastewater effluents into recipient streams and lakes that also act as sources for drinking water extracted by bank filtration (Massmann et al., 2004, Gessner et al., 2014). Advancements in wastewater processing reduced nutrient loadings into Berlin's lakes, yet in the nineteenth and twentieth century, Berlin's water management depended on sewage farms, where - at that time state of the art - untreated sewage was deposited on constructed wetlands for purification through soil filtration. This simple technique and an input of sewage exceeding the soil infiltration capacity introduced nutrient-rich and heavy metal-contaminated waters into the groundwater, streams, and lakes, leading to eutrophication and long-term sediment contamination (Ginzel and Nützmann, 1998). Severe water pollution problems were the consequences, e.g., contamination with sulfonamides (Richter et al., 2009) and acidification (Horner et al., 2009).

The lake sediment stratigraphy is a natural archive for environmental and anthropogenic impact and can help in evaluating past management strategies (Battarbee et al., 2005, Battarbee and Bennion, 2011). For instance, heavy metals can be seen as proxies for human activities originating from industry or mining. Stratigraphically appearing heavy metal contamination often represents the beginning of such activities and, in most cases, their decline documents the introduction of modern sanitation concepts and the advent of stricter water protection standards improved industrial production processes or depletion of natural resources (Bindler et al., 2010, Thevenon et al., 2011). To evaluate vertical variation of elemental composition in lake sediment, one can either use conventional quantitative techniques (Gredilla et al., 2012), which require pre-treatment of the samples, or non-invasive analytical techniques like X-ray fluorescence spectroscopy (XRF), which allows to obtain only semi-quantitative data, yet with unprecedentedly high spatial resolution. To interpret the resulting matrices of compositional data, multivariate statistical methods can be used, for instance to achieve an assessment of past management measures. For environmental data and especially lake sediments, cluster analysis and principal component analysis (PCA) have been used for decades. Cluster analysis, e.g., k-means clustering, efficiently describes similarity between sets of samples but gives no information about behavior of variables in the source data. In contrast, PCA reduces the dimensions of the potentially complex original multidimensional data by extracting correlations and projecting source data on only a few latent variables. These then represent common information from variables and often align with (sometimes otherwise undetected) environmental gradients. It is a widely used technique in paleolimnology and sediment quality assessment (Arambarri et al., 2003, Borůvka et al., 2005, Reid and Spencer, 2009, Comero et al., 2011, Rydberg and Martinez-Cortizas, 2014, Schreiber et al., 2014, Kleeberg et al., 2015, Lin et al., 2016, Rydberg et al., 2016). An alternative approach is to use self-organizing maps (SOM), which are a type of artificial neural networks and give extended classification details (Alvarez-Guerra et al., 2008). A SOM has the profound advantage to visualize the multidimensional data on a two-dimensional plane, while to sufficiently explain most variance in a PCA model more than two PCs would have to be used. SOMs have found widespread use in sediment assessment studies (Nadal et al., 2004, Alvarez-Guerra et al., 2008, Yang et al., 2012, Subida et al., 2013, Olawoyin et al., 2013, Pandey et al., 2015) as they are able to visualize the similarities between multiple sites by further establishing their relationship to an environmental background. One type of SOM

is the "Kohonen" map, in which, expressed in a simplified way, multivariate data is sequentially presented to a grid which consists of units, each with a randomized weight vector (Kohonen, 1998). The algorithm picks a random vector from the multivariate data and looks for the best matching unit in the grid. In an ensuing competitive step, the found unit and its neighbors get updated to become more similar to the input data. After presenting all input vectors from the multivariate data, the grid should converge to represent similarities between sites of the original data set. Both, PCA and SOM, are descriptive techniques, which support pattern recognition and formulation of hypotheses rather than being instruments of inductive, hypothesis-testing statistics themselves.

This study focuses on Lake Tegel, the second largest lake in the city of Berlin, Germany, which is crucial for Berlin's water management due to drinking water production via bank filtration. In the 1950s, a linkage of upstream sewage farms into Lake Tegel was created and resulted in substantial input of nutrients and heavy metals into the lake. Ensuing eutrophication became critical in the 1970s, with oxygen depletion in the deep water, mass development of cyanobacteria (Schauser and Chorus, 2007a), and a loss of the lake's submerged vegetation and reed belts (Hilt et al., 2010). First restoration measures in this decade diverted discharge from the inflow into other surface waters and connected nearby settlements to the public sewage system (Heinzmann and Chorus, 1994). The construction of the wastewater treatment plant (WWTP) Schönerlinde, in the area of the former sewage farms, and the launch of the surface water treatment plant (SWTP) Tegel, which eliminates phosphorus from the north-eastern inflow, in 1985 resulted in the restoration of the lake (Heinzmann and Chorus, 1994). Furthermore, a lake pipeline was built to collect water from the lake outflow and bypass it to the SWTP Tegel to dilute influents and to maintain a minimum discharge. There are time series of water quality parameters as well as sediment investigation studies that provide further helpful insights into Lake Tegel's history (Pachur, 1989, Heinzmann and Chorus, 1994, Schauser and Chorus, 2007b, Kleeberg et al., 2012b).

In this study, the recent and historical composition patterns in urban lake sediments are investigated using a multivariate assessment of sediment data obtained by a fast non-invasive analytical technique. Sediment cores from heavily impacted Lake Tegel were collected and analyzed via XRF. For comparison, further sediment cores were taken in an additional urban lake (Lake Großer Wannsee) and a lake with low urban impact (Lake Userin). Using PCA and SOM, the sediment stratigraphy of each core is analyzed and should serve as a basis for a sophisticated sediment quality assessment. In addition, these data may help to evaluate the threat of future remobilization of heavy metals from the sediments of lakes used for drinking water abstraction like Lake Tegel and Lake Großer Wannsee. The hypotheses are that (1) management measures such as those that were applied at Lake Tegel are successful in reducing the abundance of heavy metals both in the water and in the sediment phase and (2) the recent sediment of urban lakes is less contaminated with heavy metals than in the past but still has a higher contamination than a lake with low urban impact. Here, the main question remaining is whether the recent sediments of Lake Tegel feature a lower abundance of heavy metals than in the past. Finally, (3) urban water management causes spatial heterogeneity in the sediment composition within and between urban lakes in the same catchment. Distinct hot-spots that differ vastly from other locations in the same lake should be recognized and handled by urban water management strategies.

2.3 Material and methods

2.3.1 Study sites

All investigated lakes (Fig. 2.1) are connected to River Havel and are roughly the same size (Table 2.1). Lake Tegel and Lake Großer Wannsee, in contrast to Lake Userin, can be considered as bays to the River Havel. Along the River Havel, the catchment is strongly changing from rural to urban dominance, here represented by the three lakes: Lake Userin as the less-affected lake close to the source of the River Havel, Lake Tegel as the first lake the River Havel enters during its passage through Berlin, and Lake Großer Wannsee as the final lake the River Havel passages as it leaves Berlin.

Lake Tegel (52.5761° 13.2533°) is a lowland urban lake situated in North-Western Berlin. It borders densely populated urban areas at the eastern, southern, and western shores as well as harbors and industrial sites at the eastern shore while the northern shore consists mainly of forests. Seven islands divide the lake into a northern main basin and a southern more river-like part integrated with the River Havel. The main inflows are the River Havel at the south-western boundary of the lake basin and the composite inlet of Nordgraben and Tegeler Fließ in the north-east, which receives the treated effluents of a wastewater treatment plant and, in the past, discharges from a sewage farm. The mixing of the River Havel into the lake - the lake enters the basin either via a northern or a southern passage - depends on wind circulation and river discharge itself which is controlled by a downstream watergate (Schimmelpfennig et al., 2012a).

Lake Großer Wannsee (52.4275° 13.1730°) is a bay of the River Havel in the south-west of Berlin. It has two main inflows: in the north, the River Havel and in the south, the artificial Teltow channel entering via the Lake Kleiner Wannsee. The southern inflow can also act as outflow depending on the hydraulic regime. Just like Lake Tegel, Lake Großer Wannsee is used for drinking water abstraction by the Berlin water works. The Teltow channel is infamous for high sewage loads and pollution originating from shipping and industry. About half of its discharge enters Lake Großer Wannsee over the passage by Lake Kleiner Wannsee (Heberer, 2002). Increased concentrations of pharmaceuticals sourced from industry are documented for Lake Kleiner Wannsee (Heberer, 2002).

Lake Userin (53.3411° 12.9694°) is a lowland lake situated in Southern Mecklenburg-Western Pomerania near the town Userin. The lake is part of the Müritz national park and belongs to a nature protection area with the aim to keep the surface waters in their original state with low anthropogenic impact. The River Havel has its spring approximately 12 km upstream from Lake Userin and crosses the lake from north to south.

Table 2.1: Morphological parameters of investigated lakes

	Lake Tegel, Berlin	Lake Großer Wannsee, Berlin	Lake Userin, Mecklenburg-Western Pomerania
Area [km^2]	3.9[a]	2.8[a]	3.3[b]
Volume [Mio. m^3]	26.1[a]	15.4[a]	17.2[b]
Maximum depth [m]	15.9[a]	9.8[a]	9.9[b]
Mean depth [m]	6.6[a]	5.5[a]	4.6[b]

[a] Jahn et al. (2002)
[b] Provided by the state departments for agriculture and environment, Mecklenburg Lake Plateau

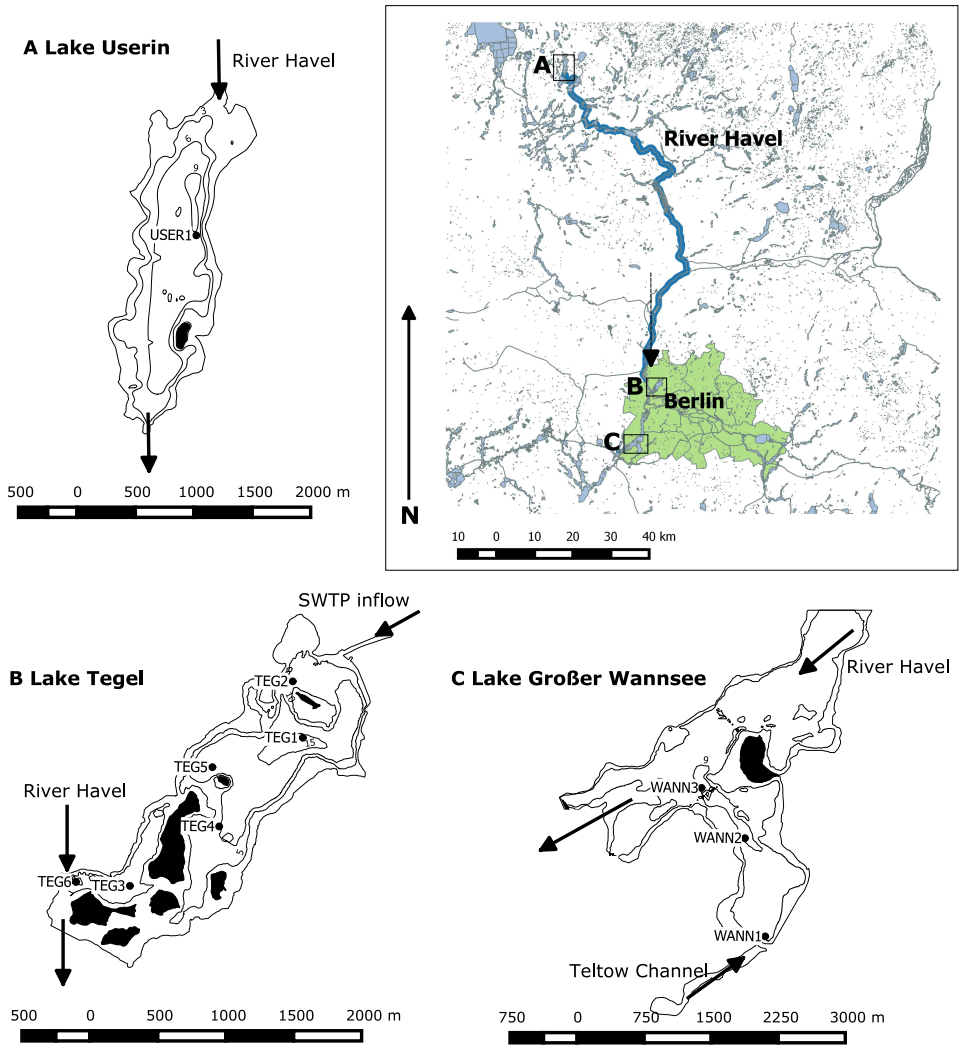

Figure 2.1: Location of the sampling sites (SWTP surface water treatment plant), black patches represent islands

2.3.2 Sampling

Sediment cores were taken at various locations (Table 2.2, Fig. 2.1) between September 2015 and March 2016 with a modified Kajak sampler (inner diameter 6 cm, UWITEC®) and were split in halves vertically before transport to the laboratory for XRF analysis at GEOPOLAR, University of Bremen. An additional sediment core was taken at the position of Lake Tegel's deepest site (TEG1), vertically subdivided into 1-cm layers, freeze-dried, and prepared for radioisotopic sediment dating at the Institute of Environmental Physics, University of Bremen.

Table 2.2: Assessment of the different sites regarding their location and urban impact (SWTP surface water treatment plant, WWTP wastewater treatment plant)

Site	Location	Core length [mm]	Anticipated urban impact
USER1	Middle of Lake Userin	346	Weak: nature protection area
TEG1	Deepest site of Lake Tegel, main lake basin	790	Strong
TEG2	Inflow of treated wastewaters	652	Strong: inflow of SWTP and WWTP, close to harbor
TEG3	Close to inflow of River Havel	572	Moderate
TEG4	Southern edge of main lake basin	730	Moderate
TEG5	Northern edge of main lake basin	401	Moderate
TEG6	Inflow of River Havel	235	Weak: inflow with agricultural impact
WANN1	Inflow/outflow of/to Lake Kleiner Wannsee and Teltow Channel	234	Strong: receives discharges of treated wastewaters and industry
WANN2	Deepest site of Lake Großer Wannsee	342	Strong
WANN3	Inflow/outflow of/to River Havel	316	Strong: River Havel catchment area now includes the city of Berlin

2.3.3 Analytical methods

All sediment cores were scanned in sections for major and trace elements with an ITRAX XRF-core scanner, COX analytical systems (Croudace et al., 2006)). Scanning was done with a Mo-tube with a step size of 1 mm and a count time of 30 s per step; tube settings were kept constant for all cores using a voltage of 40 kV and a current of 25 mA. Element data produced by the scanner are semi-quantitative and are expressed as total counts (cnts), i.e., integrated peak area. In addition to the scanning, high resolution photographs (256 dpi) and 16-bit radiographs of the sediment cores were produced. To minimize bias resulting from matrix changes and tube aging and to increase comparability between cores from different sites, the data were normalized by division with the measured coherent scatter. Therefore, data are expressed as total element counts to coherent scatter ratios (cnts/coh-

ratios). As proxy for organic carbon and water content, the ratio of incoherent to coherent scatter measured by XRF was used (Phedorin and Goldberg, 2005, Liu et al., 2013, Davies et al., 2015). We further used the ratio of normalized Fe to Mn total counts as proxy for redox conditions (Naeher et al., 2013, Davies et al., 2015, Rothwell and Croudace, 2015). High/low ratios of Fe:Mn point to reducing/oxidizing redox conditions. The non-processed XRF data are available in Online Resource 1.

Radioisotopic sediment dating was achieved by analyzing abundance of ^{210}Pb, ^{226}Ra, ^{214}Bi, ^{137}Cs, ^{40}K, and ^{7}Be by γ- spectroscopy using an n-type coaxial Ge-detector (Canberra Industries). Using a constant flux:constant sedimentation (CF:CS) model, in which the flux of ^{210}Pb is assumed to be constant, the chronology for TEG1 was formulated (Sanchez-Cabeza and Ruiz-Fernández, 2012, Bonotto and García-Tenorio, 2014).

2.3.4 Data analysis

XRF data were pre-processed as follows: (1) discarding of element data due to unreliable measurement, noisy signals, or intensities close to background level and (2) discarding of all elements with ubiquitously low intensity. Furthermore, only those elements complying with these restrictions in all ten sediment cores were considered. Valid elements for statistical analysis were K, Ca, Ti, Rb, Zr, Sr, Mn, Fe, Cr, Cu, Zn, and Pb.

To efficiently describe patterns in the multivariate dataset, we used PCA based on data from all depth layers of all cores. Data were logarithmically transformed to improve linear relationships between the elements, and scaled to a mean of zero and a standard deviation of one to ensure equal weight of all variables. We further computed the correlation of each element to the respective PCs. For clustering, we used the k-means method with the Hartigan-Wong algorithm, 25 random starts, and a maximum amount of 1000 allowed iterative runs (Hartigan and Wong, 1979). The pre-processed (logarithmically transformed) data were used to differentiate between a total number of five clusters, which were chosen visually by the "elbow method". Here, the sums of squared errors for k from 1 to 20 were calculated and plotted (Everitt and Hothorn, 2009). The interpretation of the clusters was done using box-and-whisker- plots. For filtering and smoothing, we either used a moving average filter implemented by convolution kernel or the Savitzky-Golay algorithm (Savitzky and Golay, 1964). For the latter, the smoothing was established by fitting a first order polynomial model on the data set with a set window size of 31 data points.

For data visualization and further clustering, we additionally used a SOM as implemented in the "kohonen" package (Kohonen, 1998, Wehrens et al., 2007) in R (R Core Team 2016). We provided a hexagonal grid of six times six units. This total number of 36 nodes was iteratively chosen to ensure that the amount of empty nodes in the final grid is low. As training data, the sediment data from sites of all lakes up to a depth of 150 mm were used. For training, the default algorithms of the package were applied (complete data was presented to the network 100 times, learning rate vector (0.05 0.01), circular neighborhood shape). The algorithm converged the grid into a map with clustered units after 40 iterations. The amount of clusters was determined by k-means clustering and the "elbow method".

2.4 Results

2.4.1 Sediment characteristics of Lake Tegel

Sediment cores of Lake Tegel were mainly composed of mud and, in deeper layers, sapropel-like material. The sediment core photographs and respective radiographs display that brighter, brownish colored zonations in deeper sediment layers appear in conjunction with

dark grayscale values referring to denser material, especially in TEG2 and TEG4 (Fig. 2.2). This agrees with a change in the visible sediment stratigraphy changing from a brownish to a black sediment color in the middle of most sediment cores together with a white grayscale value and therefore less-dense material. This indicates two general zonation types for most sediment cores: either denser material visible by a brownish sediment color or less-dense material with a black sediment color.

2.4.2 PCA model

The first two principal components capture 39 and 23 % of the overall variance, which totals to 62 % (eigenvalues and eigenvectors of the PCA are given in Appendix Table 2.3). The distance bi-plot (Fig. 2.3a) displays a strong heterogeneity of Lake Tegel's sites with points scattered across bivariate space, while Lake Großer Wannsee shows dominant dispersion along PC1 and Lake Userin is constricted to relatively limited location in the top left side. The clustering divided the data points into five groups, plotted on the bivariate space of the first two components. Clusters 2, 3, and 5 mainly consist of data points from sites of Lake Tegel as well as Lake Großer Wannsee, whereas cluster 1 incorporates data from all three lakes and cluster 4 only data from Lake Tegel and Lake Userin. The elements Cr, Pb, Zn, Cu, and Fe correlate positively with PC1 relating this axis to heavy metals, whereas Ti, Rb, K, Sr, Mn, and Ca are negatively correlated to PC2 (Fig. 2.3b). The latter elements are predominantly lithogenic in origin (Rb, Zr as well as Sr, in clay minerals or aluminosilicates) (Boës et al., 2011, Schreiber et al., 2014). Further support for PC2 being a proxy for the geological background of the respective catchment areas comes from Mn and Ca, which mostly originate from sedimentary rock, e.g., carbonates like rodochrosite or from calcareous mud (Pachur, 1989). Masking Lake Großer Wannsee and Lake Userin, the heterogeneity among individual sites of Lake Tegel becomes obvious (Fig. 2.3c). The sites in or close to the main basin (TEG1, TEG4, TEG5) disperse along an axis from the upper left side to the lower right side indicating a simultaneous increase of heavy metals and lithogenic elements. The inflow site TEG2 displays the highest horizontal dispersion indicating pronounced changes in the abundance of heavy metals while lithogenic elements remain constantly high in abundance. In contrast, the inflow site of River Havel, TEG6, displays only a vertical dispersion. The chronology of TEG1 by radioisotopic dating suggested the 1950s as the timeframe for the observed maximum abundance of heavy metals which coincides with the start of intensified wastewater discharge originating from sewage farms. Furthermore, we established clusters using the data of all Lake Tegel sites, which overlap and are close to identical with the previously formulated five clusters are as follows:

- Clusters 1, 2, and 3 mainly include data points that show the transition from deeper sediment layers to more recent layers of sites from the main basin
- Cluster 4 contains the recent sediment layers of the sites TEG2, TEG3, and TEG4, which are situated either close to the inflow of the SWTP or are at the edge of the main basin
- Cluster 5 incorporates recent sediment layers of sites from the main basin (TEG1, TEG5) and the River Havel inflow TEG6, as well as deep layers from the SWTP inflow site TEG2

To show simplified stratigraphic patterns, a moving average filter over 100 data points (equal to 10 cm) was applied to the scores of each core ordered along the depth axis (Fig. 2.3d). In the deeper layers, the development of most sites is marked by a sharp U-turn at

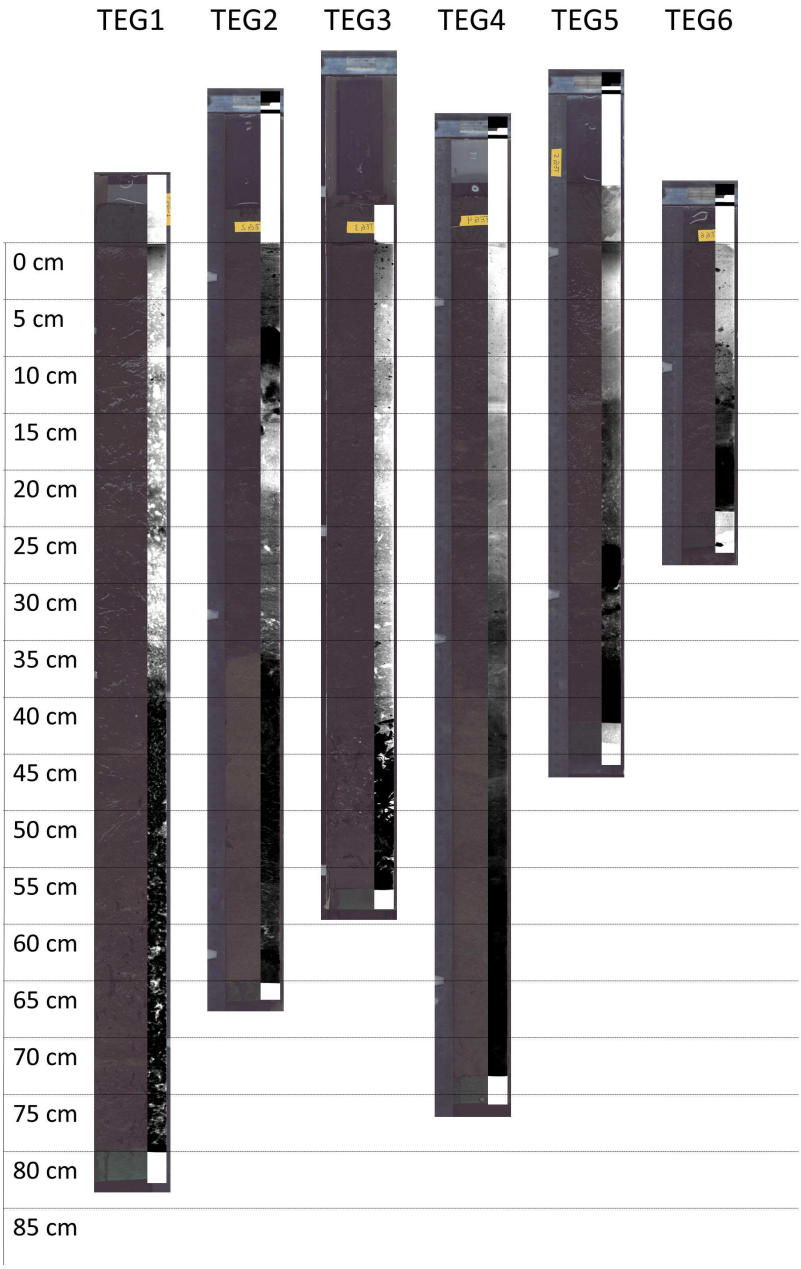

Figure 2.2: High resolution photographs of all sediment cores from Lake Tegel and the respective grayscale radiographs: darker grayscale values correspond to a visibly lighter sediment color, indicating the settling of a brown, dense material, e.g., visible in TEG2 and TEG4

times of heavy metal contamination. In recent layers, most sites move towards the lower left edge characterized by low heavy metal contamination.

2.4.3 Clustering with k-means

The spatial distribution of the established five clusters (Fig. 2.4a) over Lake Tegel as well as over the sediment depth visualizes for TEG1, TEG2, TEG3, TEG4, and partially TEG5 a sequence mostly changing from cluster 1 in deep layers over cluster 2 and cluster 3 to cluster 4 in the upper sediment layers. Cluster 5 occurs in recent sediment layers of TEG5 and TEG6, as well as in the deep sediment of TEG2. The box-and-whisker-plots (Fig. 2.4b) characterize the clusters as follows (due to the negative correlation of lithogenic elements to PC2, high/low PC2 scores represent a low/high abundance of lithogenic elements):

- Cluster 1: high organic carbon content, high Fe/Mn ratio, low abundance of Zn, Fe, Ca, and K, low PC1 score, and highest PC2 score
- Cluster 2: high abundance of Zn and Fe, high PC1 score, high Fe/Mn ratio, high content of organic carbon, high PC2 score, and low abundance of Ca and K
- Cluster 3: high abundance of Zn and Fe, high PC1 score, low Fe/Mn ratio, moderate PC2 score and content of organic carbon, and low abundance of Ca and K
- Cluster 4: high abundance of Ca, low PC2 score, low abundance of Zn, Fe, and K, low PC1 score as well as a low Fe/Mn ratio and organic carbon content
- Cluster 5: high abundance of K, high PC1 score and lowest PC2 score, high Fe/Mn ratio, similar abundance of Zn, Fe, and Ca like the clusters 2 and 3, and lowest content of organic carbon

2.4.4 Vertical distribution of redox zonations

For the sites TEG2, TEG3, and TEG4, a relationship between the abundance of heavy metals (represented by PC1) and the Fe/Mn ratio can be established (Fig. 2.5). Deep layers feature a low Fe/Mn ratio probably related to oxidizing redox conditions. In the vertical course of the sediment cores, we observed an increase of the Fe/Mn ratio concomitant with increasing abundance of heavy metals. The uppermost, recent sediment layers still display an increased abundance of heavy metals, compared to deeper layers, but mostly decreased Fe/Mn ratios. The development of TEG1 begins with an already increased abundance of heavy metals probably due to higher sedimentation rates at this site. Afterwards, the stratigraphy is similar to previously described ones. Both TEG5 and TEG6 also feature the decrease of heavy metals resulting in lower Fe/Mn ratios.

2.4.5 Classification with SOM

We clustered the converged SOM into 11 groups (Fig. 2.6a). Lake Tegel is stretching from the lower left side of the map, representing the inflow sites, to the upper right side, where the edges of the main basin (TEG3, TEG4, and TEG5) are located. The deepest site is at the center of the map close to Lake Userin, which is located on the left side of the map close to the SWTP inflow of Lake Tegel and next to Lake Großer Wannsee's Teltow channel inflow site. The remaining sites of Lake Großer Wannsee are situated at the lower right corner of the map. The scaled segment plots of each unit reveal different weighting towards

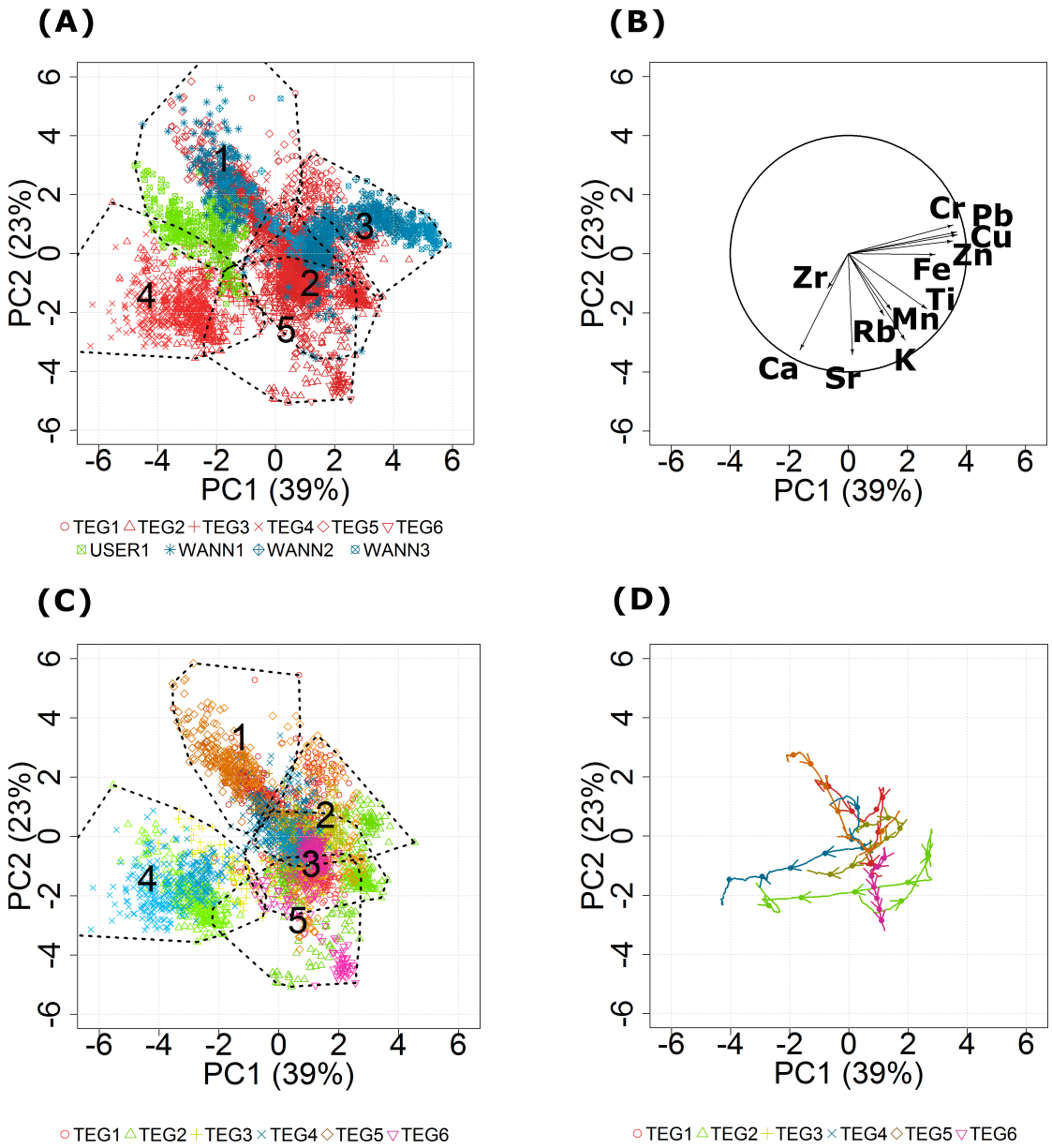

Figure 2.3: Distance bi-plots for the PCA. **a** Scores of the first and second principal component. **b** Arrows show structural coefficients of various elements on the PCA axes with unit circle, PC1 correlates with Cr, Pb, Zn, and Fe (heavy metals) whereas PC2 correlates mainly with Sr, Ca, Rb, Mn, K, and Ti (lithogenic elements). **c** Sites of Lake Tegel are visualized separately; hereby, deeper to recent layers are represented by the transition from dark to lighter colors. **d** Filtered lines (moving average of 10 cm) illustrate the historical change in sediment composition of Lake Tegel's sites, arrows represent the direction from deeper to recent sediment layers

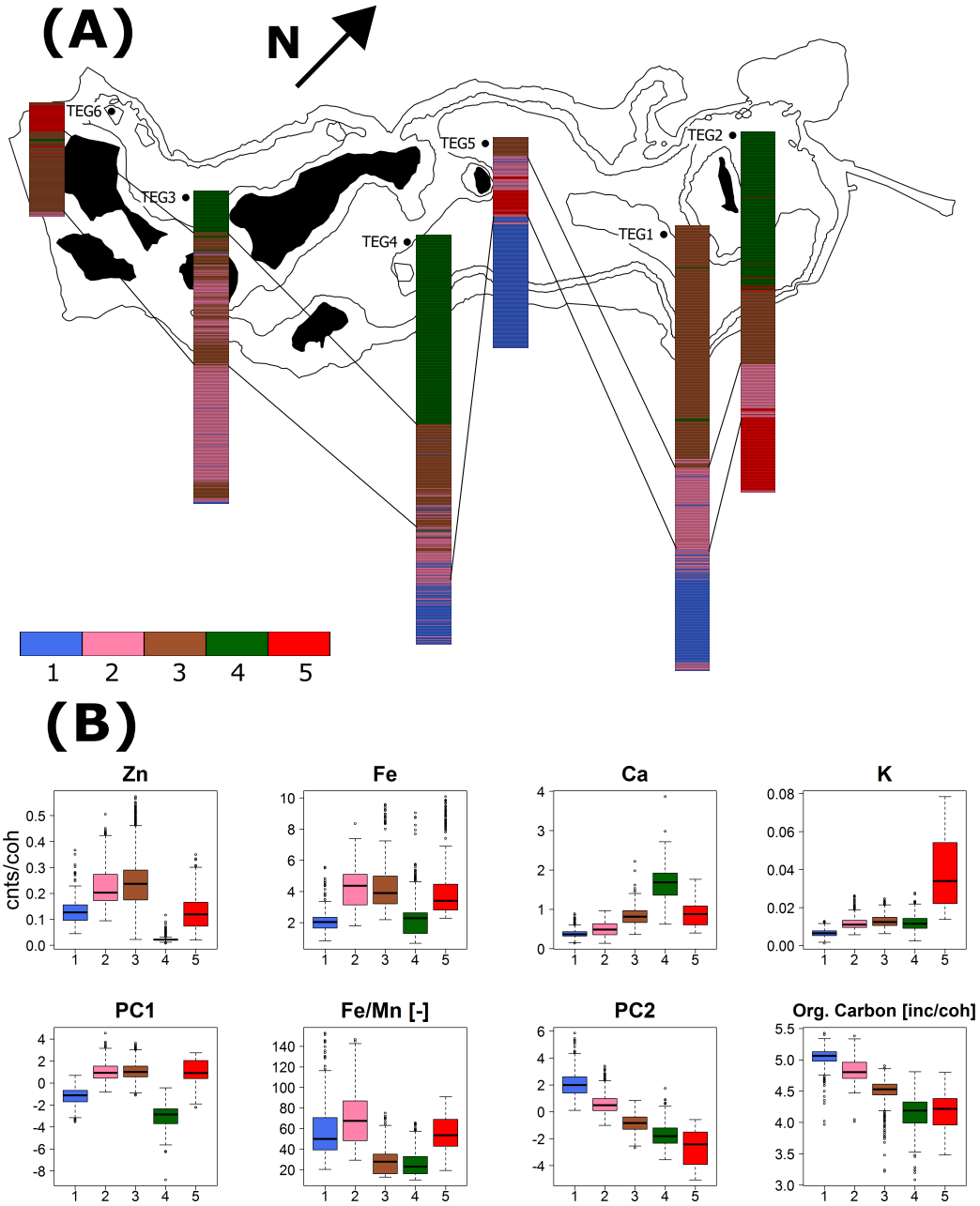

Figure 2.4: Clustered vertical profiles of the sediment cores at Lake Tegel. **a** Map of Lake Tegel, rotated about 45°, the color profiles at each site represents the respective cluster established by k-means for the vertical sediment layers. **b** Box-and-whisker-plots for the respective elements, scores or proxies, the colors represent again the respective clusters established by k-means (here the organic carbon is presented by the ratio of incoherent to coherent scatter)

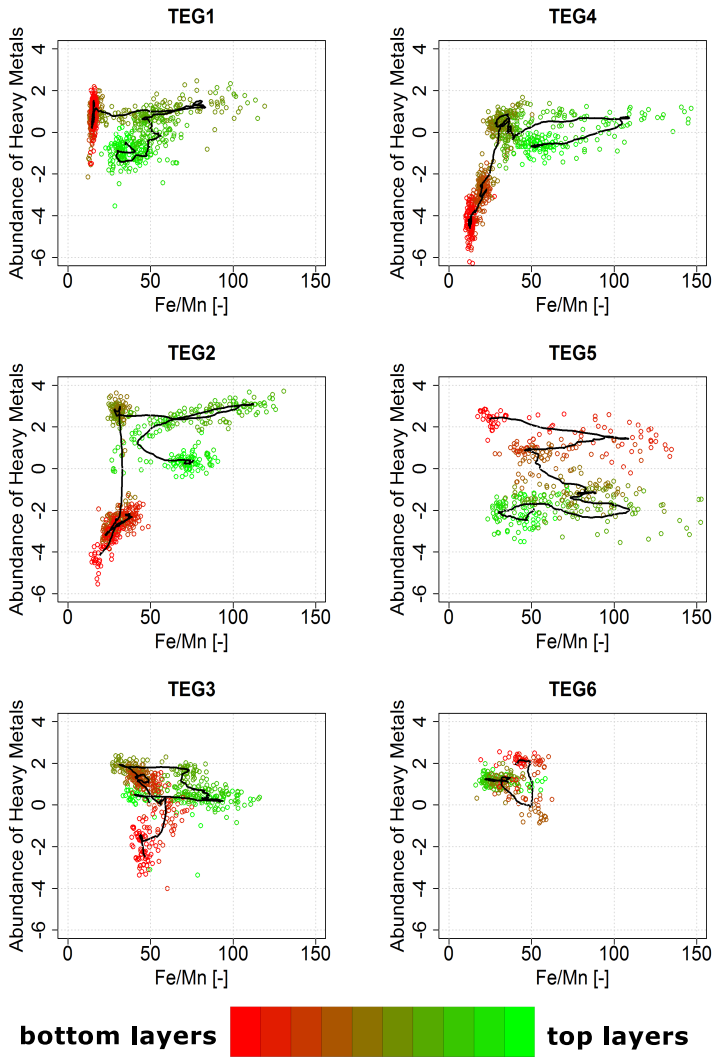

Figure 2.5: Normalized Fe/Mn ratio vs. abundance of heavy metals represented by PC1, data points were filtered with Savitzky-Golay algorithm, the color gradient goes from red (lower or deeper sediment layers) to green (upper or recent sediment layers); for TEG 1, TEG2, TEG 3, and TEG4, a lower Fe/Mn ratio in the deep layers implying oxidizing redox conditions in the past.With an increase of heavy metals in upper layers, the Fe/Mn ratio increases (reducing redox conditions); recent sediment layers are mostly characterized by a lower abundance of heavy metals and lower Fe/Mn ratios

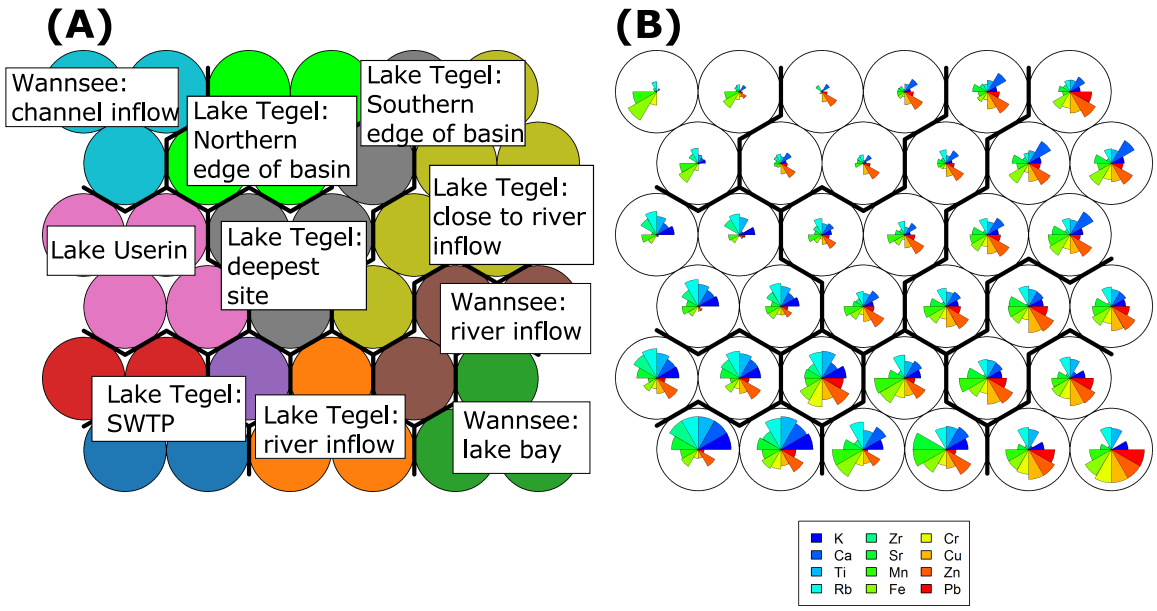

Figure 2.6: Self-organizing map. **a** Clustered map of the similar neighborhoods, the TEG sites in the center are bordering the less heavy metal contaminated sites on the left edge of the map (Lake Userin, Lake Großer Wannsee channel inflow) and the more contaminated sites on the right side (Lake Großer Wannsee bay and river inflow). **b** Code map showing contributions of elements as segment plots, there is a distinction between lithogenically imprinted sites on the left and heavy metal contaminated sites on the right

the respective elements (Fig. 2.6b). The heavy metal contamination consisting of Cr, Cu, Zn, and Pb is mainly related to the Havel inflow on the lower right corner. The lithogenic elements like K, Ca, Ti, Rb, and Sr as well as Zr are located at the lower left edge of the map. This is the location of Lake Tegel's SWTP inflow site as well as the Havel inflow into Lake Tegel. For Lake Tegel, the part close to the SWTP inflow shows increased loadings of the lithogenic elements, whereas the sites near the River Havel are related to an increased weighting to heavy metals. The recent layers in the main basin of Lake Tegel still have a slightly increased abundance of heavy metals in contrast to Lake Userin. But nonetheless, the map converged to a close neighborhood between Lake Tegel's deepest site and Lake Userin. The sites of Lake Großer Wannsee can be divided in the southern site with only an increased weighting to Mn and Fe, and the northern river-influenced sites showing higher contributions by heavy metals.

2.5 Discussion

2.5.1 Reconstruction of the management history of Lake Tegel

PCA identified two main gradients of sediment composition: heavy metals and geological background elements. This is in accordance to similar studies that used XRF analysis and PCA to assess the sediment composition of surface water systems, in which the first two principal components were also mainly correlated to either heavy metals or lithogenic elements (Schreiber et al., 2014, Kleeberg et al., 2015). Lake Tegel's sites are especially heterogeneous; while main basin sites show a high dispersion along the vertical axis and thus a change of the abundance of lithogenic elements, the site close to the north-eastern inflow features a horizontal dispersion implying a change of the abundance of heavy metals.

Nonetheless, all sites show a tendency towards low abundance of heavy metals and increased abundance of lithogenic elements in recent layers. In the past, the sediment of Lake Tegel was heavily influenced by an excess of heavy metals, which predominantly originated from the discharge of inadequately treated wastewaters from sewage farms. Especially the elements Zn and Pb are indicators for anthropogenic pollution (Grousset et al., 1995). The established clusters identify a sequence pattern for the sediment cores in the main basin. In deep sediment layers (cluster 1, TEG1, TEG4, TEG5), the sediment is characterized by high organic carbon content, probably already reducing redox conditions and low abundance of heavy metals and lithogenic elements. In the next step, the loading regime is changing (cluster 2, TEG1, TEG3, TEG4, and TEG5); the organic carbon content is reduced and the abundance towards heavy metals as well as lithogenic elements is increased. A slight increase of the Fe/Mn ratio as well as higher abundance of Zn and Fe suggests that during these times, the discharges from the sewage farms reached Lake Tegel and, due to a time lag, the beginning eutrophication enforced reducing redox conditions. During this transition, the sediment color changed from brownish to black implying increased abundance of sapropel-like material probably due to eutrophication. Subsequently, in cluster 3 (TEG1, TEG3, TEG4, TEG5), the organic carbon content and the Fe/Mn ratio are decreasing, but the abundance of heavy metals stays constant and the abundance of lithogenic elements is increasing. The uppermost recent layers for the cores TEG1 and TEG5 belong to this cluster, whereas the recent layers from TEG2, TEG3, and TEG4 are part of cluster 4. Here, the loadings of heavy metals are vastly reduced and the organic carbon content as well as Fe/Mn ratio are low. The applied management measures resulted in the decrease of nutrients, especially phosphorus, and heavy metals entering Lake Tegel, therefore enabling the restoration of the lake system. Our findings contradict the apprehension by Pachur (1989) about a future remobilization of heavy metals and indicate that the applied management measures are capable of restoring lakes and reducing heavy metal abundance in the sediment. The latter is still a threat for worldwide surface water systems (Chen et al., 2015b). Nonetheless, for most cores (especially TEG2, TEG3 and TEG4), the abundance of heavy metals and the tendency towards reducing redox conditions are still increased in the upper sediment layers compared to deep ones in spite of the reduction achieved by the management measures.

It should be noted that e.g. TEG2, TEG5, and TEG6 show vertical zones belonging to the fifth cluster. These layers are characterized by an increased abundance of heavy metals and lithogenic elements (especially Fe and K), as well as a low organic carbon content and an increased Fe/Mn ratio. This is probably due to soil runoffs or erosion events causing the leaching of elements from clay minerals and deposition at lake sites close to the inflows. TEG5 can be considered as a special case showing a different vertical sequence of clusters than the other cores. This could be because of the hydraulic regime under east wind conditions, when water from River Havel is entering the lake over the northern passage and transported material is settling down at the north-western sites of the main basin.

2.5.2 Assessment of recent sediment composition at Lake Tegel

The composition of the recent sediment cores at Lake Tegel varies across the SOM encircling Lake Userin and edging sites of Lake Großer Wannsee. Here, the deepest site of Lake Tegel is located next to Lake Userin, indicating similar abundances of heavy metals as well as lithogenic elements. The inflow site close to the SWTP of Lake Tegel has the highest abundance of lithogenic elements, whereas the sites close to the River Havel feature increased loadings of heavy metals. The higher abundance of heavy metals in the River Havel probably originates from natural and anthropogenic sources in its catchment area and appears only high in relation to the recent low heavy metal effluents from the urban area.

The bays of the River Havel, Lake Tegel and Lake Großer Wannsee, are characterized by their urban impact and applied water management measures. This becomes apparent in the gap between Lake Großer Wannsee's channel inflow site and its northern sites, which feature very dissimilar sediment compositions. The settling of heavy metals close to inflows and near shores is in accordance with the findings of similar studies investigating the heavy metal accumulation in lake sediments (Thevenon et al., 2011, Pang et al., 2015). The Teltow channel inflow, originally assumed to have an increased heavy metal contamination by industrial runoffs, features a low abundance of heavy metals and lithogenic elements. This is probably due to the settling of most heavy metals in the channel bed upstream of Lake Großer Wannsee. Furthermore, the increased abundance of heavy metals in the sediments of the sites at Lake Großer Wannsee close to the River Havel probably originates from industrial activities in the city of Berlin. In Hoelzmann and Zellmer (2008), the authors identified high heavy metal concentrations in the sediments of the River Spree in Berlin, which discharges into River Havel downstream of Lake Tegel. Heavy metals probably accumulated in these sediments since the beginning of industrialization, with a decline in loadings only occurring after 1990 due to economic changes and a general decline of industrial production in conjunction with improved industrial processes in Berlin (Hoelzmann and Zellmer, 2008). The increased abundance of heavy metals in Lake Großer Wannsee is therefore a direct consequence of urban effluent discharge.

2.6 Conclusions

Using a rapid, high resolution technique and assessing the results with multivariate methods, the management history of Lake Tegel could be visualized and interpreted. The management measures were successful in reducing the abundance of heavy metals in the sediment. In the past, the lake sediments from the different sites succeeded in a largely similar sequence pattern from low abundances of heavy metals as well as lithogenic elements over reducing redox conditions with an increased abundance of heavy metals to, again, low abundances of both heavy metals and lithogenic elements in recent sediment layers. Still, the vertical sediment composition of some sites differs vastly, especially close to the inflows and at the edge of the main basin. The cause for the heterogeneity of the sediment composition is probably the heavily modified urban water management which aims to optimize and control the water cycle for human needs. It results in altered inflow fluxes and hydraulic regimes. For instance, the SWTP at Lake Tegel artificially increases and maintains the inflow. Nowadays, the sediment composition of Lake Tegel, even if heterogeneous, shows reduced heavy metal contamination than in the past, less than a proximate urban lake and is, at some sites, similar to the heavy metal abundance of a less-impacted lake.

Acknowledgments

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Appendix

Table 2.3: Eigenvalues and eigenvectors for the first 12 principal components of the PCA (PC principal component)

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9	PC10	PC11	PC12
Eigenvalues [%]	38.6	22.4	12.5	8.6	5.7	4.3	2.5	1.6	1.3	1.1	0.9	0.4
Eigenvectors [-]												
K	0.22	-0.43	0.27	-0.03	0.16	-0.28	0.19	-0.59	0.40	0.06	0.20	0.05
Ca	-0.19	-0.48	-0.22	-0.24	0.07	0.03	-0.16	-0.05	-0.10	0.52	-0.53	-0.20
Ti	0.30	-0.28	0.33	0.02	0.19	-0.38	0.37	0.53	-0.32	-0.05	-0.15	0.00
Rb	0.13	-0.31	0.19	0.33	-0.85	0.10	-0.06	0.03	-0.02	0.05	-0.04	0.01
Zr	-0.08	-0.17	0.64	0.04	0.29	0.63	-0.25	0.06	-0.03	-0.04	0.03	-0.06
Sr	0.02	-0.51	-0.28	-0.27	0.00	-0.06	-0.43	0.14	-0.07	-0.55	0.26	0.08
Mn	0.16	-0.28	-0.46	0.35	0.17	0.50	0.48	-0.07	-0.17	-0.03	0.13	0.03
Fe	0.33	0.00	-0.17	0.53	0.25	-0.10	-0.43	0.30	0.43	0.21	-0.01	-0.03
Cr	0.40	0.15	0.01	0.19	0.11	-0.11	-0.35	-0.47	-0.63	-0.05	-0.15	-0.01
Cu	0.42	0.10	-0.04	-0.32	-0.11	0.11	0.02	0.07	0.01	0.14	0.32	-0.75
Zn	0.40	0.06	-0.03	-0.41	-0.07	0.19	-0.07	0.12	-0.04	0.42	0.21	0.62
Pb	0.42	0.11	-0.04	-0.22	-0.05	0.22	0.10	-0.05	0.34	-0.42	-0.64	0.04

Chapter 3

In the Present: Monitoring thermal stratification at Lake Tegel

This chapter gives an overview and discusses preliminary findings of an on-going monitoring study that started in July 2017 to get additional data for Lake Tegel aside from the regular monitoring conducted by the Senate of Berlin.

The preliminary results of the monitoring can be used as a basis for the formulation of future research questions and hypotheses.

This study was conducted by Robert Ladwig, Sylvia Jordan and Michael Hupfer. We acknowledge the support by Antje Köhler (Senate of Berlin) for the planning of the monitoring campaign and the help in the field by Philipp Wolke. We are also very thankful to helpful discussions and feedback by Georgiy Kirillin and Christof Engelhardt. Data from the upstream elimination plant were provided by Susanne Puhlmann (Berlin Water Works).

The report is in preparation as:

Ladwig, R., Jordan, S., and Hupfer, M.: Monitoring thermal stratification at Lake Tegel, Leibniz-Institute for Freshwater Ecology and Inland Fisheries, Germany, 2018, report in preparation

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3.1 Motivation

The Senate of Berlin is running a continuous monitoring at Lake Tegel to get data about physico-chemical and biological water parameters in different depths at the lake's deepest site with a temporal resolution of roughly a month. There is a lack of data in a high temporal resolution to better understand the onset and offset of stratification as well as deep water oxygen depletion.

The monitoring started at July 27 2017 and is an on-going campaign in collaboration with the Senate of Berlin. The aim of the study is to get water temperature, dissolved oxygen and electrical conductivity data in a high temporal resolution by deploying a logger chain at the deepest site of Lake Tegel. An additional aim is to use the extended data set to evaluate the impact of climate change on Lake Tegel, especially on thermal stratification. The monitoring at Lake Tegel is part of the framework of a Germany-wide long-term lake monitoring campaign conducted by Michael Hupfer's working group "Biogeochemical Processes in Sediments and Lake Management" at IGB.

Further, the impact of a hypothesized density current discharging from the PEP on the lake stratification was to be quantified. Past measurements showed that a denser inflow originating from the PEP is entraining in deeper water layers (Schimmelpfennig et al.,

2012a), therefore creating a density plume that could potentially deepen the surface mixed layer by convection and affecting the stratification. Since 2015 the PEP is receiving decreased discharges from the upstream wastewater treatment plant Schönerlinde. Nonetheless, there should still be differences of the water temperatures as well as the salinities between the respective inflows, the River Havel and the PEP, and the lake water. Additionally, the data can be used to quantify the abundance of seiches in Lake Tegel.

3.2 Study design

We deployed a CTO (electrical conductivity, water temperature, dissolved oxygen) logger chain at the deepest site of Lake Tegel (52.5814° 13.2649°). The chain consists of a buoy at the top and a weight at the bottom. Seven loggers in different depths (Tab. 3.1) are monitoring data every 30 min. Data were stored internally.

Table 3.1: Installation of the CTO logger chain

Depth [below surface]	Logger (Company name)	Monitored parameter
1 m	HOBO U24-001 (Onset Computer Corporation)	Electrical conductivity [$\mu S\,cm^{-1}$], temperature [°C]
3.2 m	*miniDO$_2$T* Logger (PME, Inc.)	Dissolved oxygen [$mg\,L^{-1}$], temperature [°C]
5.2 m	Tinytag Aquatic 2 - TG-4100 (Gemini Data Loggers)	Temperature [°C]
7.4 m	Tinytag Aquatic 2 - TG-4100 (Gemini Data Loggers)	Temperature [°C]
9.5 m	Tinytag Aquatic 2 - TG-4100 (Gemini Data Loggers)	Temperature [°C]
11.7 m	*miniDO$_2$T* Logger (PME, Inc.)	Dissolved oxygen [$mg\,L^{-1}$], temperature [°C]
13.7 m	HOBO U24-001 (Onset Computer Corporation)	Electrical conductivity [$\mu S\,cm^{-1}$], temperature [°C]

At the present, the loggers were readout twice, on November 21 2017 (117 days after deployment) and on May 16 2018 (293 days after deployment). At the current stage, electrical conductivity was calibrated using the internal factory calibration. The temperature accuracy of HOBO U24-001, *miniDO$_2$T* and Tinytag is 0.1 °C, 0.1 °C and 0.4 °C, respectively. The water temperature data were vertically interpolated.

3.3 Preliminary results

3.3.1 Thermal stratification July 2017 - May 2018

The temperature data confirmed the stratified state of Lake Tegel in summer 2017 (Fig. 3.1 A and B). The summer stratification of 2017 ended in early October and the summer stratification period of 2018 began in early April. In fall 2017 Lake Tegel was completely mixed (Fig. 3.1 C and D, the black line represents the temperature difference between surface and bottom layer, a widely accepted proxy for thermal stratification (Engelhardt

and Kirillin, 2014)). The winter period was rather discontinuous with sporadic and minor stratification events when the bottom temperature was higher than the water temperatures in the layers above. The winter stratification's onset was roughly in January and its offset in late March 2018. The isotherms confirmed the lamination of relatively warmer and therefore denser water in a depth of approx. 10 m to 12 m and water temperatures below 4 °C. The oxygen data showed a surface water peak in middle of March 2018, probably indicating a spring diatom bloom (Fig. 3.1 C). The data also confirmed that the spring overturn (mixing period) of 2018 was rather short (about a month from March to April 2018, Fig. 3.1 C and D). Subsequently the surface and bottom water oxygen concentrations were already declining since April 2018. This can cause a longer bottom oxygen depletion in bottom water layers in the summer stratification period of 2018 similar to the oxygen depletion in 2017 (Fig. 3.1 D).

The bottom electrical conductivity showed a curious pattern with sporadic high peaks during the fall mixing of 2017 and the winter stratification period 2017/2018 (Fig. 3.1 D). These peaks in electrical conductivity (EC) from January - March 2018 were happening simultaneously with increases in water temperatures (T) and a decline in dissolved oxygen (DO). Also the water temperatures above the sediment were experiencing a temperature increase after a small temporal lag (Fig. 3.2 A and B). During the winter period (Fig. 3.2 C), a closer inspection revealed that the sporadic temperature difference events happened in conjunction with strong, impulse-like increases of electrical conductivity.

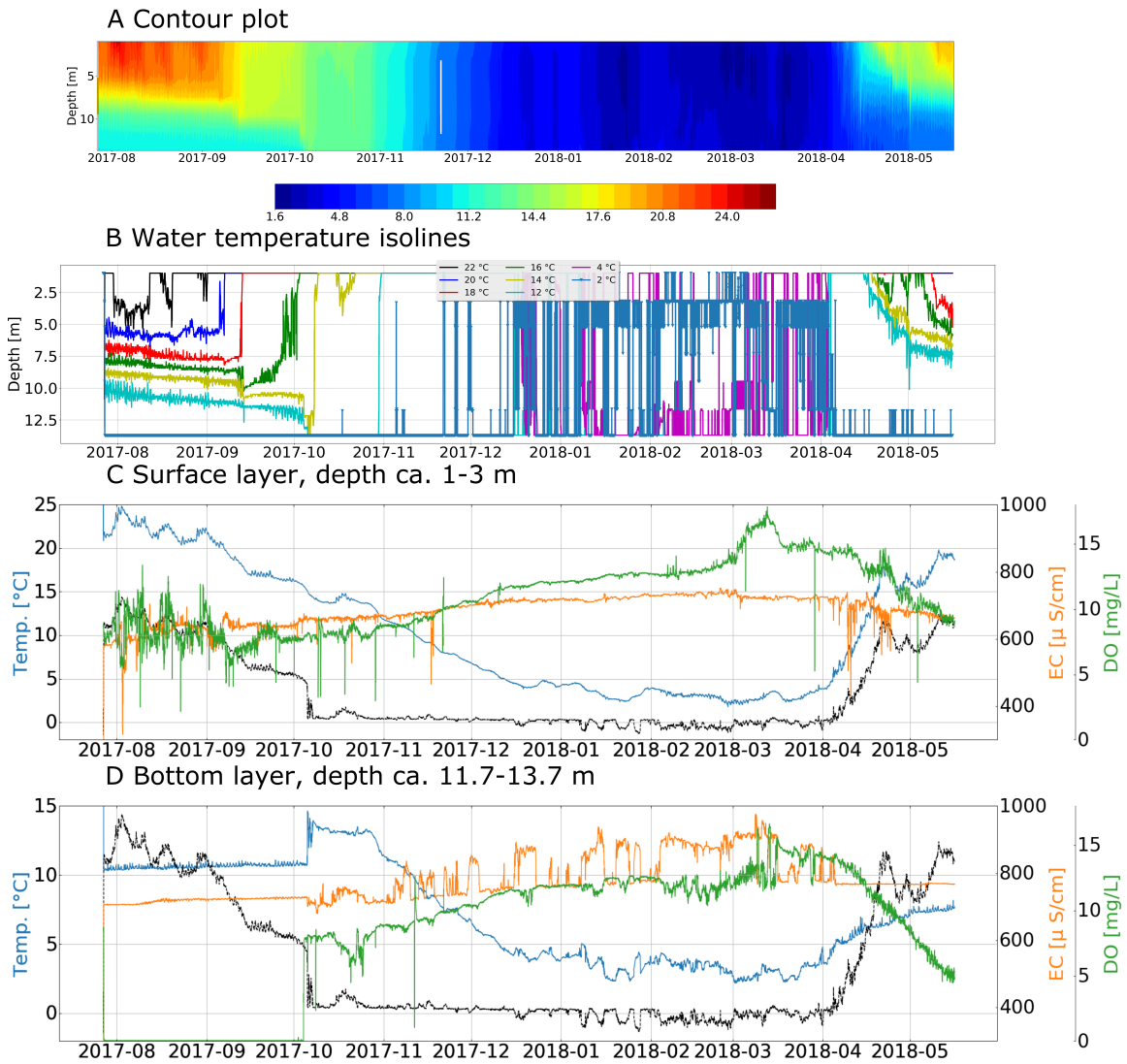

Figure 3.1: Time series of monitored data at Lake Tegel from 27.07.2017 - 16.05.2018. **A** Interpolated water temperature contour plot. **B** Interpolated isolines of water temperature. **C** Time series of water temperature, electrical conductivity and dissolved oxygen concentration in the surface layer; the black line represents the temperature difference between surface and bottom layer. **D** Time series of water temperature, electrical conductivity and dissolved oxygen concentration in the bottom layer; the black line represents the temperature difference between surface and bottom layer.

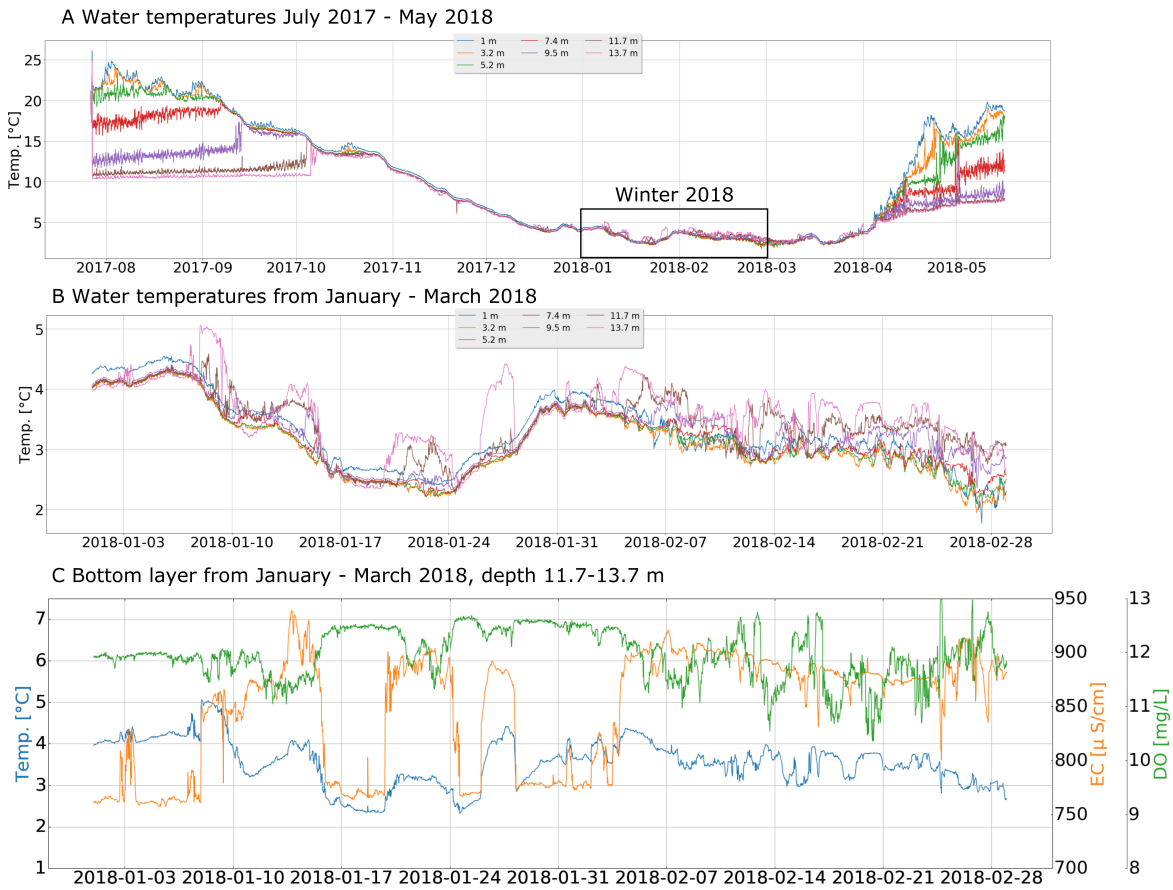

Figure 3.2: Time series of monitored data at Lake Tegel. **A** Monitored water temperatures in different logger depths from July 2017 - May 2018. **B** Monitored water temperatures in different logger depths from January - March 2018. **C** Time series of water temperature, electrical conductivity and dissolved oxygen concentration in the bottom layer from January - March 2018; dissolved oxygen concentrations were measured in a depth of 11.7 m whereas the water temperature and electrical conductivity were measured in a depth of 13.7 m.

3.3.2 Identification of seiches

The most pronounced thermal stratification occurred at Lake Tegel in August 2017 with a maximum wind velocity of $9.3\,\mathrm{m\,s^{-1}}$ and a mean velocity of $3.1\,\mathrm{m\,s^{-1}}$ prevailing from south-west (Fig. 3.3). To investigate the frequency of potential vertical seiches (V1 mode, (Boegman, 2009)) forming at Lake Tegel, we investigated the power spectral densities of the wind speed and the heat budget H of the lake:

$$H = \frac{1}{h} \int_{bottom}^{surface} T(z)dz \tag{3.1}$$

where h is the depth; and $\int_{bottom}^{surface} T(z)dz$ is the integrated water temperature [°C]. Oscillations in the heat budget can confirm the period of potential V1 mode seiches.

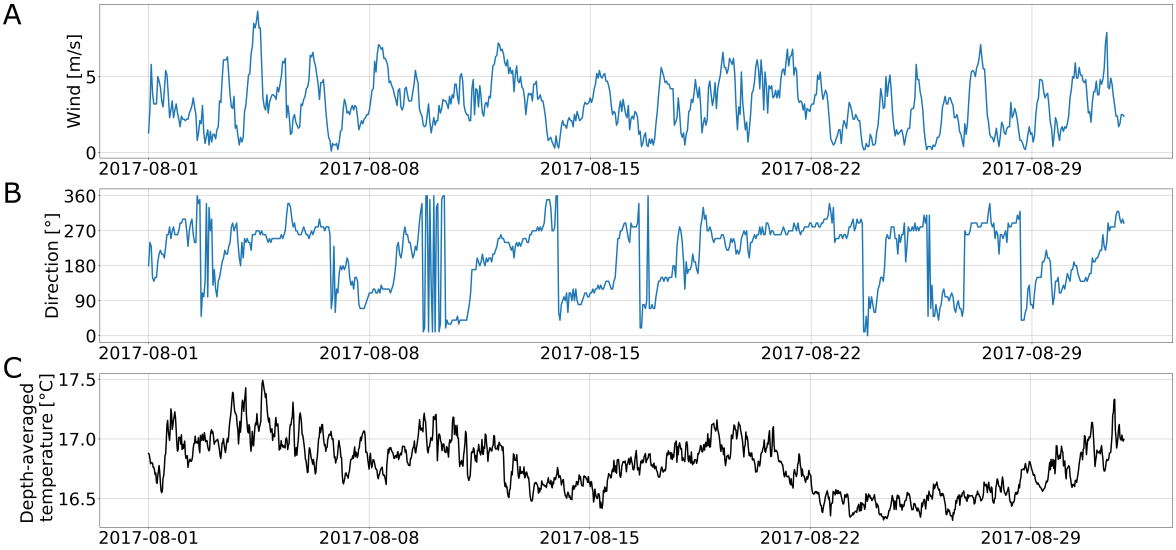

Figure 3.3: Time series of environmental data in August 2017. **A** Hourly wind velocity data. **B** Hourly wind direction data. **C** Depth-averaged water temperature [°C] reflecting the lake heat budget.

All steps to calculate the modal pattern of potential seiches were done according to Bernhardt (2013). Calculation of the power spectral densites (PSD) was done in Matlab using Welch's power spectral density estimate and the "RedNoise Confidence Levels" script by Dorothe Husson (Husson, 2014). The PSD of the wind velocity showed peaks at 24 h, 20 h, 19 h, 12 h, 8 h, 4 h and 3 h (Fig. 3.4 A). The PSD of the depth-averaged water temperature showed peaks at 24 h, 12 h, 8 h and 6 h (Fig. 3.4 B). Similar peaks for all PSDs were 24 h, 12 h and 8 h. The periods 12 h and 8 h could represent V1 mode seiches at Lake Tegel.

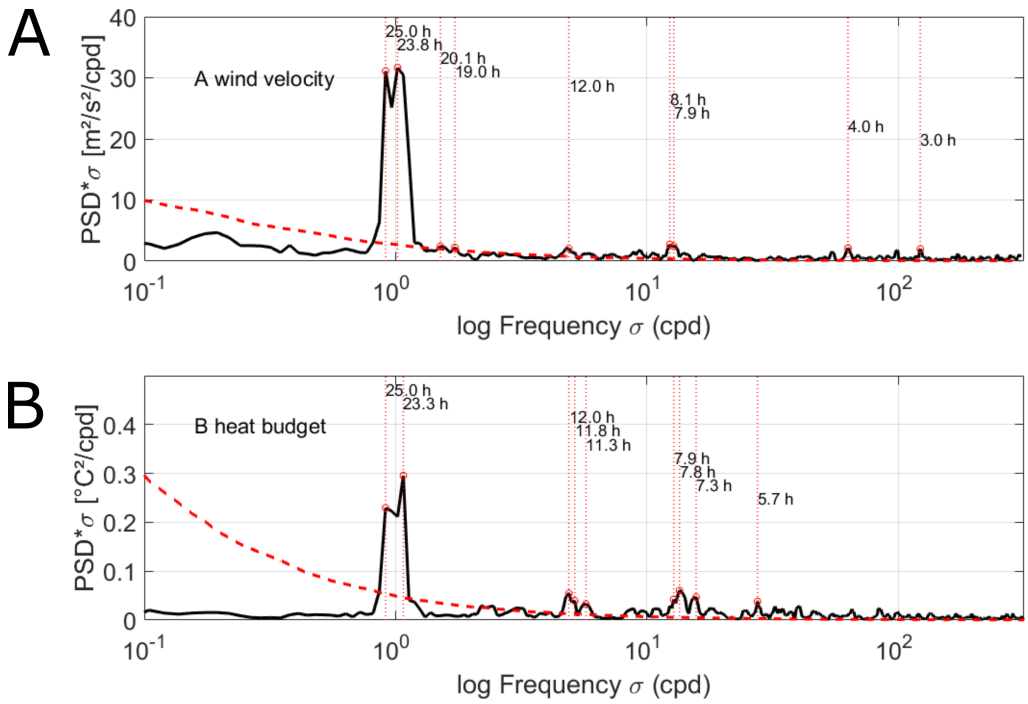

Figure 3.4: Power spectral density (PSD) plots for wind velocity and the isotherms in August 2017. The red dotted lines represent the mean red noise spectrum of the time series. **A** PSD of wind velocity data. **B** PSD of the heat budget.

3.4 Preliminary discussion

3.4.1 Winter stratification 2017/2018

The water temperature differences between surface and bottom logger identified two stratified periods: a continuous summer stratification with a water temperature difference between surface and bottom layer » 1 °C and a weak winter stratification with only some days when the difference was below 0 °C, which is typical for a winter temperature profile in a temperate lake. On closer inspection, the water temperature differences in the winter period were only sporadic and in conjunction with peaks of electrical conductivity (Fig. 3.2 C). This led to the formulation of three hypotheses to explain these winter phenomena:

1. 'Typical' winter stratification: Due to the density anomaly of water, denser and warmer water is located at the bottom of the lake during winter. During this stratified period, oxygen is depleted causing a change of redox conditions close to the sediments; an internal flux from the sediment into the water column occurred, which increases the electrical conductivity.

2. Density current: Lake Tegel is weakly stratified. A denser water plume discharging from the PEP entrains into the bottom layer due to its higher temperature and salinity (Peeters and Kipfer, 2009). These density currents are a function of the PEP's discharge, water temperature and salinity; therefore they show a sporadic and impulse-like pattern (Fig. 3.5).

3. Seiche-induced oscillations: The formation of ice during the winter period (there was ice formation during the winter 2017/2018 in Lake Tegel) could cause oscillations associated with the movement of internal waves in the bottom layer of the lake, which

caused the shifting of a thin water layer with higher electrical conductivity similar to events investigated at Lake Müggelsee (Kirillin et al., 2009).

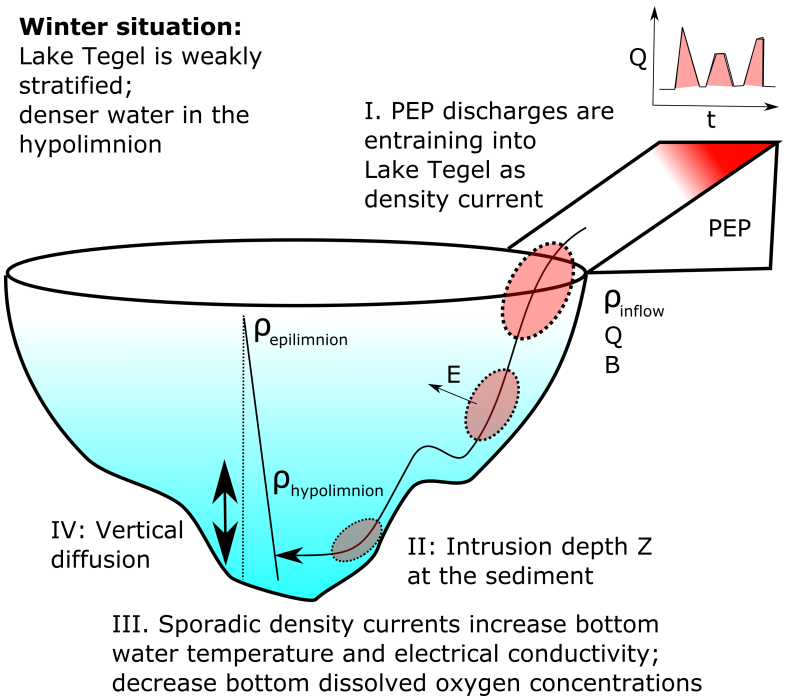

Figure 3.5: Proposed theory for the density current originating from the PEP. The respective symbols are explained in the equations below.

The first hypothesis can be rejected by inspecting the summer stratification period (Fig. 3.1 D) in the bottom layer. Here, the oxygen was already depleted, so a simultaneous internal flux was probably happening. Nonetheless, the electrical conductivity did not increase with the same magnitude as in the winter 2017/2018 period. Further, looking at the water temperatures in different depths (Fig. 3.2 B), the bottom layer was abruptly heated up, followed by a temperature increase in the above layers with a temporal lag. Under natural conditions, a bottom stratified layer should form over time, whereas the sudden bursts of temperature and electrical conductivity were probably a product of a density current entraining at the point of neutral buoyancy, which happened to be close to the sediment. Therefore, hypothesis 2 seems to be a more probable explanation for the sporadic periods of stratification in winter 2017/2018 at Lake Tegel. In this context, Lake Tegel in 2017/2018 should be classified as monomictic with a long summer stratification period and a long mixing period from fall 2017 to spring 2018.

Comparing the water temperatures of the PEP outflow with the ones measured at Lake Tegel's deepest site showed similar patterns and a time lag between both signals (Fig. 3.6). This can be interpreted in favor of the proposed density current theory.

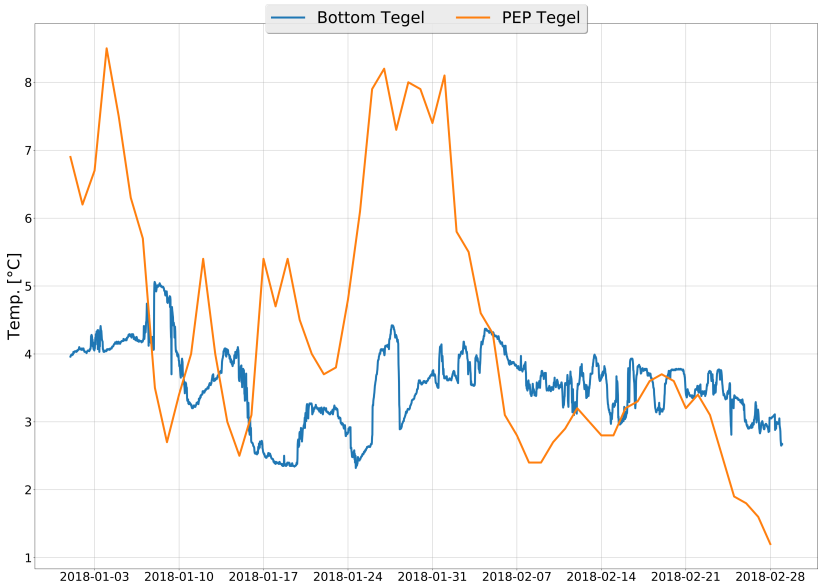

Figure 3.6: Comparison between water temperatures of the PEP inflow (orange line) and the water temperatures at Lake Tegel's deepest site (blue line) from January - March 2018.

To show that such a proposed density current could form at Lake Tegel during the winter period, we calculated the theoretical intrusion depth of such a density current. We were neglecting any potential entrainment, E, of the density current into the ambient water body. We quantified the stratification strength of the weakly stratified winter water body (during this period, Lake Tegel was weakly stratified with an electrical conductivity at the bottom of ca. 760 µS cm^{-1} to an electrical conductivity at the surface of ca. 720 µS cm^{-1}) by estimating the buoyancy frequency N:

$$N = \sqrt{\frac{g}{\rho_0}\frac{d\rho}{dz}} \tag{3.2}$$

where g is the gravitational acceleration (m s^{-2}); ρ_0 is the reference water density, which equals 1000 kg m^{-3}; $d\rho$ is the density difference between hypolimnion and epilimnion (kg m^{-3}); and dz is the depth difference between hypolimnion and epilimnion (m). Using the surface and bottom water densities measured in the field prior to the monitoring study (26.02.2017), we assumed the surface density as 1000.2 kg m^{-3} and the bottom density as 1000.4 kg m^{-3}. Therefore, the buoyancy frequency of Lake Tegel could have been quite high during the winter period of 2017/2018:

$$N = 1.2 \times 10^{-2}\,\mathrm{s}^{-1} \tag{3.3}$$

The respective buoyancy flux of the inflow can be calculated by:

$$B = g\frac{\rho_a - \rho_{inflow}}{\rho_{inflow}}Q \tag{3.4}$$

where ρ_a is the ambient water density of the epilimnion (kg m^{-3}); and ρ_{inflow} is the water density of the inflow (kg m^{-3}), which we assumed to be 1000 kg m^{-3}; and Q is the volumetric flow rate of the inflow (m^3 s^{-1}). Assuming a decreased inflow flow rate of Q = 2 m^3 s^{-1}:

$$B = 0.0039\,\mathrm{m}^4/\mathrm{s}^3 \tag{3.5}$$

Wells and Nadarajah (2009) proposed that the intrusion depth Z of a density current that flows into a stratified water body scales as:

$$Z \sim (3 \pm 1) B^{1/3} N^{-1} \tag{3.6}$$

for laboratory experiments. Although the intrusion depth Z was validated for oceanic intrusions, Lake Tegel is also a (weakly) stratified water body during winter. Calculating the intrusion depth during this winter period gives a range from $Z \sim 25.6\,\mathrm{m}$ to $51.3\,\mathrm{m}$. Therefore, the proposed density current would most certainly entrain close to the sediment. If we exclude the factor (3 ± 1), Z scales to $12.8\,\mathrm{m}$, which is closer to the maximum depth of Lake Tegel.

The third hypothesis is based on the potential abundance of winter seiches and oscillations of a denser water layer according to obvervations at Lake Müggelsee (Kirillin et al. (2009), Fig. 3.7). Such oscillations could cause sudden electrical conductivity and temperature peaks similar to the ones measured at Lake Tegel. A verification of this theory is currently not possible without additional field data. To check it, additional water temperature logger chains have to be deployed at different positions of Lake Tegel as well as temperature loggers with a higher accuracy to detect temperature differences for the calculation of potential seiche modes during winter.

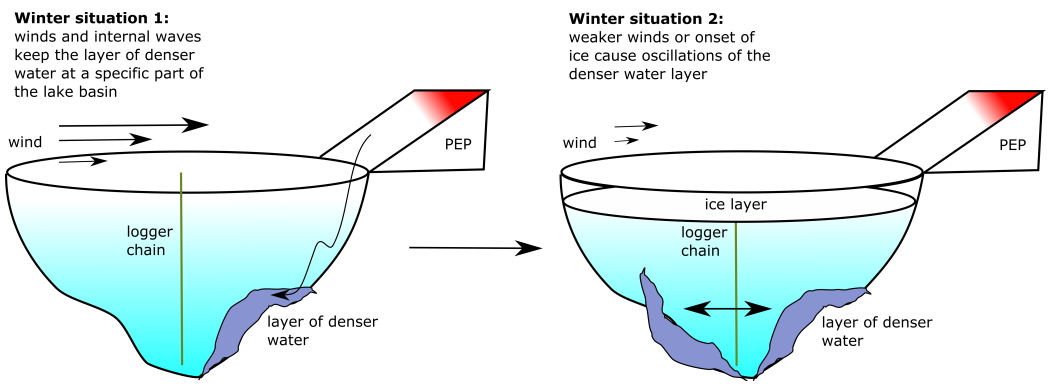

Figure 3.7: Proposed theory for seiche-induced oscillations.

3.4.2 Impact of seiches on transport processes

The PSD of the heat budget suggested the existence of vertical seiches in the periods 12 and 8 h. The former could reflect day and night cycles when the wind direction and heat fluxes are changing. Seiches have the potential to cause vertical biogeochemical fluxes even during stratified conditions (Boegman, 2009). For a more detailed investigation of potential transport processes over the thermocline, additional water temperature data in a higher spatial resolution are needed. With more data between 5 and 7 m (the typical thermocline depth), temperature isotherms could be calculated. With the help of a subsequent analysis of coherence and phase difference (CPSD), potential vertical seiche modes could be identified. For identifying winter seiches, the deployment of water temperature loggers with a higher accuracy is advisable.

3.5 Outlook

To identify probable intrusion depths of either the Havel in summer or the PEP in winter (the proposed density current), additional conductivity loggers should be installed at shal-

low depths and close to the bottom of the logger chain. Further, additional thermistors should be added in depths between 5 and 7 m to get more data about the oscillations of the thermocline depths. In the mean depth of Lake Tegel (6.6 m) additional dissolved oxygen as well as electrical conductivity loggers should support the identification of seiches. Figure 3.8 represents a comparison between the current setup of the logger chain and the envisioned future setup, which includes a finer spatial setup of loggers with additional ones to measure electrical conductivity and dissolved oxygen.

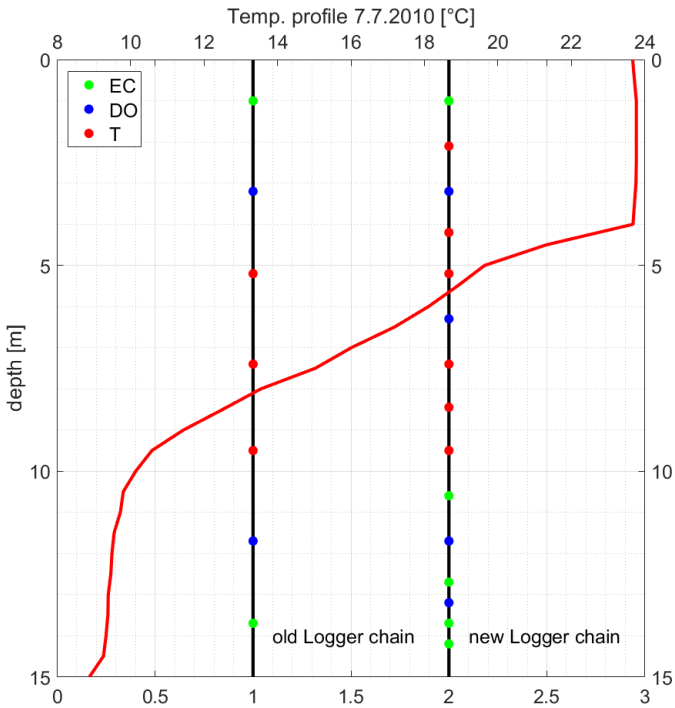

Figure 3.8: Comparison of the current logger chain and the envisioned new one; red line represents a 'typical' vertical temperature profile measured in summer 2010.

A long-term time series of vertical water temperature profiles should improve our current understanding about the mixing state of Lake Tegel, which is still classified as dimictic (although recent studies have shown the weak winter stratification). The question remains if the winter period of 2017/2018 was an outlier or a first sign of the proposed impact of climate change on lake systems (Kirillin, 2010, Ladwig et al., 2018).

The proposed density current originating from the PEP in winter is a curious phenomenon that could potentially affect the winter ecosystem and especially the oxygen budget of the bottom layer. If these density currents are consisting of oxygen depleted waters, they will decrease the concentrations of dissolved oxygen during winter in the bottom layers. The main flux of oxygen from the lake surface to the bottom happens during the spring mixing period, which was rather short in 2018. If the spring overturn duration is going to decrease in the future and, additionally, oxygen-depleted waters are entraining during winter, the oxygen concentrations of the bottom layer will decrease in the next years (the winter oxygen saturation was between 85% and 95%). This can cause a prolongation of the oxygen depletion period at the bottom of Lake Tegel during summer. Further measurements to investigate the density current should be conducted, for instance measurements of the vertical density structure (or electrical conductivity) in winter at different locations at Lake Tegel. Also, water temperature loggers with a better accuracy should be employed during the winter season. Finally, numerical 3D modeling of Lake Tegel could help investigating

the dynamics of the proposed density current.

To complement the determination of seiche characteristics, an additional logger chain should be deployed at a different position, preferably in the west from the deepest site. To calculate the horizontal seiche mode the deployment of the second logger chain (with thermistors located close to the thermocline) can be temporary and should happen at the time of the strongest stratification in August. Nonetheless, a permanent second logger chain could help in checking the third hypothesis, although Lake Tegel's complex morphometry makes choosing a suitable location difficult. At the moment the assessment of any potential vertical transport processes caused by such seiches over the thermocline at Lake Tegel is vague.

In conclusion, the monitoring study at Lake Tegel provides additional and relevant information about the internal hydrodynamics of the system and should be continued. Further, it states new hypotheses that should be tackled in future research studies.

Chapter 4

In the Future I: Application of a vertical 1D model to investigate the impact of climate change on Lake Tegel

This study was published as:

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This is the postprint version of the article.

4.1 Abstract

Lakes are known to be strongly affected by climate change as a result of their sensitivity to atmospheric forcing. The combined response of urban lakes to climatic changes and to urbanization of the catchment may be further altered by water quality management measures. We studied Lake Tegel in Berlin, Germany as a representative urban lake profoundly influenced by intense water management measures and a resulting complex hydrodynamic situation: Lake Tegel is fed by nutrient-rich river discharges and effluents from a phosphorus elimination plant (PEP). We estimated changes in water temperatures, the Wedderburn number, and the buoyancy frequency, as well as concentrations of dissolved oxygen and phosphate under climate change using a one-dimensional vertical hydrodynamic model coupled to a water quality model. Further, we investigated how four management scenarios with varying discharges of the PEP could affect the lake system. In all simulations, water temperatures increased and summer stratification extended. The modeling results demonstrated that the water management system buffers the high nutrient supply from the river inflow and can effectively mitigate negative effects of climate change on Lake Tegel, thus highlighting its importance for the lake ecosystem.

4.2 Introduction

Climate change is one of the major stressors for ecosystems (Sala et al., 2000, Walther et al., 2002). More frequent extreme weather events, rising air temperatures, intense precipitation

affecting erosion, and changing atmospheric circulation patterns are the future challenges ecosystems have to cope with (Whitehead et al., 2009). In particular, lakes are expected to act as sentinels to climate change (Adrian et al., 2009, Jiménez Cisneros et al., 2014, Landkildehus et al., 2014). Urban lakes are crucial freshwater resources for a secure water supply and adequate sanitation, as well as for recreational activities. Water management of urban lakes is an important compartment of the respective catchments and its water cycle (Grimm et al., 2008). Adaptive water management measures have the potential to mitigate effects caused by climate change as well as nutrient and contaminant loadings to lake or reservoir systems (Abdel-Fattah and Krantzberg, 2014, Graham and Georgakakos, 2009, Yasarer and Sturm, 2016). The effect of climate change on lake physics, ecosystem services and ecosystem structures has been intensively studied in the last decades (e.g., Jeppesen et al. (2014), O'Reilly et al. (2015)). Numerous authors have suggested the future dominance of cyanobacteria in lakes as a result of climate change increasing water temperatures and affecting the stratification strength (Havens and Paerl, 2015, Paerl, 2014, Trolle et al., 2014). Therefore, high water temperatures in summer in conjunction with a high buoyancy frequency suggest an increased probability for the formation of cyanobacteria blooms. Further, vertical thermal stratification was found to be particularly sensitive to the changing meteorological conditions (Kirillin, 2010, Sahoo et al., 2016, Magee and Wu, 2017), but the specific impact on lakes can be spatially and temporally diverse (Zhang et al., 2017). The among-lake coherence to climate change, particularly in the surface layers, is a well-established observation, but the individual properties of a lake can, to a certain degree, affect how deeper water layers respond to climate change (Rose et al., 2016, Snortheim et al., 2017). This individual response of a lake to climate change can be diverse even for regionally proximate lake systems (Read et al., 2014).

In contrast to rural or less anthropogenically affected surface waters, urban lakes, which are important parts of the urban water cycle, are often deeply intertwined with technical interfaces in the form of water management systems (Gessner et al., 2014). A semi-closed water cycle is common in megalopolises (Jekel et al., 2013b), in which case the treated effluents of wastewater treatment plants (WWTPs) are discharged into urban surface waters where they are further abstracted for drinking water production, for example, via bank filtration, before entering the WWTP again. The strong impact of water management measures on the system is a shared characteristic of both urban lakes and freshwater reservoirs. It is up for debate to what degree the urban management system, similarly to reservoirs, can also mitigate a lake's response to climate change. The impact of climate change in conjunction with urbanization will have a profound effect on lakes, with increased mass loadings of nutrients and contaminants originating from the urban catchment (Jeppesen et al., 2017, Kaushal et al., 2015, Sahoo and Schladow, 2008). Finding effective adaptive strategies of water management systems to diminish the vulnerability of the freshwater system to climate change is an essential task for freshwater resource managers worldwide (Garrote, 2017, Simonovic, 2017). Numerical modeling can be used to obtain a better understanding of how water management measures can adapt to ongoing challenges caused by climate change (Goonetilleke and Vithanage, 2017, Wang et al., 2016).

Although several studies have pointed out the importance of adaptive water management measures in times of climate change, for instance, for regional lakes and watersheds (Ludovisi et al., 2013, Tzabiras et al., 2016, Zhang et al., 2015), locally in the region of Berlin, Germany (Germer et al., 2011) or in general (Andrew and Sauquet, 2017, Fant et al., 2017), our focus was on the adaption of a specific management measure, the phosphorus elimination plant (PEP) at Lake Tegel in Berlin, Germany. Lake Tegel underwent a strong eutrophication period from 1950 to 1985 as a result of high external loadings of nutrients as well as heavy metals originating from an upstream sewage farm, resulting in blooms of cyanobac-

teria and the loss of the lake's submerged macrophyte population (Schauser and Chorus, 2007b, Hilt et al., 2010). To restore the lake system, which was and still is crucial for Berlin's drinking water production, the lake was subjected to various management measures: (1) the construction of an upstream WWTP, (2) the launch of the PEP treating inflowing waters, (3) the construction of a lake pipeline for bypassing outflowing water back to the PEP to maintain a steady discharge, and (4) the launch of hypolimnetic aerators in the deep water basin (Heinzmann and Chorus, 1994). Because of Lake Tegel's utter importance for Berlin's drinking water supply and for recreational activities, the lake was intensively investigated and monitored in the last decades. Past sediment studies investigated Lake Tegel's sediment affinity to an additional supply of iron and concluded that most of the iron was bound to sedimentary sulphur (Kleeberg et al., 2012a) as well as that the past management measures had a profound effect on Lake Tegel's sediment composition, resulting in a heterogeneity between different sites (Ladwig et al., 2017). Previous studies have also highlighted that the reduction of external loads was the main mechanism for the restoration of Lake Tegel, particularly the construction of the WWTP and the PEP (Schauser and Chorus, 2009, 2007b). In contrast, the performance of the hypolimnetic aerators was concluded to be more similar to bubble plume generators and therefore caused an increased mixing between hypolimnion and epilimnion instead of hypolimnetic aeration (Lindenschmidt and Hamblin, 1997). In recent years, modeling studies have proved that Lake Tegel is very sensitive to river-induced mixing caused by wind and that an optimal management to keep phosphate as well as pharmaceutical concentrations in the lake low was not feasible (Schimmelpfennig et al., 2012a,b).

The objectives of our study were (1) to determine if a one-dimensional (1D) vertical model configuration is applicable for the evaluation of management scenarios for Lake Tegel, (2) to check if an assumed shift of the lake type to a monomictic mixing regime and the formation of favorable conditions for cyanobacteria can happen as a result of climate change, and (3) if the PEP can mitigate the impact of climate change on Lake Tegel in the near future. In contrast to previous modeling studies on Lake Tegel (Lindenschmidt and Hamblin, 1997, Schauser and Chorus, 2009, Schimmelpfennig et al., 2012a), our study was focused on the simulated projection of the impact of climate change on Lake Tegel by using projected meteorological data and the simulation of physical variables as well as nutrients.

4.3 Materials and methods

4.3.1 Study site

Lake Tegel (52.5761°, 13.2533°) is a dimictic shallow lake located in Berlin, Germany. The lake consists of a northern basin with water depths of up to 16 m and a southwestern basin, which is characterized by islands and shallow water depths of around 2 to 4 m (Figure 4.1). The lake volume is 26.1 Mio. m^3, and the mean depth is 6.6 m. The lake receives nutrient-rich discharges from the River Havel in the southwest (mean discharge for 2008–2014 of $\bar{Q} = 12\,m^3\,s^{-1}$) and the treated effluents of a WWTP from the northeast (mean discharge for 2008–2014 of $\bar{Q} = 2.5\,m^3\,s^{-1}$), which are further processed by the upstream PEP. Additional management measures are an active lake pipeline, which collects water close to the southwestern outflow and bypasses it to the elimination plant to maintain a minimum discharge and to dilute influents, and several groundwater abstraction wells around the lake, as well as hypolimnetic aerators in the main basin.

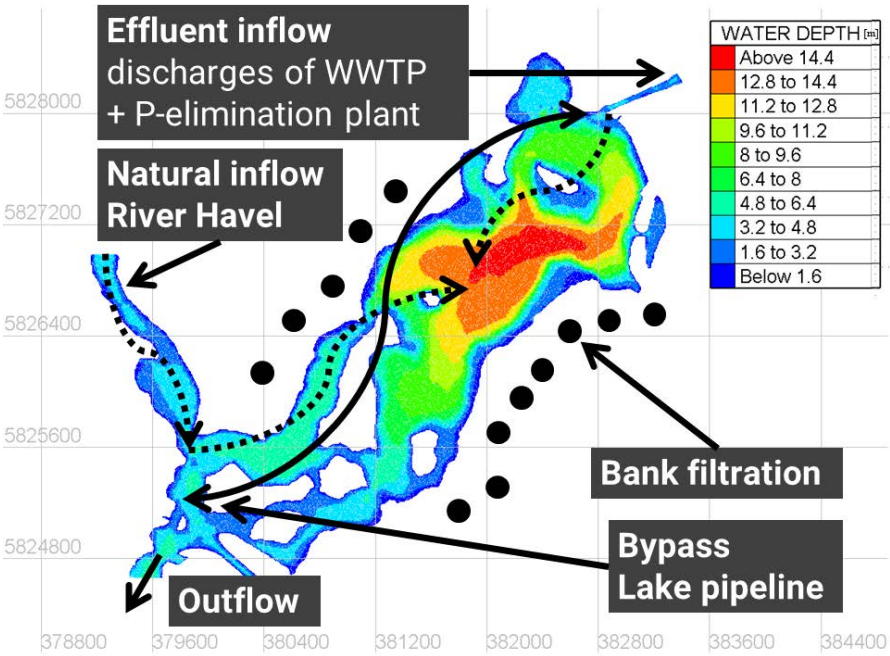

Figure 4.1: Bathymetric map of Lake Tegel including the main inflow conditions (water depths in meters, positions of groundwater abstraction wells are idealized, white spots represent islands, and the black line represents the lake pipeline).

4.3.2 Model description and input data

To check if applying a 1D vertical model is a reasonable approach for Lake Tegel, we evaluated the ratio R of the internal Rossby radius R_i (m) to the lake width B (m) and the lake number L_N [-], which was calculated with the LakeAnalyzer software tool (Read et al., 2011). The former checked the effect of the earth's rotation on the lake (Patterson et al., 1984, Gill, 1982), and the latter calculated the ratio of stabilizing forces to destabilizing forces affecting the water column Robertson and Imberger (1994), Imerito (2015). The internal Rossby R_i radius was calculated using summer field data measured in 2016–2017, during which a two-layer stratification existed:

$$R_i = \frac{c_{ws}}{f} = \frac{\sqrt{g' * h}}{f} \simeq 2016\,\mathrm{m} \tag{4.1}$$

where c_{ws} is the internal wave speed ($\mathrm{m\,s^{-1}}$); f is the Coriolis acceleration ($\mathrm{s^{-1}}$); $g' = g \cdot \Delta\rho/\rho_0$ is the reduced gravitational acceleration ($\mathrm{m\,s^{-2}}$); g is the gravitational acceleration ($\mathrm{m\,s^{-2}}$); $\Delta\rho$ is the density difference between hypolimnion and epilimnion ($\mathrm{kg\,m^{-3}}$); ρ_0 is the reference water density, which equals $1000\,\mathrm{kg\,m^{-3}}$; $h = \frac{h_1 h_2}{h_1 + h_2}$ is the equivalent lake depth (m); h_1 is the eplimnion thickness (m); and h_2 is the hypolimnion thickness (m). Subsequently, we calculated the ratio R:

$$R = \frac{R_i}{B} \simeq 2.0 \tag{4.2}$$

As input for the calculation of the lake number, we used observed field water temperature data from 2008 to 2014 measured by the Senate of Berlin at the deepest site, as well as daily wind data from the weather station Berlin-Tegel. The 1D assumption can be used for lake systems with $R > 1$ Patterson et al. (1984) and $L_N \gg 1$ Imerito (2015). With a

calculated ratio R of 2.0, indicating an absence of rotational effects, and an average value $L_N \sim 5.8$, suggesting a horizontal density structure of the lake, Lake Tegel matched these assumptions.

As a modeling tool, we applied the General Lake Model (GLM v. 2.0.0). GLM is a vertical 1D hydrodynamic model employing a flexible Lagrangian layer structure to adapt the thickness of individual layers during mixing processes (Hipsey et al., 2014). GLM incorporates water balance, surface energy budget, meteorology, vertical mixing, stratification and boundary flow dynamics. The atmospheric component of the long-wave radiation was calculated on the basis of cloud cover data. We used the implemented coupling with the Aquatic Ecodynamics Model Library (AED2 v. 1.0) to simulate water quality processes (Hipsey et al., 2013). We kept the water quality configuration simple by focusing on the inorganic biogeochemical variables phosphate and nitrate. Here, phosphate represents the soluble reactive phosphorus fraction ortho-phosphate, $o - PO_4 - P$, and nitrate represents $NO_3 - N$. To represent biological primary production, we included one phytoplankton group representing diatoms in the model, which are a dominant species in Lake Tegel (Chorus and Schauser, 2011).

In the following paragraph, we list the main conceptual model assumptions of the respective boundary conditions to simulate Lake Tegel. We used a constant sediment flux model, which acted as a sink/source for dissolved oxygen, nitrate and phosphate for each layer under the dependence of water temperatures and the respective area ratio to the benthic area. As open lateral boundary conditions, we prescribed daily inflow rates and loadings from the PEP (first inflow, representing the lake pipeline by the combined discharge of both the elimination plant and the lake pipeline) and the River Havel (second inflow). Assuming complete mixing of the River Havel inflow because of its narrow and shallow inlet between several islands, we interpolated the monthly water temperature values of the inflow. This was done by linear regression between the River Havel water temperature data and the air temperature data as well as between the River Havel water temperature data and PEP water temperature data. For each day, the maximum value of either regression was used as the water temperature for the River Havel inflow to ensure a shallow entrainment into Lake Tegel. The model included two outflow conditions: a simplified outflow by bank filtration with a constant discharge, and the main lake outflow in the southwest, which was implemented as an overflow boundary. We neglected the artificial aerators on the basis of their uncertain operation mode. Meteorological data were provided with a daily resolution.

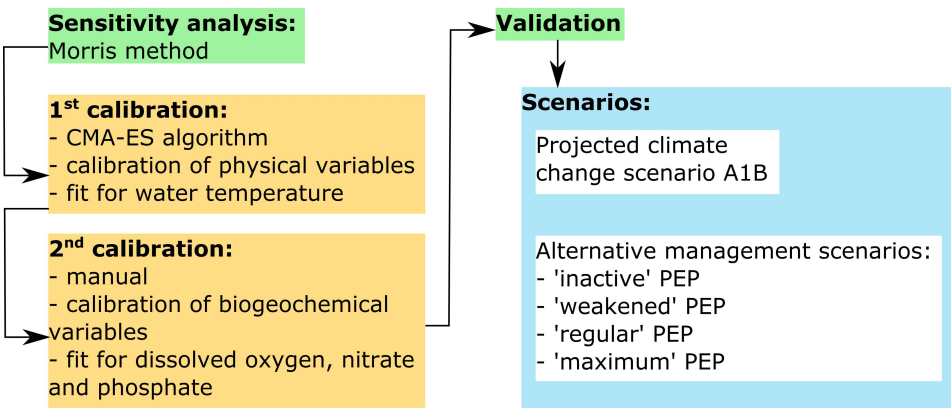

Figure 4.2: Flowchart illustrating the main modeling framework.

For the model calibration and validation, we used field data from the period 2008–2014.

The data are summarized in Table 4.1 together with the applied preprocessing steps. Further calculations and evaluations were done by using MATLAB R2017a (The MathWorks Inc., Natick, USA), and lake-specific variables were calculated using the LakeAnalyzer software (Read et al., 2011). An overview of the modeling framework is given in Figure 4.2, and the specific methods are explained in the following sections.

Table 4.1: Model boundary data: missing data were assumed to be constant to the next neighbor; values under detection limit were set to half of the detection limit concentration.

Boundary Condition	Variable	Source	Preprocessing
Morphology	Area (m^2)	SB	
	Depth (m)		
Meteorology	Air temperature (°C)	WT	
	Relative humidity (%)	WT	
	Wind speed ($m\,s^{-1}$) (height of 10 m)	WT	
	Precipitation ($m\,d^{-1}$)	WT	
	Cloud cover (-)	WT	
	Shortwave radiation ($W\,m^{-2}$)	CP	Hourly shortwave radiation was transformed to mean daily values
Inflow	Discharge ($m^3\,s^{-1}$)	TO, PEP	
	Water temperature (°C)	OH, PEP	
	Salinity ($mg\,l^{-1}$)	OH, PEP	Salinity was derived from measured electrical conductivity using factor 0.65 (Tikhomirov, 2016)
	Dissolved oxygen conc. ($mmol\,m^{-3}$)	OH, N	
	Phosphate conc. ($mmol\,m^{-3}$)	OH, PEP	
	Nitrate conc. ($mmol\,m^{-3}$)	OH, PEP	
	Ammonium conc. ($mmol\,m^{-3}$)	OH, PEP	
	Dissolved organic carbon conc. ($mmol\,m^{-3}$)	OH, PEP	
	Particulate organic carbon conc. ($mmol\,m^{-3}$)	OH, PEP	
	Silica conc. ($mmol\,m^{-3}$)		Assumed to be constant
Outflow	Discharge ($m^3\,s^{-1}$)	BWB	Constant mean discharge was used
First calibration	Water temperature (°C)	SB	Deepest site of Lake Tegel
Second calibration	Dissolved oxygen conc. ($mmol\,m^{-3}$)	SB	Deepest site of Lake Tegel
	Nitrate conc. ($mmol\,m^{-3}$)	SB	Deepest site of Lake Tegel
	Phosphate conc. ($mmol\,m^{-3}$)	SB	Deepest site of Lake Tegel

* SB: Senate of Berlin; WT: Weather station Berlin-Tegel (DWD); CP: Climate station Potsdam (DWD); TO: Stream gauge Tegelort (Senate of Berlin); PEP: Phosphorus elimination plant Tegel (Berlin Water Company); OH: Oberhavel, Konradshöhe (Senate of Berlin); N: Nordgraben (Senate of Berlin); BWB: Berlin Water Company.

4.3.3 Calibration and validation

We used the Morris method (Morris, 1991, Sohier et al., 2014) to globally identify sensitive model variables for subsequent use in the calibration procedure. The method gives a qualitative estimation of the respective variables' sensitivity by calculating the average of the absolute elementary effect (EE). The elementary effects are relative changes of the model outcome when changing a respective variable, and the Morris method ranks the variables according to their sensitivity. Using this procedure, we investigated the sensitivity of a group of 24 model variables by calculating the model outcome, which is represented here by the root-mean-square error (RMSE) between simulated and observed water temperatures in 2008, which were measured at the depth range of 0.5 to 14 m (below 1 m under the surface with a distance between measurements of 1 m). The group of model variables consisted of those given in Table 4.2 under "Calibrated by CMA-ES", except for the penalty factors and the shortwave radiation factor F_{sw}. Instead, the group checked for sensitivity included the length and width of the outflow, L_{out} and W_{out}, as well as the light extinction coefficient K_W (m^{-1}). For each variable, a normal distribution was assumed, characterized by an arithmetic mean equal to the respective default value and a σ of 1/6 of the arithmetic mean. The sensitivity analysis was run for 20 iterations. We conducted the calibration in two steps. First we used the recent data from 2008 to 2011 (n = 4 years) to calibrate physical lake parameters by comparing simulated water temperatures with field temperatures. Although the variables were calibrated globally, each year was evaluated individually by simulating the period from April to March of the next year, using the first field data of water temperatures and salinities as initial conditions. Prior to the calibration, the model variables were rescaled into the variable space $[0; 10]$. We applied upper and lower boundary conditions to each variable and started with the default values as initial values X_0 Hipsey et al. (2014). We applied the derivative-free, evolutionary Covariance Matrix Adaption Evolution Strategy (CMA-ES) algorithm Hansen (2006) to the objective function OF, effectively trying to minimize the normalized root-mean-square error (NRMSE) of the water temperature:

$$OF = min(\frac{\sqrt{\frac{\sum(T_{sim}-T_{field})^2}{n}}}{max(T_{field}) - min(T_{field})}) \tag{4.3}$$

where n is the number of observations. We chose 24 variables (Table 4.2) for the automatic calibration procedure, focusing on those that had a high average elementary effect determined by the Morris method. Further, we explored whether the optimization would benefit from a penalizing filter to better represent the river mixing due to wind dynamics. The river-induced mixing is strongest during easterly wind conditions (Schimmelpfennig et al., 2012a). The wind data obtained from the weather station Berlin-Tegel suggested that during the months of January, March, April, May and October, the lake experiences conditions that are favorable for river-induced mixing. To implement this information in the model, we added two extra calibration variables, which were used as multipliers affecting the River Havel discharge corresponding to the above-mentioned favorable months. We ran the calibation several times with changing values for the population size (number of candidate solutions per iteration) and the maximum nunmber of iterations to account for poor optimization runs converging to local minima.

In the second step, we manually calibrated the biogeochemical variables (nine variables; Table 4.2) to adjust the fit between the simulated and measured concentrations of dissolved oxygen, nitrate and phosphate for each year from 2008 to 2011. We used field data of dissolved oxygen, nitrate and phosphate as initial conditions for each year. The field data depicted fluxes of dissolved oxygen below the summer thermocline but also stable thermal

conditions. We assumed that these oxygen fluxes were caused by the activation of Lake Tegel's artificial aerators, which we wanted to neglect in the model. Therefore, we limited the calibration of the biogeochemical variables by only including days during early summer when oxygen depletion happened. To account for primary production, we included diatoms as one phytoplankton species in the model using default values, although we slightly adjusted the values for the diatom sedimentation and growth rates (see Section 4.4.1). We quantified the fit by using the RMSE and the Nash–Sutcliffe coefficient of efficiency (NSE). We validated the findings of the calibration of the physical and biogeochemical variables for the years 2012, 2013 and 2014 (n = 3 years).

Table 4.2: Model variables (initial values either refer to values given in exemplary files or from the GLM and AED2 manuals (Hipsey et al., 2014, 2013); model values are the actual values used in the calculations).

Variable	Description	Initial Value	Model Value
Calibrated by Covariance Matrix Adaption Evolution Strategy			
φ_{PEP} (°)	Streambed slope, phosphorus elimination plant (PEP)	1.0	1.1
φ_{Havel} (°)	Streambed slope, Havel	1.0	0.52
α_{PEP} (°)	Stream half angle, PEP	65	73
α_{Havel} (°)	Stream half angle, Havel	65	30
$C_{D,PEP}$ (°)	Drag coefficient, PEP	0.016	0.018
$C_{D,Havel}$ (°)	Drag coefficient, Havel	0.016	0.026
Q_{PEP} (-)	Inflow factor, PEP	1	2
Q_{Havel} (-)	Inflow factor, Havel	0.5	0.6
$k_{eastwind}$ (-)	Penalty for East/South wind conditions	1.0	0.74
$k_{remaining}$ (-)	Penalty for non-East/South wind conditions	1.0	0.96
Q_{Out} (-)	Outflow factor bank filtration	1.0	0.5
H_{Out} (m)	Outflow elevation bank filtration	29	29
C_K (-)	Convective overturn	0.125	0.2
C_W (-)	Wind stirring	0.23	0.34
C_S (-)	Shear production	0.20	0.25
C_T (-)	Unsteady turbulence	0.51	0.38
C_{KH} (-)	Kelvin–Helmholtz billowing	0.30	0.23
C_{HYP} (-)	Hypolimnetic turbulence	0.50	0.17
F_{wind} (-)	Wind factor	1.0	1.5
F_{rain} (-)	Rain factor	1.0	1.4
F_{sw} (-)	Shortwave radiation factor	1.0	1.2
C_E (-)	Latent heat transfer	0.0013	0.00266
C_H (-)	Sensible heat transfer	0.0013	0.001
C_M (-)	Transfer of momentum	0.0013	0.00107
Manually calibrated			
$F^{oxy}{}_{max}$ (mmol m^{-2} d^{-1})	Max. sediment flux, dissolved oxygen	-15	-20
$F^{nit}{}_{max}$ (mmol m^{-2} d^{-1})	Max. sediment flux, nitrate	-0.5	-0.1
$F^{amm}{}_{max}$ (mmol m^{-2} d^{-1})	Max. sediment flux, ammonium	3.0	17
$F^{phs}{}_{max}$ (mmol m^{-2} d^{-1})	Max. sediment flux, phosphate	0.2	0.04
$\Theta^{oxy}{}_{sed}$ (-)	Temperature multiplier for oxygen sediment flux	1.08	1.03
$\Theta^{DOC}{}_{miner}$ (-)	Temperature multiplier for dissolved organic carbon (DOC) mineralization	1.08	1.08
$R^{DOC}{}_{miner}$ (d^{-1})	Max. rate of DOC mineralization	0.001	0.002
$K^{oxy}{}_{sed}$ (mmol m^{-3})	Half saturation constant for oxygen dependence of sediment oxygen flux	150	50
$K^{DOC}{}_{sed}$ (mmol m^{-3})	Half saturation constant for oxygen dependence of sediment DOC flux	31.25	32
Phytoplankton			
ω_{phy} (m d^{-1})	Sedimentation rate	-0.86	-0.1
R_{growth} (d^{-1})	Growth rate at 20 °C	3	2.75
T_{std} (°C)	Standard temperature	20	20
T_{opt} (°C)	Optimum temperature	25	25
T_{max} (°C)	Maximum temperature	32	32
$\Theta^{phy}{}_{growth}$ (-)	Temperature multiplier for growth	1.06	1.06
$\Theta^{phy}{}_{respiration}$ (-)	Temperature multiplier for respiration	1.12	1.12
K_N (mmol m^{-3})	Half saturation concentration for nitrogen	3.5	3.5
K_P (mmol m^{-3})	Half saturation concentration for phosphorus	0.15	0.15

4.3.4 Scenarios

To project how climate change will affect Lake Tegel, we combined a climate change scenario with different management scenarios of the PEP. We used a realization of future meteoro-

logical conditions generated by Wetterlagen-basierte Regionalisierungsmethode 2010 (WETTREG2010) (Kreienkamp et al., 2010, Enke and Spegat, 1997, Spekat et al., 2007) for the weather station Berlin-Tegel until 2100. WETTREG2010 is a statistical method to calculate regional weather data by combining past data of the individual station with projections by global climate models. Here, the data followed the A1B scenario based on ECHAM5/MPI-OM T63L31 from the Intergovernmental Panel on Climate Change, assuming a balanced use between fossil and non-fossil energy sources, rapid economic growth combined with the development of efficient technologies, and a peak of the global population in the middle of this century (SRES et al., 2010). WETTREG2010 projects future daily meteorological variables for air temperature, relative humidity, wind speed, precipitation and cloud cover. As a simplification, we used the daily mean shortwave radiation averaged over the specific day of the year in the period 2008–2014 as future values. The WETTREG2010 method created several independent time series, each with a good replication of future climate variability. Instead of an ensemble, we utilized only one projected time series for the evaluation of the future impact of climate change on Lake Tegel. We investigated four management scenarios to quantify the impact of alternative discharge regimes of the PEP under climate change on the lake system. In the following, the mean annual discharge and its respective standard deviation are stated, whereas in each management scenario, either a constant value (inactive and maximum scenarios) or a time series of daily mean discharges averaged over the specific day of the year in the stated time periods (weakened and regular scenarios) were used:

1. Inactive: discharge is set to a constant value of $0\,\mathrm{m^3\,s^{-1}}$, and the elimination plant becomes deactivated: $Q = 0 \pm 0.0\,\mathrm{m^3\,s^{-1}}$.

2. Weakened: for each year, we used the mean daily discharges from the period 1996–2001, when the lake pipeline, supporting the elimination plant, was deactivated: $Q = 1.47 \pm 0.3\,\mathrm{m^3\,s^{-1}}$.

3. Regular: for each year, we used the mean daily discharges from our field data for 2008–2014: $Q = 2.53 \pm 0.4\,\mathrm{m^3\,s^{-1}}$.

4. Maximum: for each year, we set the daily discharge to a constant value of $3.5\,\mathrm{m^3\,s^{-1}}$: $Q = 3.5 \pm 0.0\,\mathrm{m^3\,s^{-1}}$.

For water temperatures, salinity, and concentrations of dissolved oxygen, ammonium, nitrate, phosphate, dissolved organic carbon (DOC), particulate organic carbon (POC) and silica, we calculated the daily mean values averaged over the specific day of the year in the period 2008–2014 and assumed the future values to have a steady annual pattern. We evaluated the impact of the scenarios on the individual years 2020, 2040, 2060, 2080 and 2100 by quantifying the following:

- The surface water temperatures (°C).

- The differences between surface and bottom water temperatures as a proxy for stratified conditions (Engelhardt and Kirillin, 2014, Wilhelm and Adrian, 2008); here we used the simulated bottom water temperatures at a depth of 6.5 m, which represented the mean depth of Lake Tegel.

- The duration of stratification between onset and breakdown; we determined the onset and breakdown of stratification as the day on which the temperature difference was over or under 1 °C and the mean temperature difference of the next 14 days was also over or under 1 °C.

- The thermocline depths (using the LakeAnalyzer software); the thermocline depths were normalized between 0 and 1.
- The dimensionless Wedderburn number $W = \frac{g'h^2}{{u_*}^2(L/2)}$ (Thompson and Imberger, 1980), where h is the depth of the mixed layer (m), u_* is the water friction velocity due to wind stress (m s^{-1}), g' is the previously explained reduced gravitational acceleration, and L is the fetch length (m); W is an indicator for the breakdown of lake stratification (Kirillin and Shatwell, 2016) (using the LakeAnalyzer software).
- The buoyancy frequency $N^2 = \frac{g}{\rho}\frac{d\rho}{dz}$ (s^{-2}) as an indicator for phytoplankton habitat conditions (using the LakeAnalyzer software).
- The duration of critical bottom oxygen concentrations under 2 mg L^{-1}; we determined the start and end date of oxygen depletion as the day on which the mean oxygen concentration at depths from 10 to 15 m was over or under 2 mg L^{-1} and the mean oxygen concentration of the next 14 days was also over or under 2 mg L^{-1}.

Each year was run from March 15 until December 31 of the respective year, and we assumed mixed initial conditions with uniform vertical profiles of water temperatures (5 °C), dissolved oxygen (10 mg L^{-1}), nitrate (2.6 mg L^{-1}) and phosphate concentrations (0 µg L^{-1}), which were assumed from past field data.

4.4 Results

4.4.1 Sensitivity analysis, calibration and validation

The Morris method attributed the highest EEs to the bulk aerodynamic coefficient for the wind factor F_{wind} (EE: 0.5), the latent heat transfer C_E (EE: 0.2) and the sensible heat transfer C_H (EE: 0.2) (Figure 4.3). The next sensitive parameters were the inflow factors of the PEP and the River Havel, Q_{PEP} and Q_{Havel}. We included most of investigated parameters because of their similar EEs. We dropped the length and width of the outflow as well as the light extinction coefficient because of their low sensitivity for the model outcome. Instead we added the wind penalty variables and a factor for the shortwave radiation for the calibration. During the first calibration step, which aimed to adjust the water temperatures, the best result was achieved by a CMA-ES run over 500 iterations with a population size of 10. The biogeochemical variables were calibrated manually in a second calibration step by checking the respective NSEs of dissolved oxygen, nitrate and phosphate concentrations. Further, we changed the sedimentation rate of diatoms ω_{phy} to -0.1 m day^{-1} (Reynolds, 1997) and manually adjusted the growth rate R_{growth} to 2.75 day^{-1}. An overview of the final model parameters is given in Table 4.2.

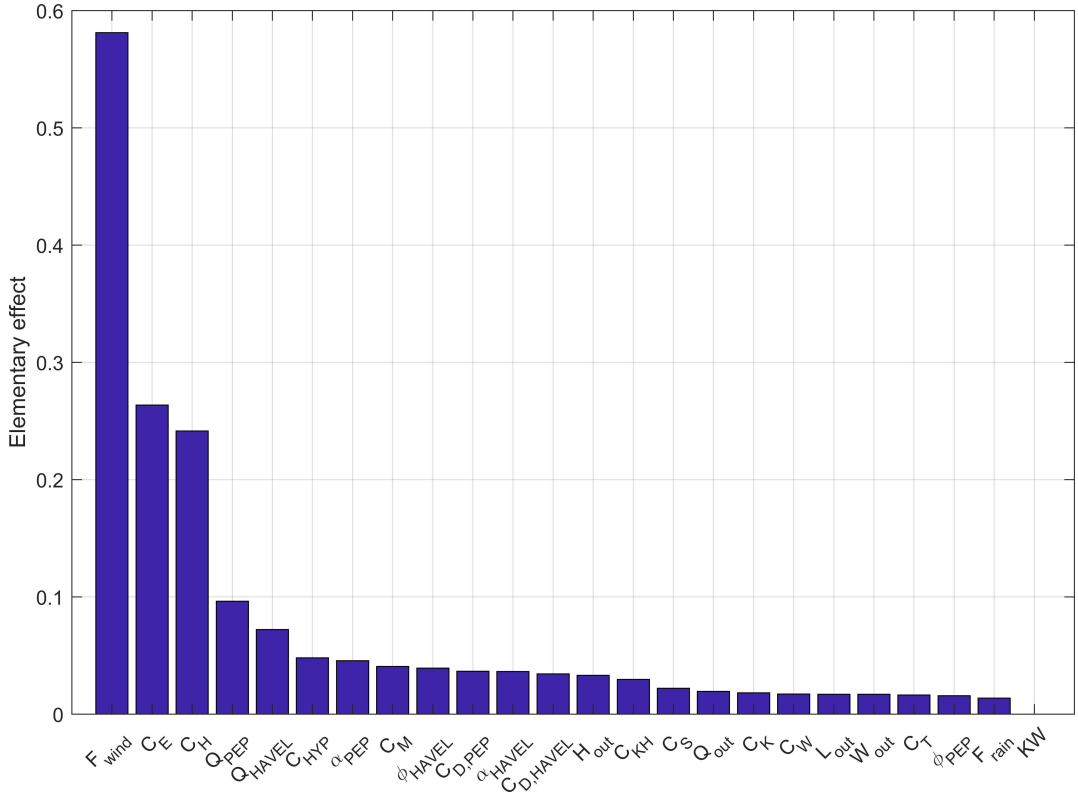

Figure 4.3: Elementary effects of the parameters derived by the Morris method (variable symbols are explained in Table 4.2; L_{out} and W_{out} represent outflow length (m) and width (m), respectively; KW is the light extinction coefficient).

The calibrated years 2008, 2009, 2010 and 2011 achieved NSEs for water temperatures of 0.89, 0.84, 0.9 and 0.83, respectively (Figure 4.4 and Appendix Figure 4.7A–C, showing the hydraulic and water quality dynamics produced by the calibrated model). For dissolved oxygen, the fit between the simulated and field data, with NSEs for 2008, 2009, 2010 and 2011 of 0.63, 0.57, 0.59 and 0.59, respectively, was sufficient. Here the oxygen depletion during summer at the bottom was adequately replicated, whereas the simulated oxygen concentrations in the surface layer were below the measured oxygen concentrations (Figure 4.4, here shown for 2008). Surface oxygen peaks during the summer season were achieved by simulated blooms of diatoms enabling an internal biological production of oxygen. Although the RMSEs for nitrate for the years 2008–2011 over the whole water column were low, between 0.84 mg L^{-1} and 1.1 mg L^{-1}, the NSEs were negative. The fit between measured and simulated phosphate was similar to the fit of nitrate: the RMSEs were between 12 µg L^{-1} and 27 µg L^{-1} and the NSEs were negative. The simulated surface temperatures were in very good agreement with the field data, whereas there were discrepancies between the simulated and measured bottom water temperatures (Figure 4.5, showing the fit between measured and simulated data). The depth-specific time series of surface as well as bottom nitrate concentrations depicted that the bottom nitrate concentrations were depleted during summer, whereas in the field, there was still an abundance of nitrate. Still, for most years, the RMSE of simulated to measured bottom nitrate concentrations was only about 0.4 mg L^{-1} (Appendix Table 4.3). During summer, the surface phosphate concentrations were mostly overestimated, whereas the model was able to replicate the surface phosphate concentrations during the mixing events in autumn. The model was able to simulate a similar range of the measured sediment phosphate flux, although there were temporal dis-

crepancies. The model reproduced the annual stratification patterns of the shallow dimictic lake and was capable of reproducing the seasonal patterns of the nutrients, particularly the general depletion of oxygen and nitrogen concentrations and an internal phosphate flux during summer, as well as the replenishment of bottom layers with oxygen and nitrate concentrations in autumn.

The results for the validated years were similar to the results for the calibrated years. The years 2012, 2013 and 2014 achieved NSEs for water temperatures of 0.87, 0.85 and 0.87 and for dissolved oxygen of 0.56, 0.24 and 0.73 (Appendix Figure 4.7D–F). The bottom nitrate concentrations of all validated years were underestimated (Figure 4.5). The replication of bottom phosphate concentrations was in a good agreement for 2012 and 2013. In 2014, the bottom phosphate fluxes were underestimated (RMSE: 29 mg L^{-1}; Appendix Table 4.3).

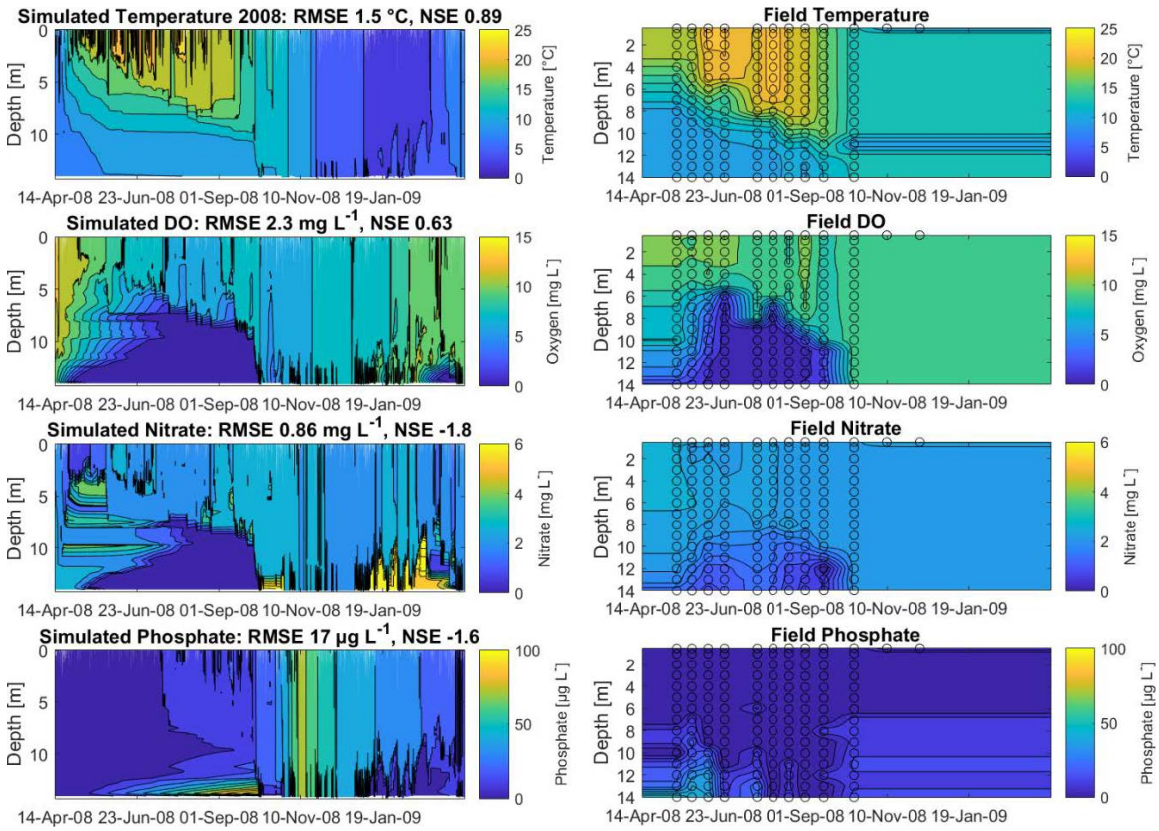

Figure 4.4: Contour plots for 2008, expressing the simulated dynamics of water temperature (°C), dissolved oxygen (mg L^{-1}), nitrate (mg L^{-1}) and phosphate concentrations (µg L^{-1}), as well as linear interpolated field data; the calculated root-mean-square errors (RMSE) and Nash–Sutcliffe coefficients of efficiency (NSE) are given for the total water column; the open circles represent available measured data.

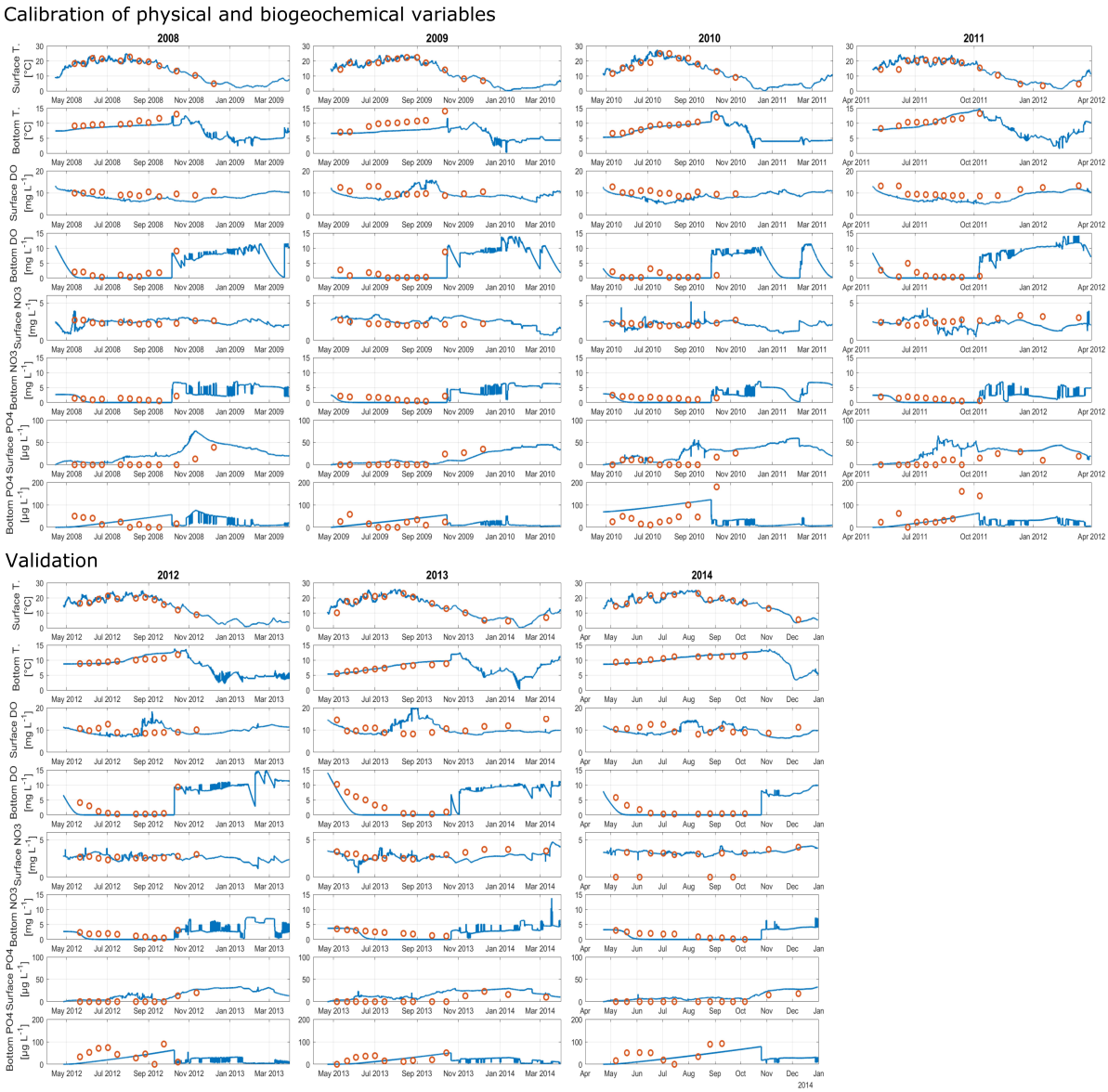

Figure 4.5: Time series expressing the model performance of water temperature (°C), dissolved oxygen (mg L^{-1}), phosphate (µg L^{-1}) and nitrate concentrations (mg L^{-1}); blue lines represent simulated results and red open circles represent field data; surface and bottom represent depths of 2 and 14 m, respectively.

4.4.2 Climate change and alternative management scenarios

The median, maximum and minimum surface water temperatures were increasing over all management scenarios before reaching levels in 2100 that were similar to those for 2040 (Figure 4.6A). In all scenarios, the highest median water temperatures were projected in the years 2060 and 2080. Because of this general temperature trend in all management scenarios, for the visualization of the time series of buoyancy frequency and phosphate concentrations, we only investigated 2020, 2060 and 2100 (Figure 4.6F,H). All scenarios with an active PEP projected similar water temperature differences (Figure 4.6B). The water temperature differences peaked in 2080 before declining at the end of the century. Compared to the other management scenarios, the inactive management scenario projected the highest

maximum and median values of water temperature differences between surface and bottom layers in 2040, 2060 and 2080. The stratification period extended in all scenarios, with a shift of the stratification onset from the middle of April to late March (Figure 4.6C). In the inactive scenario, the results of the relative thermocline depth showed signs of a disappearance of the winter stratification period (Figure 4.6D). Here, the thermocline still reached the maximum depth of Lake Tegel in December, whereas the other three scenarios determined a developing thermocline beginning in December, depicting a stratification in winter. Further, when the discharges of the PEP were increased (weakened, regular and maximum), an increased thermocline deepening could be observed between late August and September, which vanished again in the middle of September. Nonetheless, this short thermocline deepening period reduced the successive time of the summer stratification period. The simulation showed that during the prolongation of the stratification, 2060 and 2080, there were only short periods when the thermocline reached the mean lake depth. The changes in the calculated lake-wide Wedderburn number were similar for the regular and maximum scenarios, with higher values in 2020 and 2080 (Figure 4.6E). In the inactive as well as weakened scenarios, the Wedderburn numbers increased strongly until 2080 before decreasing to a similar level as in the other two scenarios. Here, the inactive scenario projected the highest mean as well as maximum values of the Wedderburn number, which were mostly over 1. The inactive scenario projected higher buoyancy frequencies over $10^{-2}\,s^{-2}$ compared to the other scenarios (Figure 4.6F). In all scenarios, the buoyancy frequency was well over $10^{-4}\,s^{-2}$ from April to October. In all scenarios, 2100 showed a slightly longer duration of the buoyancy frequency over $10^{-3}\,s^{-2}$ until the end of September. The duration of a critical oxygen depletion in bottom layers was similar over all scenarios (Figure 4.6G). The inactive scenario projected a slightly longer oxygen depletion duration in 2060 and 2080 compared to the other scenarios. The weakened, regular and maximum scenarios projected phosphate peaks during the summer months that were similar to a projected winter phosphate plateau (Figure 4.6H). In contrast, in the inactive scenario, the projected summer phosphate peak surpassed the winter plateau. The highest integrated phosphate concentrations were projected in the inactive scenario (60 $\mu g\ L^{-1}$), followed by the weakened scenario (40 $\mu g\ L^{-1}$) and the regular and maximum scenarios (both about 35 $\mu g\ L^{-1}$).

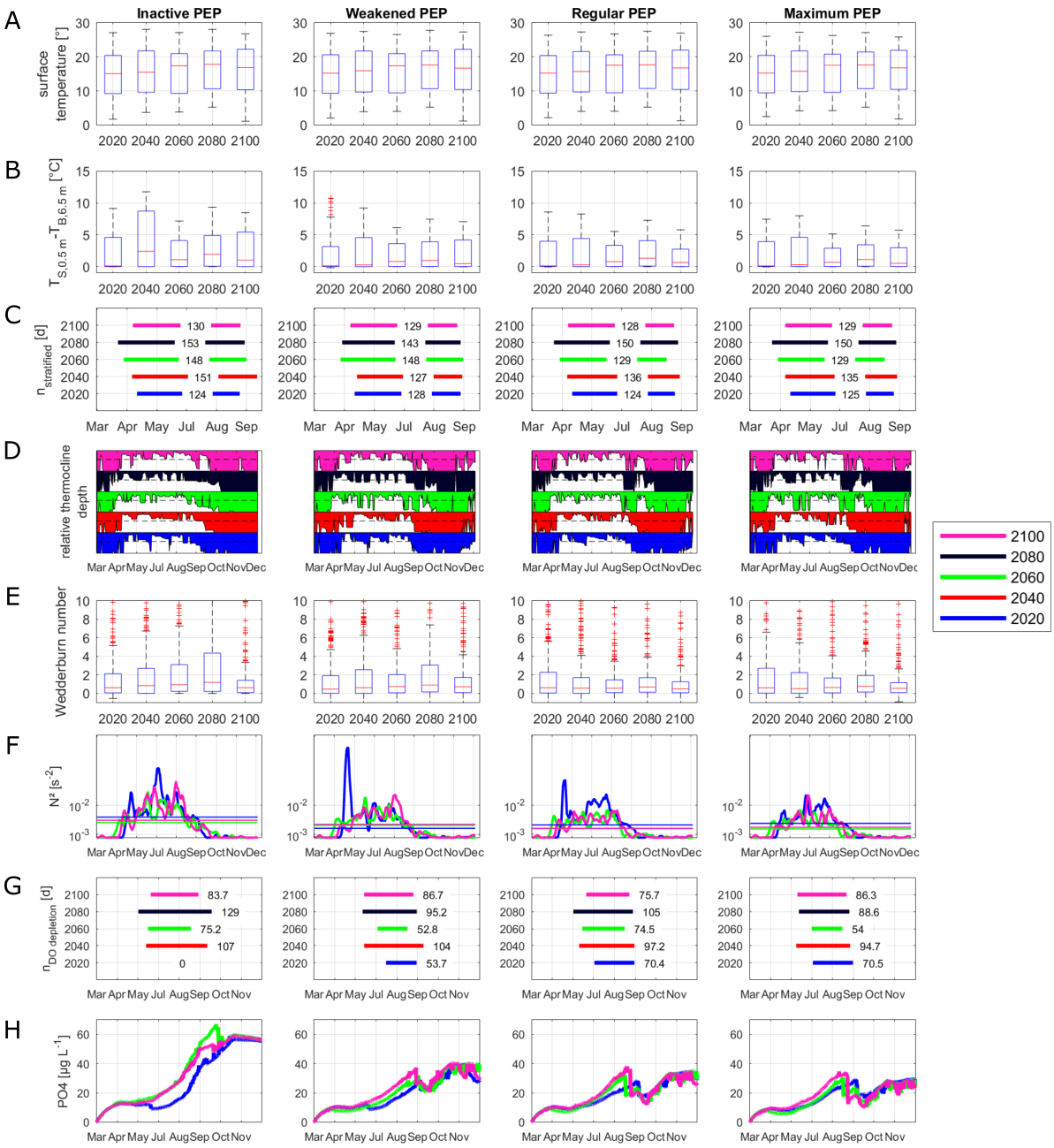

Figure 4.6: Evaluation of scenarios dealing with climate change and alternative management setups for 2020, 2040, 2060, 2080 and 2100 running from March 15 to December 31. "Inactive" represents a phosphorus elimination plant (PEP) scenario with no discharge, "Weakened" represents a decreased inflow of the PEP, "Regular" represents PEP discharges similar to those of 2008–2014, and "Maximum" represents a PEP scenario with a constant high discharge. Box plots summarize all daily values of the respective parameter and year; the central line indicates the median; the bottom and top edges of the box indicate the 25th and 75th percentiles, respectively; and the whiskers represent the most extreme data not considered as outliers: (**A**) boxplots of surface water temperatures (°C) at 0.5 m; (**B**) boxplots of water temperature differences (°C) between surface (0.5 m) and the mean depth temperatures (6.5 m); (**C**) stratification duration (days); (**D**) relative depth of thermocline between 0 and 1, where the black dashed line represents the mean depth (6.5 m); (**E**) boxplots of Wedderburn number; (**F**) buoyancy frequency (s^{-2}) filtered by a moving average filter over a window of 7 days; the vertical lines represent the respective mean buoyancy frequency including only values greater than zero; (**G**) duration of oxygen depletion in deeper layers (days) (in a depth from 10 to 15 m); (**H**) vertical integrated phosphate concentrations ($\mu g\ L^{-1}$).

4.5 Discussion

4.5.1 Model application

We considered the application of GLM-AED2 to Lake Tegel as being successful in replicating the essential processes of the lake system, namely, the lake stratification as expressed by the water temperatures as well as the seasonal patterns of the inorganic nutrients nitrate and phosphate. Although the ratio R of the internal Rossby radius to the lake width, the lake number and a prior 1D model study Lindenschmidt and Hamblin (1997) suggested that the 1D assumption was valid for the lake, the system is still characterized by a complex hydrodynamic situation including two hydraulically and chemically diverse inflows, a dendritic morphometry, wind-induced mixing events (Schimmelpfennig et al., 2012a) and an intense water management system. These stochastic, rapid and mostly temporary factors (particularly wind-induced mixing), combined with the fact that the observed field data of the deepest site does not represent the whole lake basin and spatial variations are to be expected, likely induced most discrepancies between the observed and simulated data. There were only minor differences between the calibrated and the validated years, which suggested a good model stability and the feasibility of our conceptual model for Lake Tegel. The CMA-ES algorithm achieved very good water temperature fits, and we advise the utilization of automatic calibration techniques for future lake modeling studies. Whereas the RMSE and NSE criteria of water temperatures for the calibration and validation years illustrated a very good fit, the model still had minor discrepancies simulating the water temperatures in deep layers. These simulated deep water temperature discrepancies were in agreement with other studies that have investigated the sensitivity of GLM (Rose et al., 2016, Read et al., 2014). As a result of their high sensitivity, two important calibration variables were the inflow factors for the River Havel and PEP inflows, which were decreased or increased, respectively, during the automatic first calibration step. This was done to ensure a weaker impact of the River Havel on Lake Tegel compared to the inflow of the PEP. However, the inflow factor is a direct multiplier for the prescribed discharges of the respective boundary condition and therefore affects the water budget and the hydrodynamics (e.g., flow velocity) as well as the loadings. This can cause a strong model overfitting and an overrepresentation of the PEP inflow. We kept the calibrated inflow factors to investigate the application of the automatic calibration algorithm on the Lake Tegel model and because the fit between field and simulated data was valid. Nonetheless, future work has to be done to investigate sophisticated criteria for the range of the model variables.

The model was capable of sufficiently replicating the oxygen budget of Lake Tegel with a NSE of between 0.5 and 0.6 for most years. The surface oxygen concentrations in the year 2013 were strongly overestimated, which resulted in a NSE of 0.2. Although the negative NSE for nitrate and phosphate suggested that the mean concentration would be a better predictor than the model, our simulation was still capable of reproducing seasonal patterns of nitrate, phosphate and dissolved oxygen concentrations, particularly the depletion of dissolved oxygen and nitrate concentrations, during summer. This good replication was confirmed by the RMSE criteria of the biogeochemical parameters, which suggested a good fit with either a low RMSE for nitrate of under 0.5 mg L^{-1} or a low RMSE for phosphate of between 2 and 30 μg L^{-1}. Processes weakly mirrored by the model were the patterns of surface dissolved oxygen concentrations. This was related to the simple configuration of the ecological module likely underestimating the primary production during summer and the simple atmosphere oxygen flux module. An intense calibration for phytoplankton variables and the inclusion of additional phytoplankton species in the model could help to improve the overall oxygen budget. Contrary to the field data, our model suggested a depletion of bottom nitrate during summer as a result of anaerobic conditions. This was

caused by the dependence of the nitrate sediment flux on the basis of the abundance of bottom dissolved oxygen. Recent studies have implemented a more sophisticated coupling of GLM to a geochemical sediment model (Salmon et al., 2017), which could help to improve the accurate simulation of sediment–water fluxes at Lake Tegel in the future.

The implementation of the wind penalizing filter did not improve the simulation results, and for future applications, the singular use of one inflow parameter is sufficient. Our assumption that the model calibration would suggest a higher value for months that favored mixing events (January, March, April, May and October) compared to the other months was not confirmed. The implementation of such a dynamic wind boundary could be interesting for future studies investigating similar systems that are heavily influenced by wind-induced mixing processes.

4.5.2 Assessment of scenarios

The climate change scenario projected a prolongation of the stratified summer period in future years. This prolongation was in agreement with other studies, which have showed that climate change will eventually change the stratification patterns of lakes (Jeppesen et al., 2009, Rolighed et al., 2016, Sahoo et al., 2016). Additionally, all scenarios showed that the median as well as minimum and maximum annual surface water temperatures of the 25th and 75th percentiles will increase in the near future. The latter half of the 21st century depicted the highest median annual surface water temperature, while at the end of the century, the median slightly decreased. As explained before, the A1B scenario assumed a peak of human development in the middle of the 21st century, as well as technological innovations. Therefore, the WETTREG2010 data for projected air temperatures were stagnating in the latter half of the 21st century, further causing the surface lake water temperatures to slightly drop compared to the other simulated years. Taking the assumptions by the A1B emission scenario for Lake Tegel, the strongest impact of climate change on the hydrodynamics and the lake ecosystem can presumably happen between 2050 and 2080. Afterwards, the conditions of Lake Tegel can oscillate back to the current conditions. Therefore, the impact of climate change on Lake Tegel under emission scenario A1B can be the strongest in the second half of the 21st century.

The management scenarios projected a shift of the lake state in the inactive scenario, for which the winter stratification vanished. This suggested that Lake Tegel could shift from a dimictic towards a monomictic state, because of the deactivation of the PEP. This general shift from a dimictic to a warm monomictic state was also shown to be the possible fate for other lakes in local proximity to Lake Tegel Kirillin (2010). Whether or not the PEP discharges are high or low, the elongation of the summer stratification period can severely increase the duration of a bottom oxygen depletion in Lake Tegel. This depletion of oxygen will affect the Lake Tegel ecosystem and redox reactions at the sediment. An increase in the buoyancy frequency can indicate conditions favoring the growth of cyanobacteria. Here, a buoyancy frequency of over $10^{-4}\,\mathrm{s}^{-2}$ is a critical limit for benefiting cyanobacteria dominance (Furusato and Asaeda, 2004). The critical buoyancy frequency was surpassed during summer in all management scenarios. However, the formation of cyanobacteria blooms also depends on other hydrological and ecological factors, for instance, the water retention time, the availability of nutrients and the dominant phytoplankton structures (Journey et al., 2013). Nonetheless, we argue that the projected physical lake variables, water temperature difference and buoyancy frequency, as well as the increased surface water temperatures due to climate change, can favor the formation of cyanobacteria blooms in the future in Lake Tegel. Further, the management scenario with nonexistent discharges of the PEP also projected increased concentrations of phosphate in the water column, further favoring the

possible formation of cyanobacteria. As explained previously, future water quality studies on Lake Tegel should focus on the simulation of cyanobacteria and highlight the trophic interactions between different phytoplankton species.

The differences between the weakened, regular and maximum management scenarios regarding stratification patterns, stratification strength, thermocline deepening, buoyancy frequency and the concentrations of oxygen as well as phosphate were marginal. We showed that any active discharge regime of the elimination plant was a beneficial factor to the lake system by (a) acting as a buffer to nutrient-rich river inflows by discharging phosphate-poor waters, and (b) causing a weaker summer stratification compared to the inactive scenario. Without the PEP discharges acting as a dilluting factor, Lake Tegel could be heavily influenced by discharges of the River Havel. The result of this was increased phosphate concentrations in conjunction with a slightly higher buoyancy frequency that could potentially benefit the formation of cyanobacteria blooms. The mechanism behind the slightly increased summer stability in the inactive scenario compared to the other scenarios was likely a feedback loop between increased nutrient concentrations and a resulting higher turbidity (changes in water clarity), similarly to the results of a study conducted by Rose et al. (2016). Rose et al. stated that the thermal structure of lakes with a similar depth to Lake Tegel is sensitive to changes in water clarity, because "[...] the surface temperature may have warmed faster and deeper waters more slowly than they would have if water clarity had not increased" Rose et al. (2016) (p 50). In our model, increased loadings of inorganic nutrients, for instance, phosphate, by the river inflow caused an earlier diatom bloom in the model and a subsequent increase in the light extinction coefficient/turbidity. This resulted in a decreased heat flux to the deeper water layers and thereby lower water temperatures. Additionally, the inflow of denser and warmer waters from the elimination plant was absent, which would otherwise further intrude into deeper lake layers, effectively increasing the water temperatures.

The results of the projected thermocline depths did show that the thermal lake stratification was not particularly distinctive and resulted in the formation of a relatively thin epilimnion. In the numerical model, wind-induced mixing or convective cooling events could easily deepen the thermocline at Lake Tegel. In particular, the weakened as well as the maximum management scenarios depicted several strong mixing events during summer, in which the thermocline nearly reached the maximum depth of Lake Tegel. Theses short summer mixing events can have a high relevance for future management: during these mixing events, internally released nutrients from the sediment could be transported to the surface water layers and could cause eutrophication. On the other hand, these thermocline deepening events could also transport dissolved oxygen into the hypolimnion. The management scenarios with a weakened or inactive PEP projected future lower and stagnant bottom water temperatures as a result of a stronger heating of the surface layer and a subsequent increased stability of the water column during the summer stratification period. For the latter half of the 21st century, the surface water temperatures were following the air temperature, and the bottom temperatures experienced less variance and did not drop below 5 °C. The stagnant water temperatures and the oxygen depletion could eventually negatively affect the ecosystem (Kirillin, 2010).

Important limitations of our study were the uncertainties associated to (1) the field data, (2) our conceptual model of Lake Tegel, (3) the GLM-AED2 model, (4) the projected weather data, and (5) the setup of alternative PEP management scenarios. The uncertainty due to field sampling and the data analysis could not be neglected. It could be a possible source for errors, but we minimized it by using transient and checked data by the same agency for each site. The uncertainties of the conceptual model and the simulation were minimized by calibrating and validating the model. A potential major source of uncertainty was the

future climate projection by WETTREG2010. Although the regional data set was based on ECHAM5 and therefore on physical principles, the underlying assumptions of the A1B scenario as well as the stochastic nature of climate anomalies were still important sources for uncertainty. The last uncertainty was by choice: by only using simple future management scenarios, for instance, constant low and high values, we investigated the general response of Lake Tegel to climate change and management alterations. In reality, the PEP discharge is dependent on the upstream inflow of the WWTP, its respective catchment, the mode of operation of the lake pipeline and rainfall events. Therefore, steady discharge curves are highly idealized scenarios. Further, although recent reports have suggested an increase in total discharges as a result of climate change (Reusswig et al., 2016), we neglected the effect of climate change on the discharges of the flow boundary conditions and applied the same discharge curves for every future year. We also neglected the impact of an increasing frequency of extreme weather events on the lake system causing short-term high run-off and possible erosion events. These assumed simplifications should enable the model applications to focus on the effects of changing meteorological variables in conjunction with alternative management scenarios on the lake's thermal stratification and composition of oxygen as well as phosphate. Additionally, investigating factors such as increased surface and subsurface runoffs or complex inflow boundaries would extend the scope of this study and should be approached by coupling a catchment model to a hydrodynamic lake model.

4.5.3 Implications for the lake water management

In the context of this study, we considered adaptive lake water management as a management that is not based on a fixed restoration strategy/management plan but one that "[...] recognizes the non-stationary nature of a system [...]" (Imberger et al., 2017) (p 73). Because of the recent concerns regarding micropollutants in the urban water cycle of Berlin, particularly for Lake Tegel (Jekel et al., 2013b, Schimmelpfennig et al., 2016), there are future plans to divert the discharges of treated effluents from the upstream wastewater elimination plant away from Lake Tegel. In this case, the PEP could shut down as a result of the financial unfeasibility of operating a treatment plant and only treating discharges under the capacity. At the least, the discharges of the PEP into Lake Tegel would certainly decrease. However, as the results of our modeling study and former studies (Schauser and Chorus, 2009, Schimmelpfennig et al., 2012b) have suggested, the low phosphate discharges of the PEP have a diluting effect on the lake system. Decreasing these additional discharges can increase the phosphate concentrations in the water column. This can enable the formation of phytoplankton blooms and, later, increase water turbidity, further increasing the surface water temperatures. This vicious cycle has the potential to enhance the impact of climate change on the lake thermal stratification. Neglecting the economic unfeasibility of operating a PEP under capacity, using the lake pipeline to bypass water to the northeastern inflow for treatment has the potential to be an efficient measure to adapt the water management to climate change. The lake pipeline has a mean average flow of $0.65\,\mathrm{m^3\,s^{-1}}$ and can be increased to a maximum flow capacity of about $1.9\,\mathrm{m^3\,s^{-1}}$. This discharge then would be similar to the results of the weakened scenario and could counter the heavy loadings originating from the River Havel as well as the increased water column stability.

Another potentially useful strategy to adapt Lake Tegel's water management to climate change could make use of the hypolimnetic aerators at Lake Tegel, particularly under the condition that cyanobacteria would be established in Lake Tegel. Former studies have stated that the aerators cause a lifting of hypolimnetic waters into the epilimnion and, therefore, decrease the thickness of the metalimnion (Lindenschmidt and Hamblin, 1997, Heinzmann and Chorus, 1994). Artifical circulation measures are a widespread technique to avoid hy-

polimnetic oxygen depletion conditions and the formation of cyanobacteria blooms (Visser et al., 2016). Although the installed aerators have the potential to cause more harm during future strong stratification events by transporting nutrients and oxygen-depleted waters from the hypolimnion to the epilimnion, destratification could also hinder the formation of toxic algae blooms. If these hypolimetic aerators could be modified to cause a complete mixing of the water column of Lake Tegel, they could have a positive effect in the latter half of the 21st century when the impact of climate change could be the strongest. Nonetheless, this management strategy also needs the additional discharges from the PEP; otherwise the aerators would only mix phosphate-rich waters into the hypolimnion. A combination of a still active PEP, even with low discharges, and artificial mixing or even oxygenation events could mitigate the projected severe impact of climate change on Lake Tegel's thermal structure as well as oxygen and phosphate composition in the latter half of the 21st century.

Although there is a wide range of in-lake management measures to control internal nutrient release from the sediment or to manipulate the water column stability (Visser et al., 2016, Bormans et al., 2016), the best long-term management measure to prevent a future eutrophication of Lake Tegel is the reduction of external loadings of phosphate originating from the River Havel (Schimmelpfennig et al., 2016). Particularly as a result of climate change, a future reduction of the nutrient availability in lakes can become crucial because of its positive feedback on eutrophication (Matzinger et al., 2007). Our study demonstrated that the inflow of the PEP can be efficient enough without artificial destruction of stratification. According to Schimmelpfennig et al. (Schimmelpfennig et al., 2012b), an effective management strategy should consider the reduction of the nutrient input combined with the redirection of the wastewater discharge to the River Havel by "reverse" application of the pipeline (flow from PEP to the River Havel). This would require a long-term strategy of regulating the agriculture in the catchment. In the meanwhile, the PEP appears to be effective in mitigating the negative effects of climate change and should be kept active in the next decades.

4.6 Conclusions

Our 1D vertical model coupled to a water quality configuration was applicable to the evaluation of water management scenarios for Lake Tegel. According to projections made by the 1D model and using a realization of future meteorological conditions projected by WETTREG2010, Lake Tegel's annual stratification patterns will change as a result of climate change. The winter stratification will decrease, whereas the summer stratification will intensify. Additional nutrient-free discharges by an active elimination plant can mitigate an increase in the stability of the summer stratification period. Lake Tegel could potentially even shift from a dimitic seasonal-mixing type to a monomictic type. Ultimately, these physical changes will affect the lake's water quality. An increased summer stratification period combined with a higher buoyancy frequency will act as a favorable habitat for the formation of cyanobacteria blooms. Nonetheless, our study has showed that the elimination plant acts as an important "life-support system" for Lake Tegel, because the discharges from the plant act as a buffer against nutrient-rich waters from the River Havel. We conclude that the urban lake management system, similarly to reservoirs, has the potential to mitigate some of the manifold effects of climate change on an urban lake ecosystem, and a sophisticated adaption of management measures is required to deal with future challenges.

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Abbreviations

The following abbreviations are used in this manuscript:

AED2	Aquatic Ecodynamics Model Library
CMA-ES	Covariance Matrix Adaption Evolution Strategy
DOC	Dissolved organic carbon
EE	Elementary effect
GLM	General Lake Model
NRMSE	Normalized root-mean-square error
NSE	Nash–Sutcliffe coefficient of efficiency
PEP	Phosphorus elimination plant
POC	Particulate organic carbon
RMSE	Root-mean-square error
WETTREG	Wetterlagen-basierte Regionalisierungsmethode (regionalization method)
WWTP	Wastewater treatment plant

Appendix

Table 4.3: Depth-specific root-mean-square errors for surface (0.5 m) and bottom (14 m) layers of water temperature T (°C) and dissolved oxygen DO (mg L^{-1}), nitrate N (mg L^{-1}) and phosphate P (µg L^{-1}) concentrations.

Year	**Surface**				**Bottom**			
	T	DO	N	P	T	DO	N	P
2008	0.17	2.1	0.17	6.6	0.51	0.48	0.54	10
2009	0.41	2.7	0.19	2.6	0.89	0.94	0.45	8.6
2010	0.74	2.1	0.09	5.3	0.24	0.72	0.4	21
2011	0.73	1.9	0.22	6.1	0.4	0.72	0.41	17
2012	0.31	2.6	0.12	2.3	0.32	0.53	0.40	11
2013	0.53	3.1	0.18	3.1	0.2	1.0	0.52	5.7
2014	0.36	2.7	0.51	2.0	0.2	0.51	0.36	29

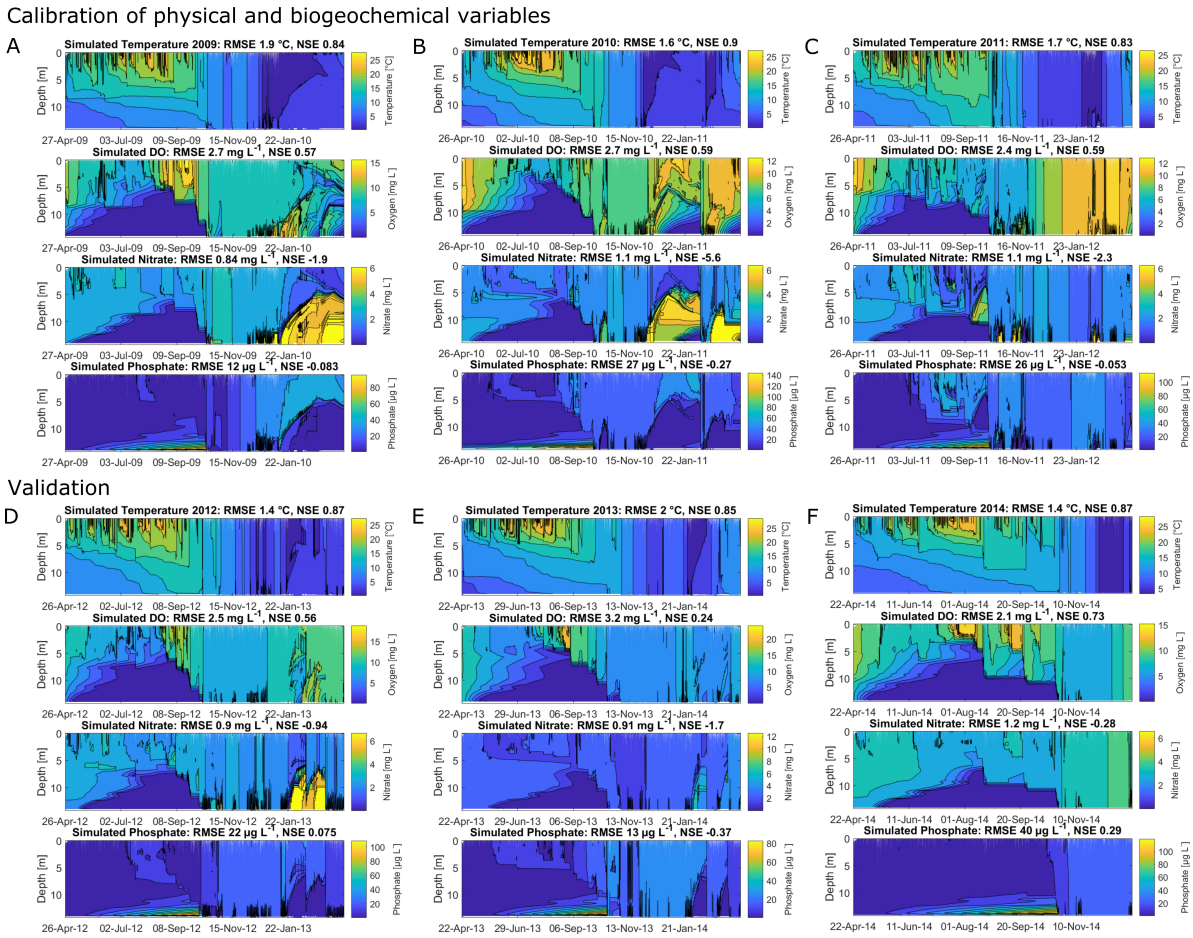

Figure 4.7: Contour plots expressing the model performance of water temperature (°C), dissolved oxygen (mg L^{-1}), nitrate (mg L^{-1}) and phosphate concentrations (µg L^{-1}); the calculated root-mean-square errors (RMSE) and Nash–Sutcliffe coefficients of efficiency (NSE) are given for the total water column: (**A**–**C**) calibrated years 2009, 2010 and 2011; (**D**–**F**) validated years 2012, 2013 and 2014.

Chapter 5

In the Future II: Application of a depth-averaged 2D model to evaluate the impact of short-duration heavy rainfall events on Lake Tegel

This study was initially submitted to Environmental Fluid Mechanics (Springer) as:

Ladwig R., Matta E., Hinkelmann R., and Hupfer M.: Numerical investigation of water exchange times and phytoplankton bloom formation in an urban lake after short-duration heavy rainfall events, submitted to Environmental Fluid Mechanics on October 09 2018

This is a preprint version of the manuscript.

5.1 Abstract

Short-duration heavy rainfall events, which will become more intense and frequent due to climate change, can severely affect lake ecosystems by increasing external nutrient loadings and, therefore, benefiting phytoplankton bloom formation. Water exchange times, like the lake hydraulic residence time or the influence time distribution, are important to evaluate the impact of such rainfall events on the lake system. We calibrated a depth-averaged 2D hydrodynamic model of the urban Lake Tegel (Berlin, Germany) using a time series of 15 years and computed the water exchange times in dependence on the wind conditions. Then, we coupled a water quality model to the hydrodynamic model and ran short-duration heavy rainfall scenarios, similar to an event Lake Tegel had experienced in summer 2017, with different wind and water management settings. The influence time distribution revealed that during east-wind conditions, the river intrusion into Lake Tegel was enhanced but the local influence times were also the shortest. Further, the short-duration heavy rainfall scenarios, which were evaluated by using principal component analysis, showed that the Lake Tegel system is dominantly controlled by the wind direction, followed by the inflow discharges and, finally, the ecological reactions. To mitigate the impact of short-duration heavy rainfall events on the Lake Tegel ecosystem, we recommend to enhance inflow nutrient elimination and/or to increase external discharges to decrease the hydraulic residence time.

5.2 Introduction

Climate change is going to severely affect physical and ecological characteristics of lakes around the world (Adrian et al., 2009, Jeppesen et al., 2017). Changes in air temperatures will affect the onset as well as offset of thermal stratification periods (Kirillin, 2010). Further, changes of precipitation intensities will affect the whole catchment by contributing to surface runoff eventually affecting nutrient concentrations and turbidity in the receiving lakes. The latter can, in combination with air temperature changes, severely accelerate lake warming (Rose et al., 2016). Especially short-duration heavy rainfall events, which can become more frequent and more intense due to climate change (Westra et al., 2014, Woolway et al., 2018), are future stressors to which the urban water management has to adapt. Such strong precipitation events increase flow discharges as well as surface runoffs causing urban flash floods. The former can cause overflows at technical systems (watergates, treatment plants) and the latter increases stormwater surges that will increase the influx of contaminant loadings into nearby surface waters. In the aftermath of such rainfall events, the urban lake ecosystem structure is modified and increased loadings of nutrients as well as a deepening of the thermocline, which can affect underwater light limitation, can benefit the formation of phytoplankton blooms (Kasprzak et al., 2017). Further, increased surface runoffs will affect the lake's turbidity and can cause brownification, which is also driven by climate change (Kritzberg et al., 2014).

A common approach in evaluating the potential hazard of pollutants and nutrients on the lake ecosystem is to calculate specific water exchange times of potential interactions between the substances and the ecosystem as well as physical transport processes (Delhez et al., 2014). The lake hydraulic residence time, commonly expressed in its simple form as the ratio of the lake volume to the outflow discharge, indicates the mean time that a water parcel is theoretically retained in a lake and expresses the duration a system needs to recover from a pollution event. An alternative to the residence time is the influence time, which is the time needed for the replacement of water in a specific location of the domain and is therefore a diagnostic proxy for local influence of a substance (Delhez et al., 2014, Montaño Ley and Soto-Jiménez, 2018). Especially during short-duration heavy rainfall events, understanding the total and local times of interactions is crucial for an effective water management. The impact of such short-duration heavy rainfall events on lake metabolism was investigated by Zwart et al. (2016). A main conclusion was that the lake hydraulic residence time, which was reduced due to increased surface runoff, affected the carbon turnover rates. A similar finding was obtained in the Swedish Lake Mälaren, in which a rainy period increased organic carbon loadings into the lake, changing water color and causing blooms of cryptophyceans (Weyhenmeyer et al., 2004). Here, the hydraulic residence time directly impacted the influence of the rainfall period on the lake ecosystem. The record harmful algal bloom in Lake Erie, North America, in 2011 was also caused by the compound effects of heavy precipitation, agricultural loadings and a period of weak lake circulation, therefore increasing lake residence time (Michalak et al., 2013). Especially in lake systems with river inflows and therefore a profound effect of through-flow on the lake-wide distribution of dissolved substances, the residence and influence times can vary depending on the season (Carmack et al., 1986). The interactions between wind, lake morphometry and inflows were also investigated using field measurements and modeling in Coeur D' Alene Lake (USA), in which the authors showed their combined impact on primary production (Morillo Sebastián et al., 2008). Numerical modeling using a depth-averaged 2D hydrodynamic model was also used to estimate hydraulic residence times as well as transport dynamics during strong rain events in the Itaparica Reservoir, Brazil (Matta et al., 2018). This work was then extended by applying a 3D model to simulate the impact of extreme meteorological events and heat

dynamics (Matta et al., 2017), while the nutrient load and carrying capacity limits concerning mainly phosphorus (P) and chlorophyll-a (Chl-a) have been investigated by (Selge et al., 2016). Here, external phosphorus export rates increased during strong rain events.

The urban Lake Tegel (Berlin, Germany) is an ecosystem affected by multiple stressors and controlled by a diverse water management system. In summer 2017, a short-duration heavy rainfall event happened at Lake Tegel and caused mass development of phytoplankton in its aftermath. Lake Tegel experienced a severe period of eutrophication in the past and is, therefore, a well described, investigated and modeled system. In the 20th century, Lake Tegel's water quality deteriorated due to increased loadings of nutrients and heavy metals from an upstream sewage field. Several successful management measures (construction of a phosphorus elimination plant, water bypass, expansion of canalization) were underdone from the 1970s - 1990s to restore the lake ecosystem and to mitigate further eutrophication. In previous research studies, a wide variety of numerical models have been implemented to address research questions at Lake Tegel, from mass balance box-models (Schauser and Chorus, 2009), vertical 1D models (Lindenschmidt and Hamblin, 1997, Ladwig et al., 2018) to depth-averaged 2D models (Schimmelpfennig et al., 2012a,b). In all theses former studies, the aim was to adapt the urban water management to the external stressors in order to mitigate contamination or eutrophication, which would be a disastrous consequence for Berlin's second largest lake and crucial source for drinking water production. Although previous studies addressed the hydrodynamics of Lake Tegel, most of them did not incorporate water quality simulations based on biogeochemical reactions.

The aim of this study was to understand the environmental fluid dynamics of Lake Tegel during and after a short-duration heavy rainfall event by setting up a hydrodynamic model coupled to a water quality module. Our hypothesis was that an inflow of nutrient-rich river waters caused these phytoplankton blooms and that such river-mixing events could be controlled by an adaptive water management that artificially increases external inflows. Therefore, we were neglecting stormwater discharges from the urban catchment consisting of sewer overflows and surface runoffs into Lake Tegel. Although these stormwater flows are a profound stressor for surface water systems by affecting flow patterns and volumes as well as degrading the water quality by increased loadings of nutrients (Walsh et al., 2012, Erickson et al., 2013), they are diffuse sources and therefore hard to quantify. For this reason, we focussed in particular on the interactions between the main inflows and the lake ecosystem. Based on the works of Schimmelpfennig et al. (2012a), (1) we calibrated and validated a depth-averaged 2D model to replicate the hydrodynamics of Lake Tegel using a time series of 15 years. For evaluating the potential transport as well as the retention of contaminants and nutrients in the lake system, (2) we calculated the local influence time distributions during mean discharge and mean wind conditions. Afterwards, (3) we extended the model with a water quality module and validated this module to replicate Lake Tegel's nutrient interactions and phytoplankton dynamics. Although TELEMAC-3D was previously used to simulate water quality of Lake Müggel in Berlin, Germany (Kopmann and Markofsky, 2000), to our knowledge this is the first published study applying the water quality module EUTRO of the open TELEMAC-MASCARET modeling suite to real field data. Finally, (4) we ran short-duration heavy rainfall scenarios and modified the inflow treatment plant boundary condition to evaluate its potential to mitigate the formation of phytoplankton blooms. The results of each scenario were represented by the lake hydraulic residence time, inflow discharges and loadings, river mixing as well as phytoplankton, dissolved oxygen and nutrient concentrations in the lake basin using principal component analysis (PCA).

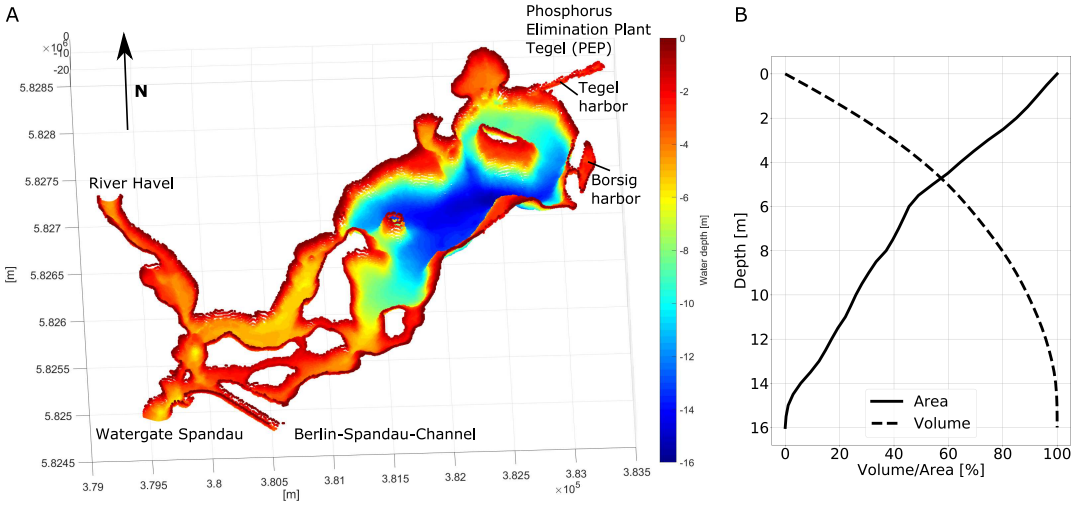

Figure 5.1: Study site Lake Tegel in Berlin, Germany. **a** Bathymetric map of Lake Tegel with the main boundary conditions. **b** Hypsographic curves of Lake Tegel expressing the lake volume and the lake area in percentage over the depth

5.3 Materials and methods

5.3.1 Study site

Lake Tegel is situated in Berlin, Germany (Fig. 5.1 A, coordinates: 52.5761° 13.2533°, V=28.5 Mio. m^3, A=4.4 km^2), and is a prominent example for an urban lake that underwent morphological degradation and is controlled by a complex water management system. A large part of Lake Tegel can be considered shallow (approx. 60 % of the lake area is above the mean depth of 6.6 m, Fig. 5.1 B). A deeper lake basin with depths up to 16 m is situated in the north-eastern part of the lake.

Lake Tegel receives its inflows from the north-east (inflow of treated wastewaters over the phosphorus elimination plant Tegel (PEP)) and from the north-west (inflow of the River Havel). Additionally, riparian lake water is abstracted by several groundwater abstraction wells around the lake. A lake pipeline connects the north-eastern inflow by the PEP with the main outflow in the south-west, which is controlled by the downstream watergate Spandau. A minor outflow is the Berlin-Spandau-Channel (BSK) located in the south-east. The mean annual water budget of Lake Tegel can be described by:

$$\overline{Q}_{Spandau} = \sum Q_{inflow} - \sum Q_{outflow} = (\overline{Q}_{Havel} + \overline{Q}_{PEP}) - (\overline{Q}_{BF} + \overline{Q}_{BSK}) \tag{5.1}$$

$$\overline{Q}_{Spandau} = [(11.23 + 2.29) - (1.4 + 0.08)]\mathrm{m}^3\,\mathrm{s}^{-1} \sim 12\,\mathrm{m}^3\,\mathrm{s}^{-1} \tag{5.2}$$

where $\overline{Q}$ are the respective mean discharges (m^3 s^{-1}) for the main outflow (Spandau), the river inflow (Havel), the phosphorus elimination plant inflow (PEP), the bank filtration abstraction (BF) and the outflow by the Berlin-Spandau Channel (BSK). Regarding the inflow, the River Havel accounts for 83.06 % and the PEP for 16.93 %. On average, about 12 m^3 s^{-1} are discharged over the main outflow. Therefore, the main outflow accounts for 89.95 % of the total outflow, the BSK for 0.54 % and the bank filtration for 9.50 %. The lake hydraulic residence time in the total model domain of Lake Tegel would be about $\tau = \frac{V}{Q_{Spandau}+Q_{BF}+Q_{BSK}} = 24.5\,\mathrm{d}$. This qualifies Lake Tegel as a lake system with a short residence time. Therefore, strong interactions between the inflow input and the lake ecosystem

are controlling the system resulting in a 'run-of-the-river' dominance system, in which the inflows determine the distribution of substances in the lake (Carmack et al., 1986). The calculated residence time for the lake domain is about a $\frac{1}{3}$ till a $\frac{1}{2}$ of the lake residence time when just considering the main lake basin, which is approx. 50-90 days (Kleeberg et al., 2012b). This mirrors the on average two- to three-times higher discharges of the River Havel into the lake system.

In summer 2017, humid air masses originating from the Mediterranean Sea caused heavy rainfall in Berlin. On June 29 2017, the daily precipitation at Lake Tegel was close to 200 mm (Fig. 5.2). Subsequently, the discharges at the inflows peaked with the discharge of the River Havel raising to approx. $280\,\mathrm{m^3\,s^{-1}}$ on the short-term and the PEP experienced increased inflow discharges of upstream streams exceeding the plant's capacity. The latter caused an overflow that resulted in the discharge of non-treated waters into Lake Tegel. Consequently, Lake Tegel's surface layer became well-mixed with turbid waters being transported close to the thermocline at approx. 7 m (Fig. 5.2). These additional water masses deepened the thermocline and widened the surface mixed layer. Phytoplankton blooms started to form (Fig. 5.2), consisting mainly of cryptophyceans, bacillariophyceans and cyanophyceans. Especially bacillariophyceans or diatoms are the dominant phytoplankton group at Lake Tegel and can be characterized by high growth and metabolic rates (Shimoda and Arhonditsis, 2016). Although diatom blooms are in principle not toxic to other species, in contrast to cyanophyceans or cyanobacteria, they can shift the lake towards a turbid state affecting underwater light climate and water temperature dynamics. In the aftermath of the heavy rainfall event, the vertical abundances of dissolved oxygen and phosphate were affected by additional water masses and biological respiration causing an oxygen depletion in the bottom stagnant water layer (Fig. 5.2). Dissolved oxygen dynamics are closely coupled to the chlorophyll-a concentrations and, thus, to primary production, increasing shortly after the mixing and decreasing afterwards. Nonetheless, oxygen depletion during the summer stratification period is common in Lake Tegel. Therefore, the hypolimnetic oxygen decline was probably not directly related to the short-duration heavy rainfall event. The phosphate concentrations were higher close to the sediment, probably related to the internal fluxes from the sediment into the water column. Figure 5.2 visualized that the effects of a short-duration heavy rainfall event can last far longer than the actual precipitation event due to a time lag between the meteorological conditions and the responses of the catchment as well as in-lake processes.

5.3.2 Model setup and governing equations

A depth-averaged two-dimensional model for Lake Tegel was set up using the open TELEMAC-MASCARET modeling suite (short: TELEMAC-2D, Laboratoire National d' Hydraulique et Environnement Hervouet and Ata (2017b)). TELEMAC-2D solves the depth-averaged free surface flow equations, namely the equations for continuity as well as momentum along the horizontal x and y directions. For water quality simulations, we used the TELEMAC-2D internal module EUTRO, which calculates spatial and temporal changes of tracers representing biogeochemical and ecological reactions (Hervouet and Ata, 2017a). Tracer conservation is governed by:

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial x} + v\frac{\partial C_i}{\partial y} - \frac{\partial}{\partial x}(\nu_{t,t}\frac{\partial C_i}{\partial x}) - \frac{\partial}{\partial y}(\nu_{t,t}\frac{\partial C_i}{\partial y}) = F \tag{5.3}$$

where C_i is the respective tracer i; u and v are the velocity vectors in x- and v-direction, respectively; $\nu_{t,t}$ is the turbulent diffusivity; and F is a tracer source or sink accounting for reactive transport and water quality interactions (Hervouet and Ata, 2017b).

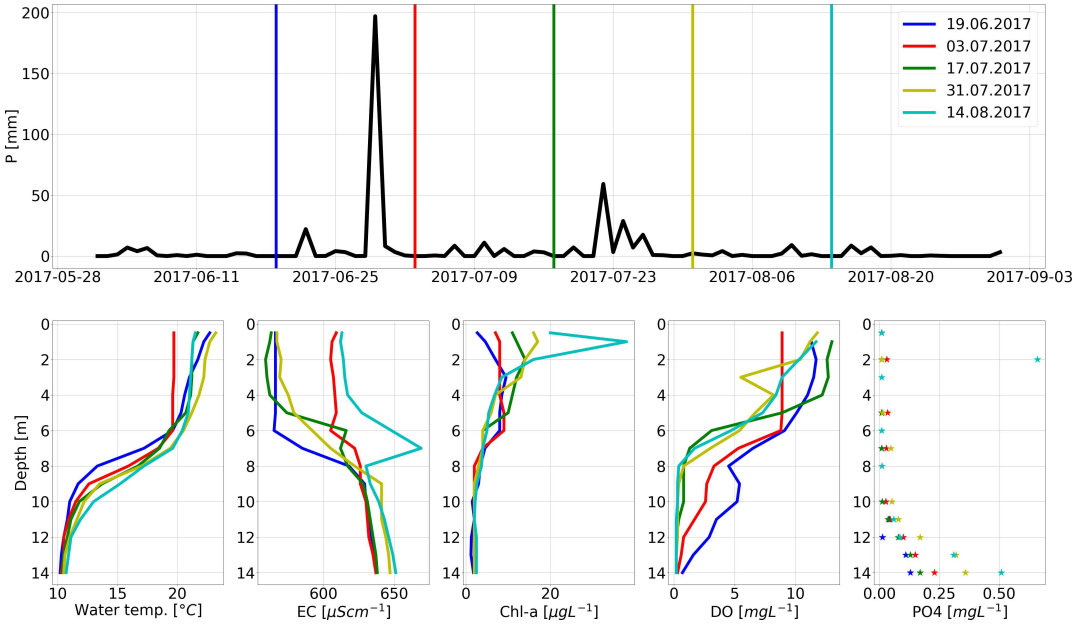

Figure 5.2: Dynamics of physico-chemical parameters, water temperature and electrical conductivity (EC), as well as chlorophyll-a, dissolved oxygen and phosphate concentrations at Lake Tegel's deepest site during a short-duration heavy rainfall event starting at June 31 2017. **Top** shows the precipitation measured at the nearby weather station Berlin Tegel Airport. **Bottom** shows vertical profiles of water temperature, electrical conductivity, chlorophyll-a, dissolved oxygen and phosphate.

First, the hydraulics of the model domain are calculated, then the tracer transport and, in the final stage, the interactions of the tracers with each other. EUTRO incorporates interactions between eight tracers (all in mg L^{-1} except Chl-a which is in µg L^{-1}): phytoplankton biomass defined per Chl-a, dissolved mineral phosphate (eventually metabolized by phytoplankton), degradable phosphate (not assimilable by phytoplankton), dissolved mineral nitrate (eventually metabolized by phytoplankton), degradable nitrate (not assimilable by phytoplankton), ammonia (assimilable by phytoplankton), organic loadings and dissolved oxygen (Hervouet and Ata, 2017a,b). All specific tracers are source and sink terms, F, in the general tracer equation (Eq. 5.3). We assumed that the soluble reactive phosphorus fraction ortho-phosphate, $o-PO_4$, is represented by phosphate, whereas NO_3-N and NH_4-N are represented by nitrate and ammonium, respectively. Further, for the meteorological boundary conditions, EUTRO uses air temperature (°C), wind speed (m s^{-1}), wind direction (°) and atmospheric radiation (W m^{-2}). The phytoplankton growth dynamics were determined by multiplicative interactions between aggregated properties of maximum growth rate at 20 °C, temperature forcing (described as a linear dependence) and nutrient limitation (minimum of phosphate and nitrate described by Michaelis-Menten enzyme kinetics). The disappearance of phytoplankton is calculated as the sum of mortality and respiration, which is multiplied by a factor for temperature forcing. We simplified the original phytoplankton growth-disappearance equation by neglecting light limitiation as well as toxicity terms:

$$F_{PHY} = (c_{max}\mu(T)\mu(lim(Phosphate, Nitrate)) - d(T)(RP + (M_1 + M_2[PHY]))[PHY] \quad (5.4)$$

where F_{PHY} is phytoplankton source/sink term; c_{max} is the maximum growth rate; $\mu(T)$ is the growth in dependence of temperature; $\mu(lim(Phosphate, Nitrate))$ is the growth limited

by the availability of either phosphate or nitrate and ammonium; $d(T)$ is the disappearance in dependence of temperature; RP is the respiration rate; M_1 and M_2 are mortality factors; and $[PHY]$ is the phytoplankton biomass. An overview of the water quality formulations is given in the Appendix.

Light limitation was neglected to focus on the phytoplankton dynamics under nutrient limitation. The default phytoplankton biomass function of EUTRO uses light forcing described by a depth-integrated Smith function, which does not represent photoinhibition. The Smith light function could be exchanged for a more sophisticated function. An overview of possible equations for phytoplankton modeling is given in Tian (2006). Other aquatic models simulating phytoplankton dynamics apply the Steele equation for light forcing, e.g. GLM (Hipsey et al., 2013) and PCLake (Janse, 2005), or exponential equations, e.g. DYRESM (Hipsey, 2008). In our model, no functional phytoplankton groups were simulated and the phytoplankton state variable represented the whole lake phytoplankton community with focus on diatoms, which are the dominant phytoplankton group in Lake Tegel.

The model domain consisted of the total lake area, downstream part of the River Havel as well as Tegel harbor and Borsig harbor (Fig. 5.1 a). Additionally a part of the BSK was also included in the model. The grid was created from interpolated bathymetric data points using Janet (v. 2.15.7, smile consult GmbH). The resulting model mesh (Fig. 5.3) consisted of 45,093 nodes and 86,880 triangular elements with respective lengths from 2.8 m to 31.7 m. Two transient flowrate boundary conditions (Fig. 5.3) were acting as inflows in the north-east (PEP Tegel) and in the north-west (River Havel), respectively. The main outflow close to the downstream watergate Spandau was incorporated as a transient water depth boundary condition in the south-west. Further, there was a constant flowrate boundary over the BSK in the south-east. Bank filtration contributed on average 9.50 % to the total outflow and was therefore incorporated in our model domain. Each bank filtration well gallery (in total seven) was simulated as a single sink term located roughly in the center of the well gallery and close to the model boundary. Further, the lake pipeline was explicitly simulated as a transient source term near the outflow and indirectly by the PEP discharge. Data for the operation of the lake pipeline was available starting on October 4 2001. Prior data was extrapolated using an auto-regressive model via Burg's method to simulate the average annual pattern of the lake pipeline from 2000 until 2001 (Kay, 1988).

5.3.3 Calibration and validation of hydrodynamics

The model calibration simulations were run using TELEMAC-2D v.7p2 and were conducted with a time step of 30 s through parallel computing on the HLRN system using 24 processors (North German Association for the Promotion of High and Maximum Performance Calculation). To replicate the field hydrodynamics in the 2D model, we calibrated the bottom friction coefficient using Strickler's friction law. We assessed the goodness of the calibration fit by comparing measured chloride data at Lake Tegel's deepest site (Fig. 5.3) with simulated tracer concentrations representing chloride from 2000-2014. This was done in accordance with former modeling studies at Lake Tegel, which also used chloride as a passive tracer (Schauser and Chorus, 2009, Schimmelpfennig et al., 2012b). We investigated the bottom friction coefficient K_{str} ranging from $30\,\mathrm{m}^{1/3}/\mathrm{s}$ to $78\,\mathrm{m}^{1/3}/\mathrm{s}$. For turbulence we used the k-ε model, which computes turbulent kinetic energy and turbulent dissipation terms automatically reducing the amount of parameters to calibrate. A mass-conservative edge by edge implementation of the N distributive scheme was used for the advection of velocities and tracers. All evaluations and post-processing were done using MATLAB R2017a (The MathWorks Inc., Natick, USA).

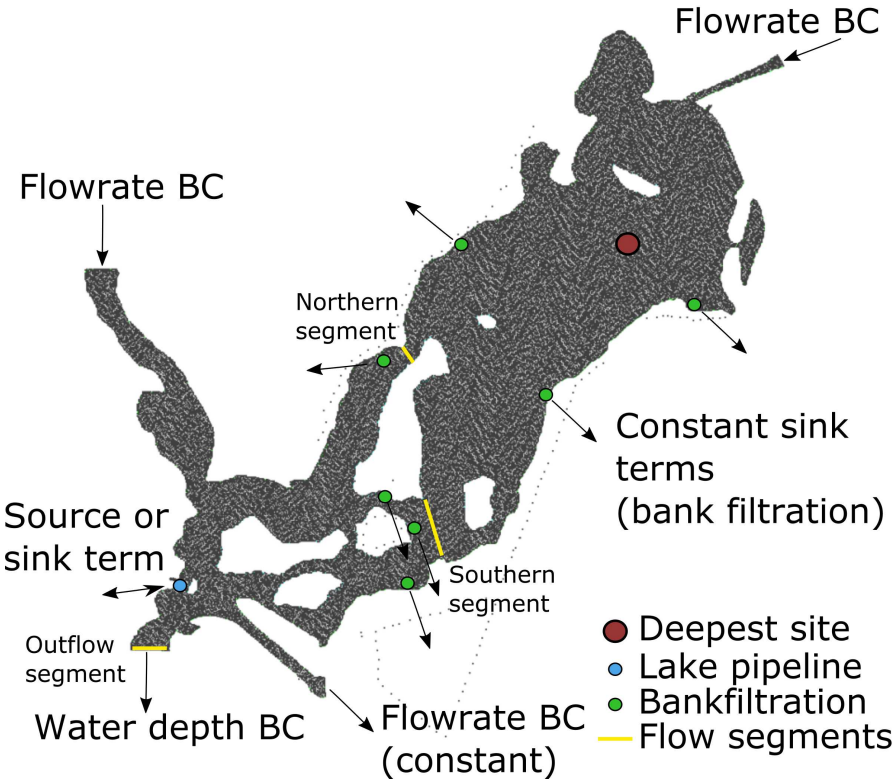

Figure 5.3: Triangular mesh of Lake Tegel with boundary conditions (flowrate boundary conditions (BC) at River Havel, phosphorus elimination plant and Berlin-Spandau-Channel; water depth BC in the south-west), sink terms (seven point sink terms representing the bank filtration wells and one source/sink term representing the bank fitlration) and specified segments for flow calculations ("Outflow", "Southern" and "Northern" segments)

5.3.4 Evaluation of the influence time distribution

Based on the results of the hydrodynamic calibration of the bottom friction, we computed the influence time by calculating the remnant function according to Takeoka (1984), Cucco and Umgiesser (2006), Montaño Ley and Soto-Jiménez (2018). A conservative tracer with an initial concentration of 100 % was uniformly released into the whole model domain. The only factors influencing the tracer concentration were the respective mean boundaries conditions, which were kept constant, as well as four wind direction setups: no wind, dynamic wind using the daily average wind speeds and directions from 2008-2014, west-wind with mean wind speed and east-wind with mean wind speed. The remnant function was then calculated accordingly as:

$$r(x,y,t) = \frac{C(x,y,t)}{C_0(x,y)} \tag{5.5}$$

where $C(x,y,t)$ is the respective tracer concentration at each point and time step; and $C_0(x,y)$ is the initial tracer concentration. For each point, the influence time τ_{IT} was computed as

$$\tau_{IT}(x,y) = \int_0^\infty r(x,y,t)dt \tag{5.6}$$

and represents the decline of $r(x,y,t)$ over time (Cucco and Umgiesser, 2006, Takeoka, 1984). In order to approach the influence time distribution, the simulations were run for a duration

of one year.

5.3.5 Validation of water quality

We validated the results of the water quality module EUTRO by comparing simulated depth-averaged concentrations of phosphate, nitrate, ammonia and dissolved oxygen with the measured depth-averaged concentrations as well as measured surface concentrations at the deepest site of Lake Tegel from May to August 2014. Initial conditions were assumed to be uniformly and were derived from measured field concentrations at the deepest site. Boundary conditions of secchi depth [m], inflow discharges and biogeochemical inflow concentrations were derived from monitored and sampled data from the Berlin Water Works and the Senate of Berlin, which were also used previously in Ladwig et al. (2018). Unknown boundary data were interpolated in time. The simulated depth-integrated phytoplankton Chl-a data were validated with surface field data of Chl-a measured at the deepest site of Lake Tegel.

5.3.6 Setup of short-duration heavy rainfall scenarios

To evaluate the impact of short-duration heavy rainfall events on Lake Tegel, we set up idealized short-duration heavy rainfall scenarios emulating the time period from June 24 - July 8 2017. Each scenario ran for 15 days with heavy rainfall setting in after the fifth day. Discharges and nutrient concentrations were derived from measured and monitored field data of the PEP, River Havel, Tegeler Fließ and Nordgraben. The latter two are small streams discharging into the PEP, and consequentially treated, before entering Lake Tegel. Meteorological data were taken from the weather station at the airport Berlin-Tegel (few kilometres away). Water levels for the south-eastern outflow condition were taken from measured water levels at the watergate Spandau. Field data of Tegeler Fließ and Nordgraben were interpolated linearily from incomplete daily data (June 14 until July 13 2017). Also, data of River Havel were interpolated linearily from incomplete daily data (June 19 until August 17 2017). In order to simplify the scenarios, the only variables alternating were the wind direction and the management of the PEP (Fig. 5.4 A). The constant wind directions were the main differences between the scenarios and the actual short-duration heavy rainfall event in June 2017. Schimmelpfennig et al. (2012a) showed that under east-wind conditions, river intrusion into Lake Tegel is the strongest and, therefore, most nutrient loadings entering Lake Tegel are occurring under east-wind conditions. These constant east-wind scenarios were compared to scenarios with constant wind coming from the west (the dominant wind direction at Lake Tegel and associated with less wind-induced river mixing). We also investigated the impact of the PEP management by altering its discharges and nutrient concentrations using three management scenarios:

- "Overflow" implies that the PEP's treatment capacity reached its limit and additional non-treated water masses were flowing directly into Lake Tegel (similar to the real event that happened in June 2017).
- "Capacity" refers to a scenario in which the PEP can treat all inflows.
- "Overcapacity" refers to the scenario in which the PEP can treat all inflows and additionally increases its discharge with the intention to reduce the laky hydraulic retention time, either by the lake pipeline or some other technological advancements (e.g. abstraction of deep lake water).

Each management scenario of the PEP differs in terms of discharge and inflow phosphate as well as nitrate concentrations (Fig. 5.4 B-D). Discharge and nutrient concentrations of the River Havel inflow as well as meteorological variables were kept constant for each scenario. To make the scenario evaluation simpler, the inflow Chl-a tracer values were kept zero for the PEP. For each scenario we evaluated the impact of short-duration heavy rainfall events on the lake system by calculating:

- the lake hydraulic residence time τ, which was calculated as the lake volume in the north of the "Northern" and "Southern" segment (approx. 2.3 Mio. m^3) divided by the sum of outflows over both segments (Fig. 5.3)
- the discharges crossing three specified boundaries ("Outflow", "Southern" and "Northern" segment) by calculating the respective flow rates, Q_i, over the respective cross-sections (Fig. 5.3)
- the mean phytoplankton biomass as Chl-a in the main basin
- the mean phosphate, nitrate and dissolved oxygen concentrations in the main basin

Here, the main basin was defined as the area consisting of all simulated points with a water depth higher than 8 m. The intrusion flow rates were calculated by integrating the products of the orthogonal flow velocity magnitudes with the water depth over the segment distance. We visualized the impact of the scenarios using PCA. The PCA input consisted of each scenarios daily information about wind direction, PEP discharge, Havel discharge, phosphate concentration in PEP as well as River Havel inflow, hydraulic residence time, flows over the specified boundaries as well as averages of Chl-a, phosphate, nitrate and dissolved oxygen concentrations in the main basin. We determined the number of principal components for evaluating the PCA using the broken-stick model (Jackson, 1993, Peres-Neto et al., 2005). Each component's eigenvalue was compared against the respective calculated eigenvalue according to the broken-stick model:

$$b_k = \frac{1}{p} \sum_{i=k}^{p} \frac{1}{i} \tag{5.7}$$

where b_k is the calculated eigenvalue for the k component; and p is the total number of variables (Peres-Neto et al., 2005).

5.4 Results

5.4.1 Hydrodynamic calibration

We investigated different bottom Strickler friction coefficients around the value of K_{str} $48\,\mathrm{m}^{1/3}/\mathrm{s}$, which was similar to a bottom friction coefficient used in a previous study Schimmelpfennig et al. (2012a). To quantify the calibration fit, we used the Nash-Sutcliffe coefficient of efficiency (NSE), the root-mean-square error (RMSE), the normalized root-mean-square error (NRMSE) and the coefficient of determination (R^2). The fits ranged from NSE's between 0.39-0.51, RMSE's between $1\,\mathrm{g\,m^{-3}}$ to $30\,\mathrm{g\,m^{-3}}$ and R^2's between 0.69-0.72 (Fig. 5.5 A). The best fit was achieved by reducing the bottom friction coefficient in the model domain to K_{str} =$42\,\mathrm{m}^{1/3}/\mathrm{s}$ achieving a NSE of 0.49, a RMSE of $1.17\,\mathrm{g\,m^{-3}}$, and a R^2 of 0.71 (Fig. 5.5 B-C).

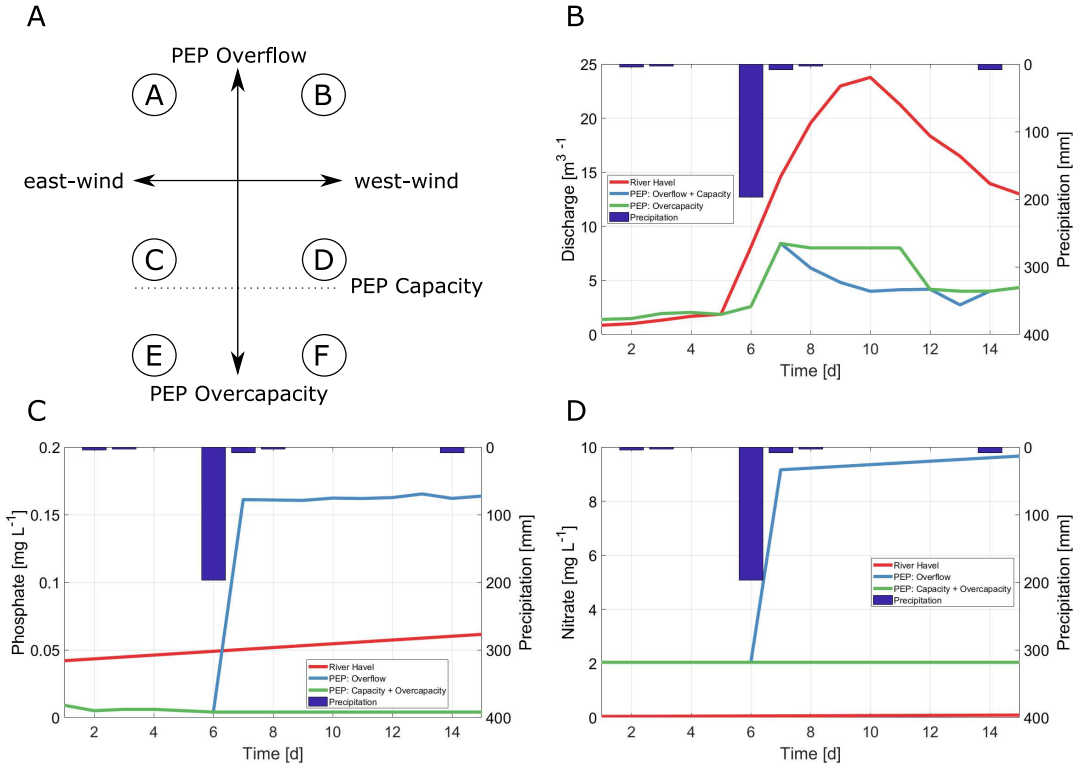

Figure 5.4: Overview of the six different scenarios that were investigated to quantify the impact of a short-duration heavy rainfall event on the Lake Tegel ecosystem. **a** Sketch showing the characteristics of each PEP scenario, either "Overflow" under east- (A) and west-wind (B) conditions, "Capacity" under east- (C) or west-wind (D) conditions, or "Overcapacity" under east- (E) or west-wind (F) conditions. **b** Discharge dynamics of the River Havel and the PEP scenarios. **c** Phosphate dynamics of the River Havel and the PEP scenarios. **d** Nitrate dynamics of the River Havel and the PEP scenarios

5.4.2 Distribution of influence times

Without wind forcing, the influence time distribution at Lake Tegel's main basin (water depth higher than 8 m) ranged from 6 to 200 days with a mean influence time of 103 days (Fig. 5.6 A). Here, also a clear flow path from the PEP to the south-western outflow emerged. Zones with influence times over a year were the "Northern" passage linking River Havel to Lake Tegel as well as smaller basins near the shore. Under dynamic wind conditions, the influence times in the main basin ranged from 80 to 111 days with a mean of 102 days (Fig. 5.6 B). Under east-wind conditions, the influence times in the main basin were the shortest, ranging from 14 to 53 days with a mean of 41 days and very short influence times in the "Northern" passage (Fig. 5.6 C). Under west-wind conditions, the influence times in the main basin were between 58 and 100 days with a mean of 86 days (Fig. 5.6 D). Therefore, the different wind setups had a ratio of dynamic to west- to east-wind of 2.7:2.0:1.0 meaning that the influence times distribution was twice as long during west-wind than during east-wind conditions and nearly three times as long during dynamic conditions compared to east-wind conditions. The mean influence times in the whole model domain for no wind, dynamic, east- and west-wind were 97, 89, 33 and 74 days, respectively.

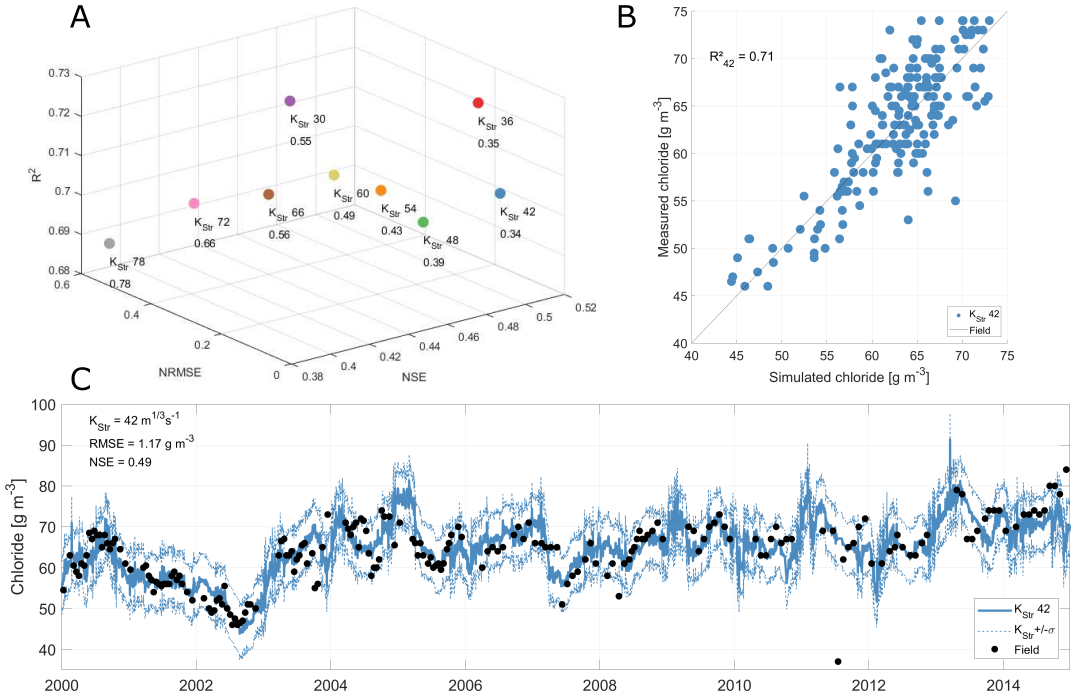

Figure 5.5: Calibration fit between simulated and measured chloride concentrations at Lake Tegel's deepest site. **a** Comparison between achieved fits of NSE, NRMSE (RMSE normalized by range of observed data) and R² of all calibration runs. The attached numbers represent the respective Euclidean distance to the 'perfect' model fit ([NSE,NRMSE,R^2]=[1,0,1]). **b** Comparison between simulated tracer and chloride field data (dots) at deepest site for the best fit of the calibration (K_{Str} =42 $m^{1/3}/s$, amount of observations n=204). **c** Comparison between simulated tracer (line), standard deviations of tracer ($\pm\sigma$, dotted lines) and chloride field data (dots) at deepest site for the best fit of the calibration (K_{Str} =42 $m^{1/3}/s$)

5.4.3 Water quality validation

We applied default as well as literature model parameters and evaluated the fit of the simulated water quality data with measured field data from May to August 2014 (Table 5.1). The mortality factor, M_1 (not in dependence of the phytoplankton biomass), the phosphorus percentage in dead phytoplankton, dtp, as well as the transformation rate from POR to PO_4, k_{320}, were slightly adjusted. The tracer concentrations for phosphate, nitrate, ammonia and dissolved oxygen ranged in the same space as the measured depth-integrated field concentrations (Fig. 5.7) and fit the measured surface concentrations very well. Further, the error bars of the standard deviations of the respective measured depth-integrated concentration fit the simulated results. The NSE were all negative indicating that the mean would be a better predictor than the model, but the RMSE's to the measured depth-averaged concentrations were in a quite good agreement with the simulation: 0.01 mg L^{-1} for phosphate, 2.8 mg L^{-1} for nitrate, 0.2 mg L^{-1} for ammonia and 7.7 mg L^{-1} for dissolved oxygen. The dynamics of phytoplankton growth (maximum in mid-June, small peak in mid-August) were replicated by the water quality model but with lower depth-integrated concentrations of Chl-a compared to the measured surface concentrations.

Table 5.1: Model values used in the water quality simulations (an overview of the water quality formulations is given in the Appendix)

Variable	Description	Value	Source
K_{Str}	Bottom friction coefficient [$m^{1/3}/s$]	42	Hydrodynamic calibration
$\mu(T)$	Max. phytoplankton growth at 20 °C [d^{-1}]	2.0	Range: 0.2-3.6 (Rigosi et al., 2011)
-	Secchi depth [m]	3 m	Field data
-	Light limitation	1	No limitation by light
KP	Phosphate half-saturation constant [$mg\,L^{-1}$]	0.006	Range: 0.000013-0.0501 (Shimoda and Arhonditsis, 2016)
KN	Nitrate half-saturation constant [$mg\,L^{-1}$]	0.014	Range: 0.0021-0.0321 (Shimoda and Arhonditsis, 2016)
RP	Phytoplankton respiration rate [d^{-1}]	0.05	Example value 0.05 (Laboratoire National d'Hydraulique et Environnement, 2018)
M_1 and M_2	Phytoplankton mortality coefficients [d^{-1}]	0.08; 0.003	Example values 0.1; 0.003 (Laboratoire National d'Hydraulique et Environnement, 2018)
fp	Phosphorus content per phytoplankton Chl-a conc. [$mg\,\mu g^{-1}$]	0.00031	Assuming 0.03 mg Chl-a/mg C (Cloern et al., 1995)
dtp	Phosphorus percentage assimilable in dead phytoplankton [%]	90	Example value 50 (Laboratoire National d'Hydraulique et Environnement, 2018)
k_{320}	Transformation rate POR to PO_4 [d^{-1}]	0.005	Example value 0.03 (Laboratoire National d'Hydraulique et Environnement, 2018)

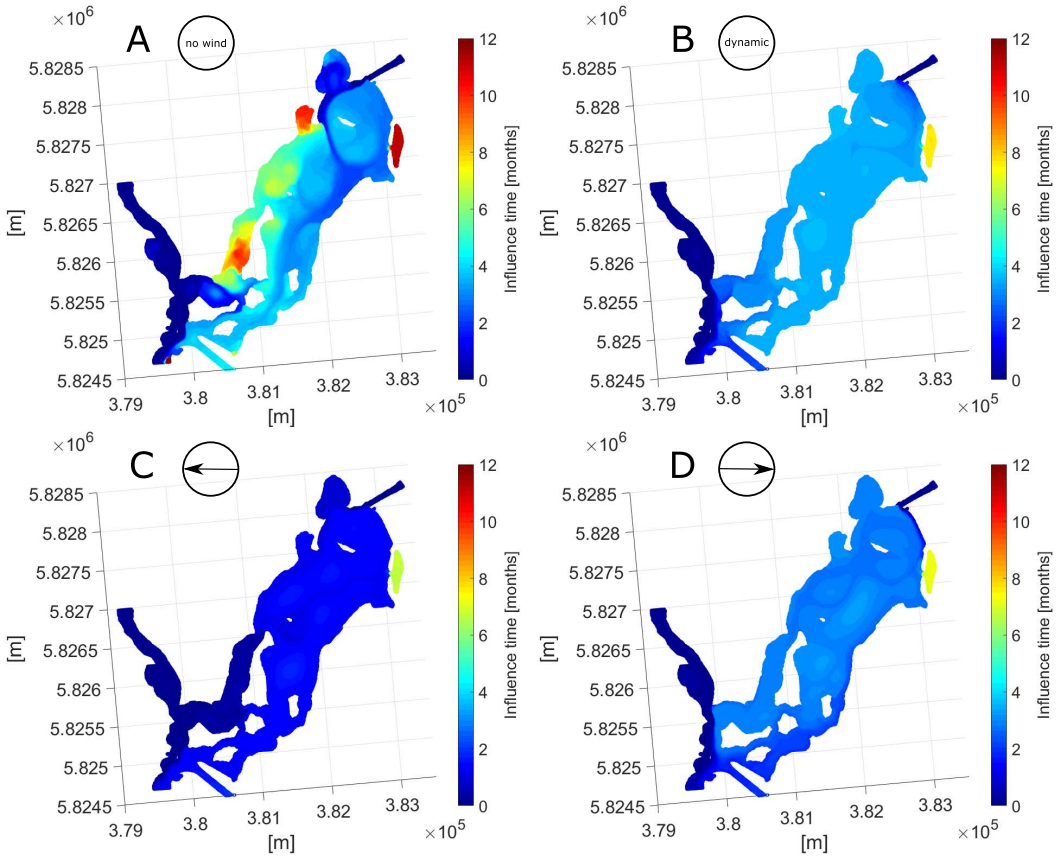

Figure 5.6: Calculated influence time distributions for Lake Tegel, the remnant function was integrated over one year, therefore integration times exceeding one year were not quantified. **a** no wind. **b** dynamic wind represented by the daily average wind speeds and directions from 2008-2014. **c** east-wind. **d** west-wind

5.4.4 Short-duration heavy rainfall scenarios

The flow over the main outflow boundary in the south-west was controlled by the discharge of the PEP with only a minor influence by the wind conditions (Fig. 5.8). During west-wind conditions, the "Southern" passage acted as an inflow and the "Northern" passage as an outflow and vice versa for east-wind conditions. When the short-duration heavy rainfall started, the respective inflows into the deep lake basin were reduced. Chl-a, phosphate, nitrate and dissolved oxygen concentrations were increasing during the "Overflow" scenario with higher values during west-wind conditions. Further, phosphate as well as dissolved oxygen concentrations had a peak and then declined. Here, dissolved oxygen had a peak at the same time as Chl-a concentrations, whereas phosphate declined after Chl-a had increased.

Using the broken-stick model, the first three components of the PCA were identified as being suitable for interpretation and explained together 89.3 % of the data's variance (Fig. 5.9). PC1 visualized the influence of the wind direction on the lake system. A positive PC1 was correlated with west-wind conditions and a river intrusion over the "Southern" and an outflow over the "Northern" passage. A negative PC1 was correlated with east-wind conditions and reversed flow patterns. Here, PC1 clearly separated the scenarios according to the wind direction and stated that the residence time was correlated to the inflow over the "Southern" segment (Fig. 5.9 A). PC2 visualized the intensity of inflow dynamics

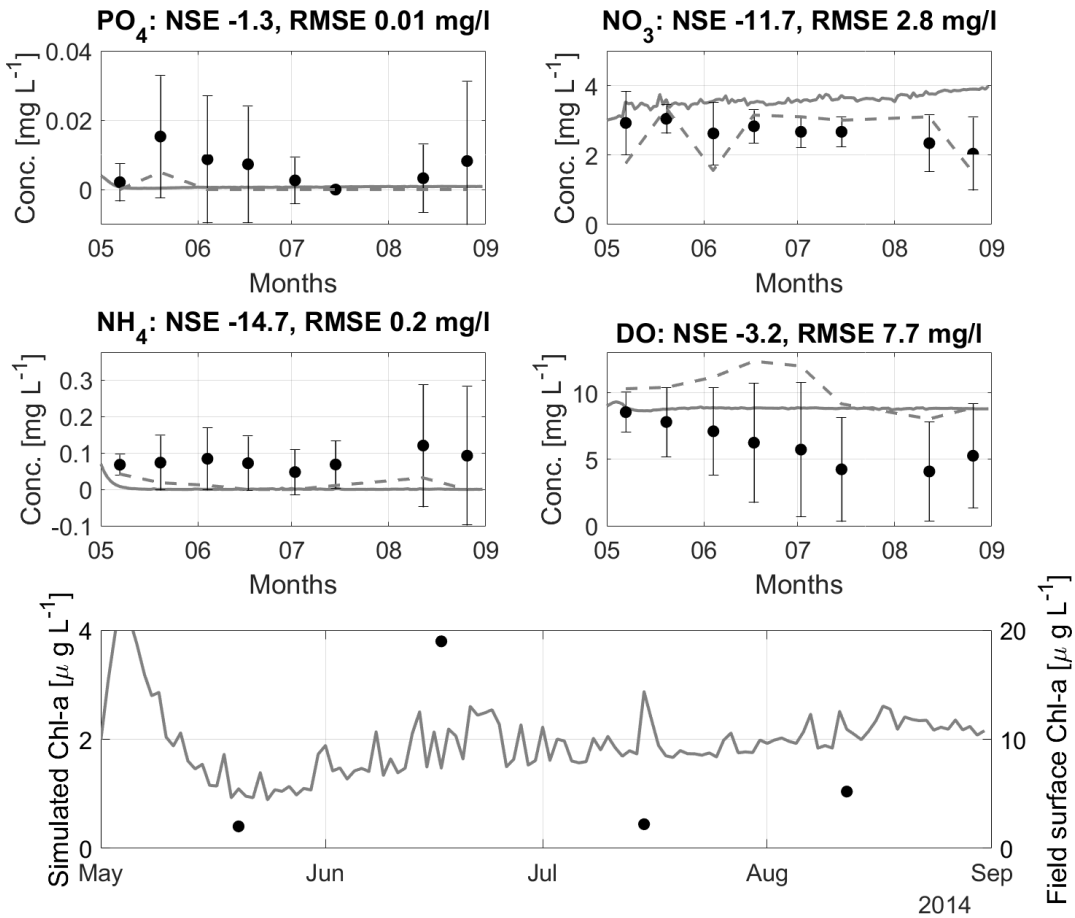

Figure 5.7: Comparison between simulated tracers (grey lines: PO_4, NO_3, NH_4, DO), the depth-averaged field concentrations (black dots) as well as their respective standard deviations (error bars) and the mean surface layer concentrations (dashed grey lines) at Lake Tegel's deepest site. The calibration criteria NSE as well as the RMSE refer to the fit between the simulated and the measured depth-averaged concentrations. Simulated Chl-a (grey line) is compared against the surface Chl-a concentrations measured at the deepest site (black dots)

against the lake hydraulic residence time. Here, a positive PC2 was correlated with inflows by the River Havel as well as the PEP, the main outflow and increased loadings of nutrients by the PEP and Havel. The hydraulic residence time and the inflow over the main outflow boundary, the "Southern" as well as the "Northern" segment were negatively correlated with PC2. Almost all scenarios, except latter stages of "Overcapacity", were positively correlated with PC2 (Fig. 5.9 A and C). PC2 also visualized that the lake hydraulic residence time was increasing with the respective inflows over the boundary segments into the lake basin (Fig. 5.9 C). Here, also the "Overflow" scenarios were correlated with Chl-a (Fig. 5.9 C). PC3 visualized the feedback mechanisms between phytoplankton biomass growth and the abundance of nutrients against the discharges and the outflow. A positive PC3 was correlated with Chl-a concentrations, phosphate loadings by the PEP and phosphate as well as nitrate concentrations in the main basin. On the other hand, a negative PC3 was correlated with the inflow rates of River Havel and PEP as well as the main outflow discharge. A positive PC3 identified scenarios favoring phytoplankton formation, which were both "Overflow" scenarios independent of the wind direction (Fig. 5.9 B and C).

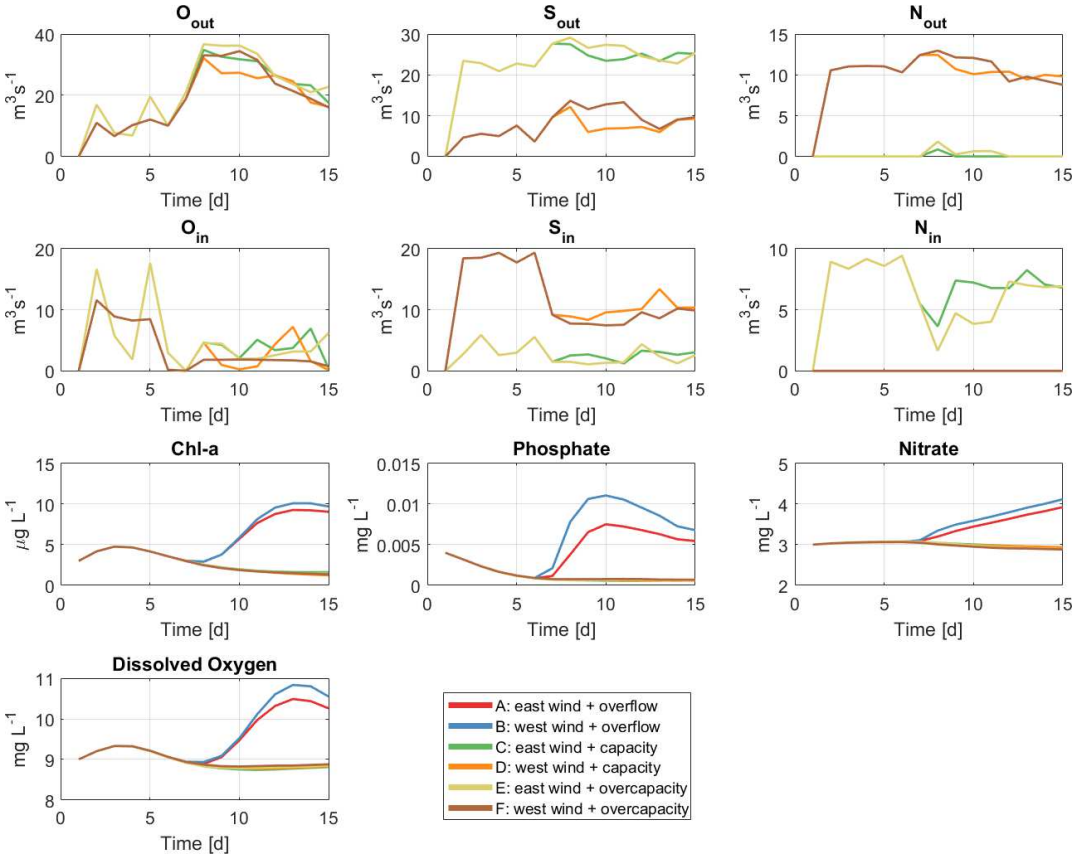

Figure 5.8: Time series of the short-duration heavy rainfall scenarios expressing temporal changes in flows at the "Outflow", "Southern" and "Northern" segments, as well as concentration changes in the main basin of Chl-a, phosphate, nitrate and dissolved oxygen

5.5 Discussion

5.5.1 Reliability of a depth-averaged model assumption for Lake Tegel

The calibration of the bottom roughness coefficient to fit a simulated tracer against measured chloride concentrations resulted in K_{Str}=42 $m^{1/3}/s$. The sediment in Lake Tegel consists mostly of mud (Ladwig et al., 2017). Therefore, high Strickler values for the bottom friction coefficient were expected to describe such cohesive material (Van, 2012). The calibrated bottom friction coefficient is in the same range as in a previous modeling study (Schimmelpfennig et al., 2012a), in which Nikuradse's law with a roughness length z_0=1 cm was used. Also, the modeling fit criteria NSE, RMSE and R^2 suggested that the calibration was as good as in previous modeling studies conducted at Lake Tegel. Schimmelpfennig et al. (2012a) achieved a NSE for the period from 1995-2010 of 0.48, which was similar to the NSE of 0.51 by Schauser and Chorus (2009) for the period 1986-1990. Our model's regression coefficient (Fig. 5.5 C) between observed and simulated data, $R^2 = 0.71$ (2000-2014), was also similar to the one by Schimmelpfennig et al. (2012a), $R^2 = 0.76$ (May to December 2009).

To our knowledge, this is one of the first published studies applying TELEMAC-2D's water quality module EUTRO to a field case with measured data. We modified the phytoplankton biomass function by neglecting light limitation and toxicity factors. On the one hand, surface phytoplankton blooms should be limited and inhibited by light, which is

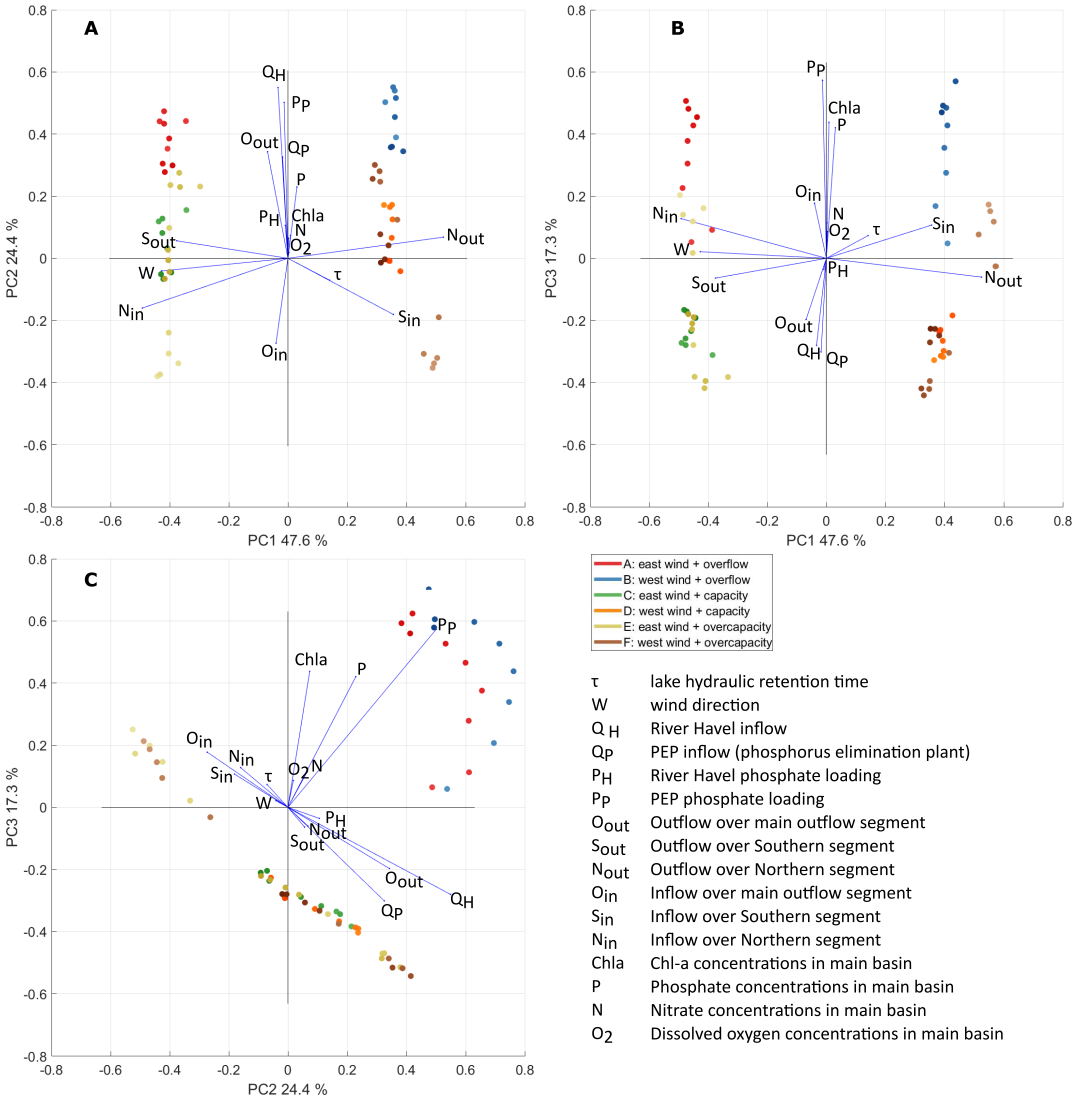

Figure 5.9: PCA model explaining 89.3 % of variance; colors of points refer to scenarios and the color intensity is decreasing with time. Abbreviations are explained in the figure. **a** PC1 against PC2. **b** PC1 against PC3. **c** PC2 against PC3

not considered in the Smith function. To better replicate phytoplankton blooms, especially diatom dynamics, alternative light functions should be implemented and checked. On the other hand, the formation of phytoplankton blooms depends primarily on the lake hydraulic residence time as well as external nutrient loadings and only secondarily on lake-specific factors like underwater light climate that shape the lake ecosystem's sensitivity towards the formation of phytoplankton blooms (Janssen et al., 2019). Therefore, we decided to neglect light limitation to focus on phytoplankton growth limited by nutrients, although short-duration heavy rainfall events should affect the underwater light climate by increasing water turbidity. The model was able to predict a phytoplankton biomass peak in the middle of June and a smaller peak in August similar to the field data. For water quality variables, the model was able to replicate the general dynamics of the field data. Here, the model replicated sufficiently the measured nutrient concentrations in the surface mixed layer, in which phosphate as well as nitrate were close to zero and nitrate as well as dissolved oxygen concentrations were nearly constant.

The simulated tracer dynamics were in a good agreement with the dynamics of the chloride concentrations measured at Lake Tegel, indicating the suitability of a depth-averaged 2D model to replicate the flow dynamics of the lake system and quantifying the horizontal distribution of substances. This assumption is based on neglecting thermal stratification and buoyancy effects in the water column. Compared to the PEP inflow and the lake water, the River Havel water is less dense and therefore limited to the surface mixed layer (Schimmelpfennig et al., 2012a). This layer also confines most nutrients and biogeochemical interactions, especially the formation of phytoplankton blooms. In addition with the short hydraulic residence time of Lake Tegel, which suggests a strong dominance by external factors, Lake Tegel can be idealized as a two-dimensional problem regarding contaminant and nutrient dynamics. Nonetheless, our depth-integrated 2D model could not replicate effects of the thermocline, acting as nutrient barrier, on the nutrient fluxes between surface mixed and bottom stagnant layer. Further, internal processes like diagenetic reactions or internal fluxes from the sediment into the water column were neglected. The latter ones were causing increased phosphate and ammonia fluxes into the bottom stagnant water layer during periods of oxygen depletion. To investigate thermal stratification and buoyancy effects in future research, a 3D numerical model solving the Navier-Stokes equation could be set up, while, to compute bottom layer biogeochemical interactions, a sophisticated sediment model needs to be added or implemented. Especially regarding internal fluxes, for instance phosphate cycling, the main processes were happening below the thermocline in the bottom stagnant layer. This is contrary to processes in the surface mixed layer, where phosphate was rapidly mineralized and transformed by bacteria and phytoplankton.

Although our model underestimated the impact of internal effects on the lake ecosystem and could have exaggerated the role of external processes, the computations of the hydraulic residence and the influence time distributions showed that Lake Tegel is dominantly controlled by external processes, which validated the mentioned model uncertainties by neglecting internal factors. The depth-averaged 2D model could sufficiently replicate the horizontal hydrodynamics of the surface mixed layer of Lake Tegel and needed less computational times compared to a 3D model, which benefited an extended calibration exercise running for 15 years with a time step of 30 seconds.

5.5.2 How to manage short-duration heavy rainfall events at Lake Tegel?

The influence time distribution of Lake Tegel was heavily depending on the wind speed and direction. Under east-wind conditions, enabling river-mixing, the influence times in the main basin were one-third of the influence times without wind and half of the times under west-wind conditions. During the usually prevailing west-wind conditions, substances can interact with the lake ecosystem for roughly 1 month, which was similar to the calculated hydraulic residence time (27.3 days). Compared to constant wind scenarios, the influences times under dynamic wind speed and direction were slightly higher. They ranged from 80 to 111 days in the main basin and were, therefore, in the same range as the previously stated residence times of 50 to 90 days (Kleeberg et al., 2012b). In order to evaluate the potential impact of contaminants and nutrients on the lake ecosystem, the influence time seems to be a sufficient local diagnostic proxy. The influence time distributions also suggested that although the River Havel can intensively mix with the lake water under east-wind conditions, the influence times were also the shortest, effectively limiting potential hazardous effects. Therefore, the impact of short-duration heavy rainfall events on the lake ecosystem could be shorter and spatially limited in dependence on the wind direction.

The short-duration heavy rainfall scenarios confirmed the results of a previous study (Schimmelpfennig et al., 2012a) that the river mixing dynamics within the main lake basin

are strongly depending on the wind direction. Under east-wind conditions, the River Havel was entraining over the "Northern" passage whereas under west-wind conditions, River Havel flowed into Lake Tegel over the "Southern" passage. Nonetheless, the "Southern" passage acts as the main outflow path from the lake basin, effectively including the discharges of the PEP. Under all wind scenarios, the inflows into the lake basin from the River Havel were reduced after the short-duration heavy rainfall event began and outflows were increased. The capacity of the PEP played a crucial role during the short-duration heavy rainfall event when nutrient loadings from the streams were overflowing the treatment plant. Then, phytoplankton blooms formed in the main lake basin due to increased concentrations of nitrate and short peaks of phosphate as well as dissolved oxygen. The PCA model confirmed our assumption that variance in the Lake Tegel system was dominantly governed by (1) the wind and mixing processes (external wind factor, PC1 with 47.6 %), the (2) respective inflow discharges and loadings (hydrodynamic factor, PC2 with 24.4 %) and (3) the formation of phytoplankton in dependence of nutrients (ecological factor, PC3 with 17.3 %). Phytoplankton biomass was positively correlated to the hydraulic residence time, signaling that a reduction of the residence time by artificially increasing boundary inflows could be a potential management strategy to control phytoplankton blooms. Additionally, the abundance of nutrients as well as phytoplankton biomass in the main basin were mainly correlated to the nutrient loadings of the PEP instead of the River Havel. In our simulations, phytoplankton biomass was originating from the River Havel inflow, but could establish high biomass concentrations in the main basin due to the abundance of nutrients entraining from the PEP. In conclusion we can state that, although phytoplankton biomass was originating from the River Havel and the mixing was controlled by the wind and the respective discharges, the main factor controlling the formation of blooms were the nutrient loadings from the PEP. This was contrary to our previously stated hypothesis that wind-induced river mixing events are the main source for nutrients and, therefore, for the formation of phytoplankton blooms. When the PEP was theoretically upgraded to eliminate also the nutrients from the additional loadings, the phytoplankton concentrations in the main basin were vastly reduced, but still slightly higher during east-wind conditions when the River Havel waters had a shorter intrusion pathway to mix directly into the lake basin. Increasing the discharges of the PEP only had a minor effect on the formation of phytoplankton blooms. Therefore, increasing the capacity of the PEP to withhold and treat additional water volumes during short-duration heavy rainfall events seems to be the best management strategy to mitigate the formation of phytoplankton blooms after future short-duration heavy rainfall events.

5.6 Conclusions

Water exchange times are important diagnostic estimators for the impact of tracers, contaminants and nutrients on the lake ecosystem. Especially under extreme external events, for instance a short-duration heavy rainfall event, a valid management strategy could consist in reducing the hydraulic residence and influence time, therefore increasing flushing. A depth-averaged 2D hydrodynamic model with water quality formulations was set up to the heavily managed Lake Tegel and was calibrated using a time series of 15 years to investigate the formation of phytoplankton blooms after short-duration heavy rainfall events. The calibration proved to be sufficient to replicate the hydrodynamics as well as the biogeochemical dynamics of the lake system. By computing the influence times in dependence of the wind, we showed that during east-wind conditions the influence times were the shortest and during no wind conditions the longest. Therefore, although river-mixing was intensi-

fied during east-wind conditions, the impact of potential substances on the lake ecosystem was the shortest. Under the prevailing west-wind and under dynamic wind conditions, the main basin had an influence time between 2 to 3 months. A PCA visualized that the Lake Tegel system is mainly influenced by the wind dynamics, the inflows and, at long last, by biogeochemical reactions. Therefore, the lake system is being dominantly controlled by external factors. Eventually, a valid management strategy to mitigate the formation of phytoplankton blooms after short-duration heavy rainfall events could be to eliminate external nutrient loadings as well as to increase inflow discharges, for instance by using a lake pipeline to bypass additional water masses. Although the latter option seems less efficient than a preferred external nutrient elimination that also avoids overflows.

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Appendix

In the EUTRO water quality module, dynamics of phytoplankton (PHY), dissolved mineral phosphate (PO_4), degradable phosphate (POR), dissolved mineral nitrate (NO_3), degradable nitrate (NOR), ammonia (NH_4), organic loadings (L) and dissolved oxygen (O_2) are simulated as tracers that are governed by advection and turbulent diffusion (see Eq. 5.3) (Hervouet and Ata, 2017a,b). The reactive component of each tracer and the tracer interactions are taken into account through the sink/source F, on the right hand side of Eq. 5.3:

$$F_{PHY} = (CP - DP) * [PHY] \tag{5.8}$$

where CP is the phytoplankton growth rate; and DP is the phytoplankton disappearance rate.

$$CP = c_{max} * g_1 * \mu(lim(Phosphate, Nitrate)) \tag{5.9}$$

in which the modified growth rate is described and where c_{max} is the maximum growth rate; g_1 is the growth in dependence of temperature = $\frac{T}{20}$, where T is the depth-integrated water temperature; and $\mu(lim(Phosphate, Nitrate))$ is the growth limited by the availability of either phosphate, PO_4, or the sum of nitrate, NO_3, and ammonium, NH_4.

$$\mu(lim(Phosphate, Nitrate)) = min(\frac{[PO_4]}{KP + [PO_4]}, \frac{[NO_3] + [NH_4]}{KN + [NO_3] + [NH_4]}) \tag{5.10}$$

where KP is the half-saturation constant of phosphate; and KN is the half-saturation constant of nitrate.

$$DP = (RP + (M_1 + M_2 * [PHY])) * g_2 \tag{5.11}$$

where RP is the phytoplankton respiration rate; M_1 and M_2 are mortality coefficients; and and g_2 is the temperature effect on phytoplankton disappearance = $(1.050)^{T-20}$.

$$F_{PO_4} = fp * (dtp * DP - CP) * [PHY] + k_{320} * g_2 * [POR] \tag{5.12}$$

where fp is the phosphorus content per phytoplankton biomass; dtp is the phosphorus percentage that is assimilable in dead phytoplankton; and k_{320} is the mineralisation rate from POR to PO_4 at 20 °C.

$$F_{POR} = [fp * (1 - dtp) * DP] * [PHY] - k_{320} * g_2 * [POR] - \frac{B_{POR}}{h} \tag{5.13}$$

where B_{POR} is the phosphorus sediment flux; and h is the water depth.

$$F_{NO_3} = -fn * (1 - Rn) * CP * [PHY] + k_{520} * g_2 * [NH4] \tag{5.14}$$

where fn is the nitrogen content per phytoplankton biomass; Rn is the proportion of nitrogen assimilated in ammonium = $\frac{[NH_4]}{[NH_4]+[NO_3]}$; and k_{520} is the nitrification rate at 20 °C.

$$F_{NOR} = [fn * (1 - dtn) * DP] * [PHY] - k_{620} * g_2 * [NOR] - \frac{B_{NOR}}{h} \tag{5.15}$$

where dtn is the nitrogen percentage that is assimilable in dead phytoplankton; k_{620} is the mineralisation rate from NOR to NO_3 at 20 °C; and B_{NOR} is the nitrogen sediment flux.

$$F_{NH_4} = [fn * (dtn * DP - Rn * CP)] * [PHY] + k_{620} * g_2 * [NOR] - k_{520} * g_2 * [NH_4] \tag{5.16}$$

$$F_L = f * (M_1 + M_2 * [PHY]) * [PHY] - k_{120} * g_3 * [L] - \frac{B_{LOR}}{h} \tag{5.17}$$

where f is the photosynthetic produced oxygen content; k_{120} is the degradation rate of organic load at 20 °C; g_3 is the temperature effect on degradation of organic loadings = $(1.047)^{T-20}$; and B_{LOR} is the sediment flux.

$$F_{O_2} = [f * (CP - RP)] * [PHY] - k_{520} * g_2 * [NH_4] - k_{120} * g_3 * [L] + k_2 * g_4 * (Cs - [O_2]) - \frac{BEN}{h} \tag{5.18}$$

where k_2 is the gas-exchange coefficient between water and atmosphere at 20 °C; g_4 is the temperature effect on reaeration = $(1.025)^{T-20}$; Cs is the oxygen saturation concentration; and BEN is the benthic oxygen demand.

Chapter 6

Synthesis

6.1 Conclusions

Small and shallow urban freshwater lakes are widespread ecosystems that shape our urban heat climate, influence recreational activities as well as provide services for the ecosystem, drinking water production and sanitation. These systems are strongly influenced by the urban catchment and water management system. In combination with global stressors (most profoundly climate change) and increasing urbanization (hence, increased usage pressure resulting in morphological degradation and water quality deterioration), these compound pressures can impact and alter urban lakes severely. Therefore, in this thesis a holistic approach consisting of a paleolimnological evaluation, a monitoring survey and two numerical modeling studies provided insights and recommendations on how to optimize the urban lake management for Lake Tegel, Berlin. This lake is a prominent representative of an urban freshwater lake dominated by a complex management system and can be used as case study for lake managers worldwide. The lake system already experiences a wide variety of management challenges and management applications:

- management challenges: legacy heavy metal contamination in the sediment, eutrophication threat, harmful cyanobacteria blooms, emerging micropollutants, microplastics, complex hydrodynamics, reduced inflow discharges, invasive species, morphological degradation
- management measures: elimination plant, lake pipeline to maintain minimum discharge and to modify hydraulic residence time, hypolimnetic aerators, bank filtration

The successful shift of Lake Tegel's water quality from eutrophic to a state with low nutrient concentrations was intensively reported in former studies, whereas changes in the spatial and vertical sediment composition were neglected. Especially due to recent insights into the interplay of wind-induced river mixing events and the lake water quality, the sediment composition of Lake Tegel was hypothesized to be quite heterogeneous. Also former studies did not include numerical formulations for water quality and ecological processes, which are crucial to set up management recommendations. The impact of climate change on urban lakes was also not intensively studied in the recent literature. Providing new observations about the heterogeneity of the sediment composition, stratification stability, the entrainment dynamics of the phosphorus elimination plant (PEP) and two climate- and stakeholder-oriented evaluations of management scenarios for Lake Tegel, this thesis filled research gaps and deepened limnological knowledge for a complex urban lake ecosystem.

Here, the main outcomes regarding the impact of past, present and potential future management measures on the lake ecosystem are listed and summarized:

Past management measures and sediment stratigraphy

- Ten sediment cores were taken and analyzed using X-ray fluorescence spectroscopy (XRF): six from Lake Tegel, three from Lake Großer Wannsee (urban lake in Berlin) and one from Lake Userin (natural lake in Mecklenburg Western Pomerania). XRF data were normalized by coherent scatter. For statistical analysis, data were logarithmically transformed and scaled to a mean of zero with a standard deviation of one. The data set was analyzed using principal component analysis (PCA), k-means clustering and self-organizing maps (SOM) to undertake an exploratory survey of the sediment composition.
- Lake Tegel's sediment is characterized by mud and sapropel-like material. A clear shift within the cores from a denser material with a brownish color to a less-dense black material can be visualized, probably indicating past eutrophication.
- The first two principal components of the PCA captured 62 % and allowed the determination of five different clusters. The bivariate space was fragmented into axes correlated either to the abundance of heavy metals or to lithogenic elements (the geological background). Most sites in the main basin depict a vertical dispersion over depth (change of abundance of lithogenic elements), whereas sites close to inflow show horizontal dispersion (change of abundance of heavy metals).
- The vertical development of nearly every site experienced a sharp U-turn during the beginning of the past heavy metal contamination/eutrophication period. In recent layers, all sites show a tendency towards a composition with low abundance of heavy metals and high abundance of lithogenic elements. The clusters differ from each other regarding their respective organic carbon content, Fe/Mn ratio, abundance of heavy metals and lithogenic elements. Most sites show a similar vertical pattern. A high organic carbon content and low amounts of heavy metals appear in deep layers. Then in intermediate layers, the abundance of heavy metals as well as lithogenic elements is increased, subsequently with occurring reducing redox conditions. The heavy metal abundance stays high but redox conditions are recovering. In recent layers, the abundance of heavy metals is low and the sediment is characterized by lithogenic elements.
- Using the SOM methodology, similarities between recent sediments of Lake Userin and Lake Tegel regarding their sediment composition were visualized. Further, the River Havel in contrast to the PEP seems to be the source of heavy metals entering Lake Tegel. Especially Lake Großer Wannsee's sediments are heterogeneous with strong variations from north to south.
- The management measures applied at Lake Tegel were successful in reducing heavy metal abundances in the sediment. Still, the vertical composition of the sediment sites differ strongly from each other. These heterogeneities are probably caused by the heavily modifying water management measures.
- The combined approach of using rapid XRF scanning technique with exploratory multivariate statistical methods was successful in investigating similarities and differences between the sediment composition of different sites.
- A calibrated depth-averaged 2D model coupled to a water quality module was able to verify Lake Tegel's heterogeneity in dependence of wind stress and inflow dynamics by computing the influence time distributions. Due to Lake Tegel's complex morphometry (large shallow area, narrow passages between islands, deep basin in the

north-east) loadings from different sources can be retained longer in certain parts of the lake basin in dependence of the aforementioned wind stress and inflow dynamics. The latter is also heavily influenced by the water management system.

- Modeling studies using a vertical 1D and a depth-averaged 2D setup, respectively, had shortcomings regarding the simulation of physical as well as water quality parameters in the bottom stagnant layer. The main reason for these shortcomings were the simple representation of sediment processes, for instance fluxes and redox reactions. In the 1D simulations, sediment processes were mostly dependent on water temperature and the availability of oxygen. In the depth-averaged 2D cases, the sediment was a permanent sink and fluxes from the sediment into the water column were neglected.

Impact of management on thermal stratification

- A CTO (electrical conductivity by HOBO U24-001, water temperature by Tinytag Aquatic 2, dissolved oxygen by $miniDO_2T$) logger chain was deployed at Lake Tegel's deepest site at July 27 2017. Seven logger internally stored data every 30 minutes. Electrical conductivity was calibrated by internal factory setting.
- Water temperature data visualized the offset of the summer stratification period 2017 as well as the onset and offset of the winter period of 2017/2018, which was characterized as discontinuous with minor stratification events. Further, the spring turnover event 2018 was short, only lasting about half a month in April 2018.
- Water temperatures measured in August 2017 were used to calculate the integrated heat budget of Lake Tegel, which was then used to calculate the power spectral density. Vertical seiches in the periods 12 and 8 h were detected. The former period is probably connected to day and night cycles.
- During the winter period of 2017/2018, sporadic peaks of electrical conductivity in combination with temperature increases and dissolved oxygen decreases were detected. These peaks could be connected to the PEP indicating the formation of a density current originating from the PEP during the winter period. These denser water masses entrain close to the bottom layer. Measured temperature data of the PEP as well as theoretical calculations affirmed the existence of the PEP density current, which can affect the oxygen budget of the hypolimnion during winter.
- A vertical 1D model was able to replicate the thermal structure of Lake Tegel for the time period 2008-2014 with NSE's (Nash-Sutcliffe coefficient of efficiency, a fit of 1 represents perfect agreement between field and simulated data) between 0.83 and 0.9. The additional data gathered by the CTO logger chain will provide better process understanding and can act as a basis for future modeling studies, e.g. serving as extended calibration data set.
- Changing the variables of the vertical 1D model caused a higher model outcome sensitivity towards simulated bottom water temperatures compared to surface water temperatures. A cause for this could be the numerical modeling of heat fluxes over the thermocline. Recent numerical improvements for vertical and deep mixing have been described in Yeates and Imberger (2003) and Gaudard et al. (2017), which could be implemented in future simulations.

- Using the calibrated vertical 1D model to simulate the annual temperature dynamics from 2008-2014 revealed that Lake Tegel could be characterized as monomictic due to only weakly stratified winter periods.

Adaptive management and climate change

- Checking two criteria, ratio of internal Rossby radio to lake width and Lake Number, it was confirmed that a vertical 1D model was applicable for Lake Tegel despite the lake's dendritic morphometry. The Morris method was used to identify global sensitive model parameters. Further, the automatic evolutionary optimization algorithm CMA-ES (Covariance Matrix Adaption Evolution Strategy: 500 iterations with a population size of 10) was coupled to the formulated GLM-AED2 water quality model (vertical 1D model) for calibrating hydrodynamic variables to improve the fit between simulated and measured water temperatures from 2008-2012. Fits were quantified by RMSE (root-mean-square error) and NSE. For validation, the years 2012-2014 were used. Biogeochemical variables were manually calibrated fitting simulated against measured concentrations of dissolved oxygen, phosphate and nitrate.

- Several alternative management scenarios were coupled with projected future meteorological data (WETTREG2010, follows A1B scenario) to quantify the impact of climate change and management alterations on surface water temperatures, stratification stability as well as onset and offset, thermocline depths, Wedderburn number, buoyancy frequency, and critical periods of dissolved oxygen concentrations as well as phosphate. The individual years 2020, 2040, 2060, 2080 and 2100 were analyzed.

- The highest sensitivity was attributed to a wind factor, latent heat transfer and sensible heat transfer. The sensitivity analysis illustrated the importance of atmosphere-surface water layer interactions. Also, the respective inflow factors were strongly influencing the model outcome.

- The GLM-AED2 model successfully replicated water temperatures (NSE about 0.9) of Lake Tegel and the general seasonal patterns of nitrate and phosphate. Also, dissolved oxygen dynamics were captured by the model (NSE about 0.6).

- Climate change is going to cause a prolongation of future summer stratification periods and an increase of surface water temperatures. Lake Tegel can shift from dimictic to monomictic.

- When deactivating the PEP, the stratification strength was high and stable (buoyancy frequency, N^2, over $1 \times 10^{-2}\,\mathrm{s}^{-2}$) potentially benefiting the formation of future cyanobacteria blooms. Also, a potential positive feedback between increased nutrient loadings by river discharges, phytoplankton growth, higher turbidity and water temperatures was detected when deactivating any PEP discharges. When activating the PEP, these additional discharges acted as buffer to nutrient-rich river inflows and caused a weaker summer stratification period.

- Using a time series of 15 years of chloride concentrations measured at Lake Tegel's deepest site, a depth-averaged 2D hydrodynamic model was calibrated with the bottom roughness coefficient. The TELEMAC-2D model applied the k-ε turbulence model as well as the mass-conservative edge by edge implementation of the N distributive scheme for computing advection of velocities and tracers. The best fit was achieved by using a Strickler coefficient of K_{str} =42 $\mathrm{m}^{1/3}/\mathrm{s}$ with a NSE of 0.49, a RMSE of

$1.17\,\mathrm{g\,m^{-3}}$, and a R^2 (coefficient of determination) of 0.71. Further, this hydrodynamic model was coupled with a water quality module, which was validated using time series data from May to August 2014. The water quality module was suitable in replicating the measured surface concentrations of phosphate, dissolved oxygen, nitrate and ammonia. However, the simulation of phytoplankton biomass had several shortcomings due to a lack of vertical field data. Nonetheless, the model could qualitatively replicate the general patterns of phytoplankton biomass dynamics.

- By computing the influence time distribution, the impact of contaminants and nutrients on the lake ecosystem over time were evaluated in dependence of different wind scenarios. Here the longest mean influence time was achieved under no wind- (97 days), followed by dynamic wind- (89 days), west-wind- (74 days) and east-wind-conditions (33 days). Although the River Havel entrained heavily into Lake Tegel's deep basin under east-wind conditions, the influence times were the shortest.
- Finally, several short-duration heavy rainfall scenarios with different discharges of the PEP ("Overflow" referring to the short-duration heavy rainfall event that happened in summer 2017, "Capacity" referring to a scenario in which the PEP can treat all inflows, and "Overcapacity" referring to a scenario in which the PEP can treat all inflows and increases its discharges) and two wind scenarios (east- or west-wind) were evaluated using PCA. The PCA identified three main dominant forces affecting Lake Tegel: (1) wind dynamics (PC1 with 47.6 %), (2) inflow dynamics (PC2 with 24.4 %) and (3) ecological reactions (PC3 with 17.3 %).
- To avoid the formation of phytoplankton blooms after short-duration heavy rainfall events, it is crucial to eliminate external nutrient loadings, which were overflowing into the lake by increasing the PEP's treatment capacity.

In general, an adaptive urban lake management has the potential to mitigate the impact of future stressors on the lake ecosystem and, therefore, can be a very positive factor. These measures are affecting crucial lake characteristics like the hydraulic retention time, thermal stratification, sediment composition and nutrient loadings. Due to severe morphological degradation and urbanization pressure, urban lakes can depend on an active management system similar to a "life-support" system. In this case, a shutdown of management measures can result in a severe trophic shift of the lake ecosystem.

6.2 Recommendations for urban lake management

The following recommendations for the management of Lake Tegel as well as other urban lakes can be concluded from the presented studies:

- The survey and rapid analysis as well as statistical evaluation of Lake Tegel's sediments revealed that the standard probing of only the deepest site in a lake has several shortcomings when making interpretations for the whole lake system. Lake Tegel's sediments are vertically and spatially heterogeneous reflecting the complex hydrodynamics and effects of past management measures. Even locally close sediment cores differed in their vertical abundances of elements. The exploratory statistical methods were successful in clustering the data according to flow dynamics as well as past management measures. These exploratory approaches can be used for future sediment surveys using big data obtained by XRF. This concludes that big sediment data sets should be used in future paleolimnological studies to make elaborate evaluations of the lake sediment composition at different sites.

- Due to its short hydraulic retention time, Lake Tegel is heavily influenced by its inflows. Therefore, the management strategy of effectively eliminating the nutrient loadings from the urban catchment (Nordgraben as well as Tegeler Fließ) proved to be effective in restoring the lake system. This also shifted the recent sediment towards higher abundances of lithogenic elements instead of heavy metals. These drastic and advanced management measures (construction of wastewater treatment plant, PEP and lake pipeline) were expensive during construction (approx. 102 Mio. Euro (Heinzmann and Chorus, 1994)) and operation (costs up to 9 Cent per treated m^3 in the PEP), but for such lake systems, which are heavily influenced by inflows, there are no plausible alternatives. An elimination of external loadings caused a return of sediment and water column quality to a former good state, probably also preventing future internal contaminant fluxes.

- Further, increasing discharges, for instance by constructing a lake pipeline, enhances outflow dynamics and therefore can disturb the formation of phytoplankton blooms. For lake systems with multiple inflows, such increased discharges by one inflow (with low nutrient concentrations) can act as a barrier. During times of climate change, such adaptive management systems can weaken the stratification stability during summer and mitigate the potential formation of toxic cyanobacteria blooms. Lake managers could use semi-closed systems to bypass water masses with relatively low nutrient concentrations (compared to the average lake concentrations) to artificially increase inflow discharges. For lakes that are also used for crucial services (e.g. drinking water production), these bypass systems could also be used to bypass otherwise complicated discharges (e.g. waters with high nutrient concentrations due to sewer overflow or short-duration rain events) around the lake. Especially for urban lake management systems that have to act on a short time scale, such bypass systems could keep a lake in a sustainable state. Nonetheless, the increase of external flows proved to be a less efficient management measure to mitigate the formation of phytoplankton blooms than the elimination of external nutrient loadings into Lake Tegel.

- Due to the emergence of micropollutants at Lake Tegel, the discharges of the upstream wastewater treatment plant into the lake were reduced by roughly 30 %. These reduced discharges could restrict future applications of the PEP to mitigate the impact of climate change on lake stratification. A solution could be to run the lake pipeline on full capacity or to build a parallel line, which was also suggested by Schimmelpfennig et al. (2012b). These measures could help to run the PEP on a higher capacity (to compensate for reduced discharges from the WWTP) and to further decrease the lake hydraulic retention time.

- Numerical lake models should account for the lake characteristics and the specific management applications. Even when simulating lakes with complex hydrodynamics, the application of a 3D model with a fine spatial resolution would not benefit the stakeholder if computational times approach management operational times. On the contrary, applying a simple model but considering the limitations can support lake management strategies. The vertical 1D model for Lake Tegel was intensively calibrated and validated. This was due to the model having very low computational times making it a perfect candidate for applying automatic calibration algorithms, which need to run iteratively for long times. Such simpler models can also be easily analyzed regarding model sensitivity (e.g. by Morris method, Bayes analysis, linear regression or SOM). The advantage of multidimensional models is their fundamental formulation of physical processes making these model results more genuine even

when an intensive calibration is not possible. Here, even for complex and stratified lake systems, the application of a depth-averaged 2D hydrodynamic model proved to be sufficient to investigate contaminant mixing patterns and the dynamics of the surface mixed layers. All investigated lake models could be easily configured to replicate hydrodynamic processes (water mass balance, water temperature as non-reactive tracer), whereas the calibration of ecological and water quality processes was more troublesome. This was mostly due to different formulations of ecological and water quality processes, as well as a lack of field data. Also the implementation of sediment processes is crucial. Most sediment interactions were either too simple or too complex. Especially the formulation of a sufficient diagenetic model that includes the most important local biogeochemical sediment reactions would be a challenging but important task. Future managers should focus more on getting vast field data for calibration. Nevertheless, all investigated models are open-source and can be modified by the user, making them excellent choices for creating specifically tailored model systems for complex urban lake systems. Here, recent advancements in machine learning could also help to improve water quality simulations for specific study sites.

- Climate change will have a profound impact on lakes by warming them faster than the trend in global air temperatures (O'Reilly et al., 2015). Most likely, future thermal stratification periods will be longer with an earlier onset (Kirillin, 2010, Hambright et al., 1994). The stable stratification in combination with increased surface mixed layer water temperatures will benefit the formation of cyanobacteria blooms (Paerl, 2014). Also future changes in atmospheric patterns will affect local wind fields, which are the profound kinetic energy sources for mixing dynamics in surface mixed layers (van Ulden and van Oldenborgh, 2006). These future external changes can affect lake ecosystems in diverse ways. For instance, Lepori et al. (2018) showed that despite an Alpine lake experiencing a reduction of phosphorus concentrations, water temperature warmings caused phytoplankton blooms. Also, short-duration heavy rainfall events can become more frequent and intense in the future. Lake managers should employ more frequent field samplings and, in the best case, on-line monitoring systems to have a shorter reaction time during unconventional ecological shifts (e.g. Fastner et al. (2018)). It is also important to think about alternative management measures to artificially destabilize the water column, for instance by artificial mixing techniques, to prevent the formation of cyanobacteria blooms. Alternatively, a reduction of the hydraulic residence time in urban lake systems could also hinder excessive phytoplankton growth periods. Nonetheless, the most important management measure seems to be the aforementioned control of external nutrient loadings into the lake.

In a final conclusion, urban lakes need a flexible management system with frequent and spatially diverse monitoring studies as well as the application of numerical modeling for the adaption of existing management measures to keep the lake system in a sustainable state. The models should account for the specific lake characteristics and applications (vertical 1D for long-term impact studies, multidimensional models for horizontal and lateral problems). Urban lake management plays a crucial role in shaping the future structure and resilience of the respective lake ecosystem.

6.3 Outlook

Future research should explicitly investigate urban lakes and their specific interactions between technical and natural interfaces. In the following paragraph, ideas for such future

research routes are addressed.

- The Research Training Group "Urban Water Interfaces" is an on-going project to promote interdisciplinary research between engineers and natural scientists regarding the urban water cycle. The results of this thesis are the basis for studies regarding the common topic group 'Interfaces in urban freshwater ecosystems' and should support the formulation of future hypotheses. Collaboration with other research networks like the Forschungskolleg "FUTURE WATER" or the "Global Lake Ecological Observatory Network" (GLEON) should enable scientists to tackle new research questions especially regarding the impact of water management and climate change on urban lakes.

- The spatial heterogeneity of urban lake sediments for the sophisticated evaluation of paleolimnological studies should be further investigated. An extended campaign can be conducted by taking additional sediment cores in different Berlin lakes and natural references and analyzing them using XRF. To get a representation of Berlin lakes, one can sample Lake Müggelsee, Lake Tegel, Lake Großer Wannsee, Lake Weißer See and Lake Schlachtensee, and for reference lakes, Lake Userin (River Havel), Reservoir Spremberg and Lake Bärwalder (River Spree). Taking at least a core at the deepest site, a core close to the inflows as well as an additional core in the main basin should enable the following multivariate analysis to distinguish between different clusters caused by either the urban or the agricultural catchment (assuming that no lake system is unaffected by anthropogenic stressors). For the statistical analysis, the presented (Ladwig et al., 2017) as well as additional methods (e.g. Positive Matrix Factorization) should be applied. An interesting approach could be to first conduct a PCA and subsequently a SOM, so to cluster the multidimensional PCA results on a two-dimensional grid. This sediment study can help in filling knowledge gaps about the spatial and vertical sediment contamination of urban lakes. By extending such a study to also include sediment cores from urban ponds, a holistic picture of the sediment composition of urban freshwater systems could be formulated. Further, these new insights could be used for the formulation of a sediment diagenesis model for urban lakes with a focus on certain substances, for instance phosphorus. Especially field data about reaction and exchange rates between the sediment and the water column are needed. Such a sediment diagenesis model should establish new insights, for instance the relationship between bottom dissolved oxygen concentrations and internal phosphate fluxes (Hupfer and Lewandowski, 2008), to improve the mechanistic understanding of sediment biogeochemical reactions.

- To improve our understanding of the hydrodynamics happening in urban lake systems, especially Lake Tegel, and to gather present data for a future evaluation of potential climate change effects, it is advisable to deploy additional monitoring buoys at different positions in urban lakes. This is especially important for the determination of seiches. At Lake Tegel, a monitoring buoy close to the PEP inflow could improve our understanding of the density current entrainment dynamics. This can be important for the management of the bottom layer oxygen dynamics and therefore for the lake ecosystem. Further, the monitoring data can be used for numerical model calibration and training of machine learning algorithms. Upgrading the monitoring equipment to allow for remote data transmission could also enable real-time monitoring of Lake Tegel, which could be used for short-term forecasts similar to flash floods forecasts.

- Satellite imaging is a powerful technique to get additional long-term and up-to-date data for lake studies, e.g. water level fluctuations or cyanobacteria blooms (Crétaux

and Birkett, 2006, Wynne et al., 2010). Satellite data (Landsat, MODIS, Sentinel) can be calibrated by in-situ measurements to improve the explanatory power. Achieving solid calibration techniques (in most cases linear regressions between satellite and field data) would be a powerful tool for future freshwater studies in Berlin, enabling stakeholders to rapidly evaluate satellite data. Limitations of this approach are meteorological conditions (clouds) and the spatial resolution of the satellite image.

- The presented calibration strategy from Ladwig et al. (2018) in combination with new in-situ data obtained by the monitoring campaign (see Chapter 3) should enable the setup of an advanced GLM-AED2+ model for Lake Tegel. The main limitation for applying a vertical 1D model lies then in the temporal resolution of the meteorological data, which should be tackled by downscaling or interpolation. Then a vertical 1D model could be run for Lake Tegel on a subdaily time step. In combination with the gathering of further sediment data, AED2+ can be configured to run diagenetic processes. Especially the high frequency vertical water temperature data (every 30 min) acquired by the monitoring campaign will support the calibration process. The recent GLM version 3.0 BETA also allows the computation of wind-sheltering and sediment heat fluxes (new features are explained in Hipsey et al. (2017)). Due to GLM-AED2+'s rapid computational times, one could couple a server with an on-line monitoring buoy to establish short-term forecasts of vertical water temperatures and nutrient compositions at Lake Tegel, similar to flash floods forecasts. Such a project can also be improved by citizen science approaches, e.g. constructing and maintaining local weather stations or analyzing water samples.

- The depth-averaged 2D model could be used to explore the movements of floating water moss at Lake Tegel. These moss are associated with high amounts of potentially toxic *Tychonema sp.*, which have caused neurotoxicosis in dogs in 2017 at Lake Tegel (Fastner et al., 2018). Such a model could support the development of maps visualizing zones of increased probability of water moss coming close to the shore lines in dependence of external factors, e.g. wind, flow dynamics.

- After having set up a finite element mesh and having calibrated the hydrodynamics for depth-averaged two-dimensional flows and tracer kinetics using TELEMAC-2D, the next logical step would be to augment the model by explicitly considering the vertical dimension. A 3D model was also tested during this PhD research using TELEMAC-3D. Here, the measured high frequency water temperature data obtained by the monitoring campaign (see Chapter 3) can be used for calibration (water temperature dynamics simulated as non-reactive tracer with atmosphere-water interactions). With such a 3D lake model, thermal stratification and ecological interactions could be intensively investigated. Of course, 3D models need more computational time and calibration. Such models could be applied to investigate the entrainment dynamics of the PEP as well as the River Havel inflow. Therefore, the proposed density current from the PEP (see Chapter 3) as well as the theoretical periods of seiches could be checked by using a 3D model.

- For a more robust simulation of urban lakes, one can apply multiple autonomously developed lake models to the same ecosystem, for instance Lake Tegel. This method is called ensemble modeling. Trolle et al. (2014) applied three lake ecosystem models to a Danish lake and achieved superior results compared to the application of a single model. Especially for complex freshwater systems like urban lakes, a robust and critical methodology is important. This methodology should consist of a thorough

sensitivity analysis, a split-sample calibration (calibration and validation) preferably with an automatic algorithm and a prediction of model results with uncertainties. The latter can be improved by using multiple models especially for the representation of ecological processes. For future Lake Tegel simulations, the combined application could consist of PCLake, GLM-AED2+ and DYRESM-CAEDYM.

- For the holistic evaluation of urban lake management scenarios for Lake Tegel, the formulation of a catchment model is advisable. Here, the lake model should be coupled to the essential natural and technical components: natural and urban runoff, natural and urban evapotranspiration, rivers, wastewater treatment and drinking water supply plants, soil infiltration and groundwater. Such a coupled interface model can be used for applications concerning 'Integrated Water Resources Management' (IWRM) for an urban catchment. Also, open questions regarding climate change and ecosystem services can only be approached by using such a coupled catchment model, in which the essential compartments are coupled to each other. Feedback mechanisms across technical and natural interfaces are crucial to quantify the vulnerability of the ecosystem.

Chapter 7

Supplementary Contributions

The chapter gives an overview of the supplementary scientific work, which I carried out during my time as a PhD student at the Leibniz-Institute of Freshwater Ecology and Inland Fisheries.

Co-authored publications:

1. Hupfer, M., Jordan, S., Herzog, C., Ebeling, C., **Ladwig, R.**, Rothe, M., and Lewandowski, J.: Chironomid larvae enhance phosphorus burial in lake sediments: Insights from long and short-term experiments, submitted to Science of the Total Environment

Conference presentations (in chronological order):

1. **Ladwig, R.**, Gillefalk, M., Romero, C., Herrero, S., Broecker, T., El-Athman, F., Schaper, J., Hinkelmann, R., and Hupfer, M.: Urban Water Interfaces: Interfaces in Urban Surface Waters, The Sixth German-Russian Week of the Young Research "Urban Studies: The City of the Future", 12.-16. September 2016

2. **Ladwig, R.**, Heinrich, L., Singer, G., and Hupfer, M.: Qualitative Beurteilung von Bewirtschaftungsmaßnahmen im Sediment eines urbanen Sees mittels multivariater Statistik, DGL Tagung Wien, 26.-30. September 2016

3. **Ladwig, R.**, Kirillin, G., Hinkelmann, R., and Hupfer, M.: Lake on life support: Evaluating urban lake management measures by using a coupled 1D-modelling approach, EGU General Assembly 2017, Vienna, Austria, 23.-28. April 2017

4. Broecker, T., Teuber, K., **Ladwig, R.**, Nützmann, G., and Hinkelmann, R.: Impact of small-scale riverbed topography on stream flow and surface detention of a tracer, EGU General Assembly 2018, Vienna, Austria, 8.-13. April 2018

5. **Ladwig, R.**, Matta, E., Hinkelmann, R., Kirillin, G., Furusato, E., and Hupfer, M.: How can we adapt urban lake management in times of climate change?, 9th Water Research Horizon Conference 2018, Dresden, Germany, 3.-4. July 2018

Conference posters (in chronological order):

1. Köhler, A., Heinrich, L., **Ladwig, R.**, Kleeberg, A., and Hupfer, M.: Optimierung von Managementmaßnahmen im Tegeler See (Berlin) Erfahrungen und neue Herausforderungen, DGL Tagung Wien, 26.-30. September 2016

2. Heinrich, L., **Ladwig, R.**, Ohlendorf, C., Perez-Mayo, M., and Hupfer, M.: Element retention rates from quantified μXRF-Scan document effects of management measures on urban lake sediment, XRF Core Scanning 2017, Taiwan, Taiwan, 20.-24. March 2017

3. **Ladwig, R.**, Matta, E., Furusato, E., Kirillin, G., Hinkelmann, R., and Hupfer, M.: Model-based assessment of urban water management strategies for a shallow dimictic lake, ELR2017NAGOYA and ICLEE 8th Conference, Nagoya, Japan, 22.-25. September 2017

4. **Ladwig, R.**, Matta, E., Hinkelmann, R., and Hupfer, M.: From 1D to 2D: Impact of extreme weather events and climate change on the heavily stressed urban Lake Tegel in Berlin, Germany, EGU General Assembly 2018, Vienna, Austria, 8.-13. April 2018

Reports:

1. Hupfer, M., Jordan, S., Herzog, C., Heinrich, L., and **Ladwig, R.**: Abschlussbericht: Sedimentuntersuchungen am Tegeler See, on behalf of Berlin Senate Department for the Environment, Transport and Climate Protection, Germany, 2016

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