



Thèse

2021

Open Access

This version of the publication is provided by the author(s) and made available in accordance with the copyright holder(s).

Assessing future effects on lake ecosystem resilience using Data Analysis and Dynamic Modelling

Mesman, Jorrit

How to cite

MESMAN, Jorrit. Assessing future effects on lake ecosystem resilience using Data Analysis and Dynamic Modelling. Doctoral Thesis, 2021. doi: 10.13097/archive-ouverte/unige:157664

This publication URL: <https://archive-ouverte.unige.ch/unige:157664>

Publication DOI: [10.13097/archive-ouverte/unige:157664](https://doi.org/10.13097/archive-ouverte/unige:157664)

UNIVERSITÉ DE GENÈVE

*Département F.-A. Forel des sciences et l'environnement
et de l'eau*

FACULTÉ DES SCIENCES

Professeur Dr. Bastiaan W. Ibelings

Groupe de Physique Appliquée (GAP)

Dr. Stéphane Goyette

UPPSALA UNIVERSITY

Department of Ecology and Genetics

Dr. Don C. Pierson

Assessing Future Effects on Lake Ecosystem Resilience using Data Analysis and Dynamic Modelling

Modelling the Effects of Extreme Weather Events and Climate Warming on Lakes

THÈSE

présentée à la Faculté des Sciences de l'Université de Genève

pour obtenir le grade de Docteur ès sciences, mention sciences de l'environnement

par

Jorrit MESMAN

de

Ter Aar (Pays-Bas)

Thèse N° 5617

GENÈVE

Atelier d'impression ReproMail

2021



**UNIVERSITÉ
DE GENÈVE**

FACULTÉ DES SCIENCES

DOCTORAT ÈS SCIENCES, SCIENCES DE L'ENVIRONNEMENT

Thèse de Monsieur Jorrit MESMAN

intitulée :

**«Assessing Future Effects on Lake Ecosystem Resilience
using Data Analysis and Dynamic Modelling»**

La Faculté des sciences, sur le préavis de Monsieur B. W. IBELINGS, professeur ordinaire et directeur de thèse (Département F.-A. Forel des sciences de l'environnement et de l'eau), Monsieur S. GOYETTE, docteur et codirecteur de thèse (Section de physique), Monsieur D. PIERSON, docteur et codirecteur de thèse (Department of Ecology and Genetics, Uppsala University, Uppsala, Sweden), Monsieur J.-L. LOIZEAU, docteur (Département F.-A. Forel des sciences de l'environnement et de l'eau), Monsieur K. RINKE, docteur (Department of Lake Research, Helmholtz-Centre for Environmental Research, Magdeburg, Germany), Madame N. SCHUWIRTH, docteure (Department Systems Analysis, Integrated Assessment and Modelling, Dübendorf), Monsieur T. BLENCKNER, docteur (Stockholm Resilience Centre, Stockholm University, Stockholm, Sweden), autorise l'impression de la présente thèse, sans exprimer d'opinion sur les propositions qui y sont énoncées.

Genève, le 23 novembre 2021

Thèse - 5617 -

Le Doyen

List of Papers

This thesis is based on the following papers:

- I. Mesman, J. P., Stelzer, J. A. A., Dakos, V., Goyette, S., Jones, I. D., Kasparian, J., McGinnis, D. F., & Ibelings, B. W. (2021). The role of internal feedbacks in shifting deep lake mixing regimes under a warming climate. *Freshwater Biology*, 66(6): 1021-1035. doi:10.1111/fwb.13704
- II. Mesman, J. P., Ayala, A. I., Adrian, R., De Eyto, E., Frassl, M. A., Goyette, S., Kasparian, J., Perroud, M., Stelzer, J. A. A., Pierson, D. C., & Ibelings, B. W. (2020). Performance of one-dimensional hydrodynamic lake models during short-term extreme weather events. *Environmental Modelling & Software*, 133: 104852. doi:10.1016/j.envsoft.2020.104852
- III. Moore, T. N.*, Mesman, J. P.*, Ladwig, R.*, Feldbauer, J.*, Olsson, F., Pilla, R. M., Shatwell, T., Venkiteswaran, J. J., Delany, A. D., Dugan, H., Rose, K. C., & Read, J. S. (2021). LakeEnsemblR: An R package that facilitates ensemble modelling of lakes. *Environmental Modelling & Software*, 143: 105101. doi:10.1016/j.envsoft.2021.105101 (* = shared main author)
- IV. Mesman, J. P., Ayala, A. I., Goyette, S., Kasparian, J., Marcé, R., Markensten, H., Stelzer, J. A. A., Thayne, M. W., Thomas, M. K., Pierson, D. C., & Ibelings, B. W. (2021). Drivers of phytoplankton responses to summer storms in a stratified lake: a modelling study. Submitted to *Limnology and Oceanography*. Preprint doi:10.31223/X5PK8H

In addition to the papers included in this thesis, I have contributed to the following papers:

- I. Reinl, K. L., Brookes, J. D., Carey, C. C., Harris, T. D., Ibelings, B. W., Morales-Williams, A. M., De Senerpont Domis, L. N., Atkins, K. S., Isles, P. D. F., Mesman, J. P., North, R. L., Rudstam, L. G., Stelzer, J. A. A., Venkiteswaran, J. J., Yokota, K., & Zhan, Q. (2021). Cyanobacterial blooms in oligotrophic lakes: Shifting the high-nutrient paradigm. *Freshwater Biology*, 66(9): 1846-1859. doi:10.1111/fwb.13791
- II. Stelzer, J. A. A., Mesman, J. P., Adrian, R., & Ibelings, B. W. (2021). Early warning signals of regime shifts for aquatic systems: Can experiments help to bridge the gap between theory and real-world application? *Ecological Complexity*, 47: 100944. doi:10.1016/j.ecocom.2021.100944
- III. Thayne, M. W., Kraemer, B. M., Mesman, J. P., Ibelings, B. W., & Adrian, R. (2021). Antecedent lake conditions shape resistance and resilience of a shallow lake ecosystem following extreme wind storms. *Limnology and Oceanography*. doi:10.1002/lno.11859
- IV. Woolway, R. I., Sharma, S., Weyhenmeyer, G. A., Debolskiy, A., Golub, M., Mercado-Bettín, D., Perroud, M., Stepanenko, V., Tan, Z., Grant, L., Ladwig, R., Mesman, J., Moore, T. N., Shatwell, T., Vanderkelen, I., Austin, J. A., DeGasperis, C. L., Dokulil, M., La Fuente, S., Mackay, E. B., Schladow, S. G., Watanabe, S., Marcé, R., Pierson, D. C., Thiery, W., & Jennings, E. (2021). Phenological shifts in lake stratification under climate change. *Nature communications*, 12(1): 2318. doi:10.1038/s41467-021-22657-4

TABLE OF CONTENTS

Summaries	1
Summary (in English)	1
Résumé (en français)	4
Sammanfattning (på svenska)	7
Introduction	10
Lake responses to extreme weather events	10
Storms ahead: extreme events and climate change	11
Perturbations and ecological stability	12
Management of climatic extreme events in lakes and reservoirs for the protection of ecosystem services – The MANTEL project	12
On the tightrope between physics and biology	13
Learning from extremes using observational studies and experiments	13
New frontiers: process-based modelling of extreme events	14
Advantages and limitations of process-based modelling	16
Good things come in threes: observations, experiments, and modelling	17
Aims of the thesis	17
Chapter 1 - The role of internal feedbacks in shifting deep lake mixing regimes under a warming climate	18
Abstract	18
Introduction	19
Physical, chemical, and biological consequences of enhanced stratification	21
Water temperatures and stratification	21
Oxygen dynamics in deep lakes	22
Influence of anoxia on nutrient distribution and other substances	22
Influence of mixing dynamics on lake phytoplankton	23
Shifts in mixing regime	24
Shift from a polymictic to a seasonally stratified regime	24
Shift from a dimictic to a monomictic regime	27
Shift from a holomictic to an oligo- or meromictic regime	28
Conclusion	31
Acknowledgements	31
Chapter 2 - Performance of one-dimensional hydrodynamic lake models during short-term extreme weather events	32
Abstract	32
Introduction	32
Methods	33
Observational data	33

Lake thermal metrics	34
Lake models	35
Calibration.....	35
Storm and heatwave events	35
Assessment of model performance	37
Results	37
Model performance for the whole simulation period	37
Observations during events	38
Model performance during events	39
Discussion.....	43
Conclusion	46
Declaration of competing interest	46
Acknowledgements.....	46
Appendix A. Supplementary data.....	46
Software availability	46
Chapter 3 - LakeEnsemblR: An R package that facilitates ensemble modelling of lakes.....	48
Abstract	48
1. Introduction.....	48
2. Methods	50
2.1 Model descriptions	50
2.2 R package description	51
3. Example application of LakeEnsemblR.....	55
3.1 Lough Feeagh: water temperature dynamics	56
3.2 Langtjern: lake ice dynamics	58
3.3 Uncertainty partitioning	60
3.4 Multi-parameter ensemble.....	60
3.5 Discussion	61
4. Summary	62
4.1 Framework.....	62
4.2 Recommendations for use	63
4.3 Outlook	64
Acknowledgements.....	64
Software and Data Availability	65
Chapter 4 - Drivers of phytoplankton responses to summer storms in a stratified lake: a modelling study	66
Abstract	66
Introduction	66
Methodology	68

Site description	68
Data collection	68
Model description and setup.....	69
Calibration.....	70
Sensitivity analysis	71
Validation	71
Numerical experiment 1: varying initial conditions before a storm	71
Numerical experiment 2: inducing storms in long-term scenarios.....	74
Results	75
Calibration and validation.....	75
Numerical experiment 1: Variables controlling phytoplankton response to storms.....	75
Numerical experiment 2: Effect of a warmer climate on phytoplankton response to storms	78
Discussion.....	79
Model validation	79
Causal factors regulating phytoplankton response to storms	80
Effects of storms on phytoplankton under a warmer climate.....	81
Implications beyond Lake Erken	81
Conclusion	83
Acknowledgements.....	83
Software availability	84
Synthesis.....	85
Lessons learned	85
A further process-based understanding of the interactions between lake physics and biogeochemistry during extreme events.....	85
Complex interactions between long-term climate warming and short-term extreme events.....	85
Modelling as a viable approach to study short-term effects of extreme events.....	86
Next steps.....	86
Incorporation of three-dimensional processes.....	86
Precipitation events and catchment inflows	87
Biogeochemical modelling to study shifts in mixing regimes	87
Repeated perturbations and different durations of perturbations	87
Effect of short-term events on long-term dynamics.....	87
Concluding remarks.....	87
Supplementary Material.....	89
Acknowledgements	90
References	92

SUMMARIES

SUMMARY (IN ENGLISH)

Extreme weather events can have large and long-lasting impacts on lake ecosystems. Wind storms mix stratified water layers and resuspend sediment, heatwaves promote stratification and may cause heat stress for aquatic organisms, and high rainfall events affect nutrient inflows into the lake. The intensity and frequency of such events are shifting as part of anthropogenic climate change, but simultaneously the changing lake conditions will also affect how extreme events interact with lakes. For example, earlier and stronger stratification will change vertical profiles of nutrients and increase resistance to wind mixing, which may alter the link between storms and phytoplankton.

The terms “resistance” and “resilience” describe how an ecosystem responds to and recovers from a perturbation. Extreme weather events are natural perturbations and in this thesis we investigate the resistance and resilience of lake ecosystems to such events, and how this may change with climate warming. The main methodology explored here is process-based modelling, which has recently been applied more and more to study the effect of extreme weather events on lakes. There is uncertainty connected to model simulations, but a large advantage is the ability to explore many different climate and extreme event scenarios. This thesis is a small part of the larger MANTEL project, which oversees multiple PhD theses on the topic of studying the effects of extreme weather events on lakes.

Before starting with modelling, we need to explore the links between thermal stratification and lake biology that extreme weather events will act upon. The first chapter of this thesis is a review in which we discuss the overall effects of climate warming on lake physics, chemistry, and biology, with a specific focus on mixing regimes, i.e. seasonal patterns in lake density stratification. The paper then proceeds by identifying feedback loops between lake processes that could lead to an accelerated shift to a new mixing regime or that could make a mixing regime resistant to change. Three mixing regime shifts are investigated: 1) from polymictic to seasonally stratified, 2) from dimictic to monomictic, and 3) from holomictic to either oligo- or meromictic. Polymictic lakes mix multiple times per year, but if such lakes are deep enough (c. 3-10 m mean depth) they may experience temporary stratification events due to decreases in water transparency. Under select circumstances, this stratification may trigger a further decrease in transparency (through increased dissolved carbon or phytoplankton concentrations) and so the stratified regime may stabilise. However, this feedback is unlikely to provide stability over multiple years, as stratification is lost in winter. Ice-covered (dimictic) lakes are shifting to ice-free (monomictic) lakes due to climate warming, and a reduced ice-albedo feedback may accelerate this transition in very deep lakes (mean depth 50 m or more). However, the majority of studies on this topic suggest that a gradual transition is more likely. Holomictic lakes mix from top to bottom in winter, oligomictic lakes experience irregular top-to-bottom mixing, and meromictic lakes never mix completely due to a heavier deep-water layer (due to accumulated solutes). Climate warming induces a trend towards less frequent complete mixing. Normally, the warming of deep waters ensures that complete mixing occurs occasionally, therefore promoting oligomixis. However, if water density increases due to the accumulation of solutes, and exceeds the water density decrease due to warming, a meromictic regime may form. At the end of the chapter, we mention modelling as a potential pathway to study some of these feedback loops, specifically those related to the loss of polymixis and the possible formation of meromixis.

The second chapter was a necessary step before starting modelling studies on short-term effects of extreme events. Model performance is commonly assessed on a calibration or validation period, usually spanning multiple years. However, model performance on short time scales during extreme weather events was largely unknown. Here we assessed the performance of one-dimensional hydrodynamic models to reproduce observed trends in water temperature and stratification metrics. We included three lake models (Simstrat, GOTM, GLM) and high-frequency data from three lakes (Lough Feeagh - IR, Lake Erken - SW, and Müggelsee - DE), and in each

lake we defined ten storms and ten heatwaves to test the models on. The models reproduced the direction and magnitude of change during both storms and heatwaves well. Statistically significant over- or underestimation was only found in a few cases. Any time lags of the simulated changes tended to be less than 1 hour. However, compared to reference (i.e. non-extreme) time periods, the model error during the extreme events was 30-100% higher (with the exception of storms in the shallowest lake). In conclusion, we can use 1D hydrodynamic models to assess effects of extreme weather events on lakes, but we should take into account the decreased accuracy. The latter could be done for example by adopting a model ensemble approach. Together, the first two chapters form the basis for the rest of the thesis: theoretical framework and methodology. Additionally, both studies can be used as building blocks for further studies on extreme events.

Ensemble modelling is a promising step forward for the aquatic modelling community, especially when modelling extreme weather events. To facilitate the use of ensemble modelling within the lake modelling community, we developed an R package, *LakeEnsemblR*, which is presented in Chapter 3. Users will require only a single set of input files and one configuration file to run and calibrate five different one-dimensional hydrodynamic models (FLake, GLM, GOTM, Simstrat, and MyLake) and to store the results in a single output file. The package can also be used to visualise and analyse the model output. In the paper we also demonstrated the use of the package on two lakes, Lough Feeagh in Ireland and Langtjern in Norway. The advantage of the ensemble approach was apparent in the generation of a credible confidence band around the mean prediction, but also in the fact that the ensemble mean sometimes outperformed the best single-model fit. The potential for ensemble modelling was one of the outcomes of the second chapter, but was also widely recognised in the lake modelling community. More widespread use of this method could lead to improvements in forecasting studies, both short- and long-term.

The last chapter of the thesis followed from the first two chapters, and looked at the effect of multiple potential drivers on how phytoplankton reacts to storms. The investigated drivers were wind speed, mixed layer depth, surface water temperature, incoming shortwave radiation, and hypolimnetic nutrient concentration. Each driver was scaled independently in a full factorial design while inducing a 24-hour wind perturbation. Wind speed had a non-monotonic effect, where moderate wind speeds (c. 5-10 m/s) could increase phytoplankton concentrations after storms, but high wind speeds (> 10 m/s) had weaker or even negative effects. When the mixed layer was deeper than approximately 8 m, the effect of the storm was strongly reduced. Incoming shortwave radiation, surface temperature, and hypolimnetic nutrients also affected how storms influenced phytoplankton, with higher radiation and nutrients promoting positive effects of storms, and higher surface temperature stimulating negative effects of a storm on phytoplankton. Lastly, the effect of climate warming was assessed by scaling the air temperatures to a level projected in 2040-2070 according to the RCP8.5 emission scenario. While climate warming affected summer averages of many lake variables, the response of phytoplankton to storms did not markedly change in a warmer climate. This chapter includes the modelling of lake ecosystems, rather than only lake physics as in chapters 2 and 3. It also focuses on the study of the resistance (i.e. magnitude of response) of lakes to an extreme weather event, under the influence of climate warming. At the same time, one of the key results is that not only the extremes are important, but rather the entire range of possible weather conditions. The diverging responses of phytoplankton to storms, observed in other studies, are caused by both storm characteristics and antecedent lake conditions. Our modelling approach could study the effects of the different drivers individually and provided an assessment of potential future effects.

In conclusion, this thesis has contributed to a further process-based understanding of how extreme events influence lake thermal structure and biogeochemistry. Process-based understanding is instrumental to assess in what types of lakes certain responses occur, and also to construct predictive models that can inform lake management. The thesis also showed some of the interactions between long-term climate warming and short-term extreme weather events that may be expected to occur. This topic is not often considered and may be important for forecasting efforts. Lastly, the chapters in this thesis form further evidence that process-based modelling is a viable approach to study the effects of extreme weather events on lakes. More exciting new paths

for further investigation remain open, which are especially important considering the rising global temperature trends and the increasing role of extreme weather. Lakes are important ecosystems, both considering their unique biodiversity and their role for humans. Better understanding of the impacts of extreme events on lakes helps us to improve management of these systems and to anticipate future conditions.

RÉSUMÉ (EN FRANÇAIS)

Les événements météorologiques extrêmes peuvent avoir de graves conséquences sur les écosystèmes lacustres à long terme. Les tempêtes mélangent la colonne d'eau et remettent les sédiments en suspension ; les vagues de chaleur stimulent la stratification et peuvent causer un stress thermique pour des organismes aquatiques ; et des événements de fortes précipitations affectent l'apport des nutriments dans les lacs. L'intensité et la fréquence de tels événements changent dans le cadre du réchauffement climatique, mais simultanément, l'évolution des conditions lacustres affectera également la manière dont les événements extrêmes interagissent entre lacs. Par exemple, une stratification plus tôt et plus forte modifiera les profils verticaux des nutriments et renforcera la résistance au mélange par le vent, ce qui pourrait modifier le lien entre les tempêtes et le phytoplancton.

Les termes « résistance » et « résilience » décrivent comment un écosystème répond à une perturbation et s'en remet. Des événements extrêmes météorologiques sont des perturbations naturelles et dans cette thèse nous étudions la résistance et la résilience des écosystèmes lacustres contre de tels événements, et comment cela peut changer avec le réchauffement climatique. La principale méthodologie explorée est la modélisation basée sur les processus. Cette dernière est de plus en plus appliquée pour rechercher l'effet des extrêmes météorologiques aux lacs. Il existe une incertitude liée aux simulations de modèles. Néanmoins, l'avantage de cette méthode est la possibilité d'explorer beaucoup de scénarios climatiques et des différents événements extrêmes. Cette thèse est une petite partie du projet MANTEL, qui comprend plusieurs thèses doctorales sur le sujet des effets des événements climatiques extrêmes sur les lacs.

Avant de commencer avec la modélisation, il est nécessaire d'explorer les connections entre la stratification thermique et la biologie lacustre, sur lesquelles les événements extrêmes agiront. Le premier chapitre de cette thèse est une revue sur effets globaux du réchauffement climatique sur la physique, la chimie, et la biologie des lacs, avec un accent spécifique sur les régimes de mélange, i.e. les tendances saisonnières de la stratification thermique des lacs. Par la suite, l'étude identifie des boucles de rétroaction entre des processus lacustres, qui pourraient conduire à un passage accéléré à un nouveau régime de mélange ou qui pourraient rendre un régime de mélange résistant aux changements. Nous avons examiné trois changements de régimes de mélange : 1) de polymictique à stratifié, 2) de dimictique à monomictique, et 3) de holomictique à oligo- ou méromictique. Des lacs polymictiques se mélangent plusieurs fois par année, mais si ces lacs sont suffisamment profonds (c. 3-10 m de profondeur moyenne), ils peuvent avoir des événements de stratification temporaires en raison de la diminution de la transparence de l'eau. Dans certaines circonstances, cette stratification peut déclencher une nouvelle diminution de la transparence (par une augmentation du carbone dissous ou des concentrations de phytoplanctons) et le régime stratifié peut alors se stabiliser. Cependant, il est peu probable que cette rétroaction assure la stabilité sur plusieurs années, car la stratification disparaît en hiver. Des lacs gelés (dimictique) se transforment en lacs sans glace (monomictique) à cause du réchauffement climatique, et la rétroaction de l'albédo de la glace peut accélérer cette transition dans les lacs très profonds (plus de 50 m de profondeur moyenne). Cependant, la majorité des études sur ce sujet suggèrent qu'une transition graduelle est plus probable. Les lacs holomictiques se mélangent de haut en bas en hiver, et les lacs oligomictiques subissent un mélange irrégulier de haut en bas, et les lacs méromictiques ne se mélangent complètement jamais à cause d'une couche d'eau profonde plus lourde (en raison des solutés accumulés). Le réchauffement climatique cause une tendance à un mélange complet moins fréquent. Normalement, le réchauffement des eaux profondes assure un mélange complet occasionnel, ce qui favorise l'oligomixie. Néanmoins, si une augmentation de la densité en raison d'accumulation des solutés dépasse un abaissement de la densité en raison de réchauffement, un régime méromictique peut se former. À la fin du chapitre, nous mentionnons la modélisation comme une possibilité pour étudier certaines de ces boucles de rétroaction, plus précisément celles liées à la perte de polymixie et la formation éventuelle de méromixie.

Le deuxième chapitre était une étape nécessaire avant de commencer avec les études de modélisation sur les effets à court terme des événements extrêmes. La performance d'un modèle est normalement évaluée sur une

période de calibration ou validation, qui couvre habituellement plusieurs années. Toutefois, la performance des modèles sur des échelles de temps courtes pendant des événements météorologiques extrêmes était largement inconnue. Ici, nous avons évalué la performance des modèles unidimensionnels hydrodynamiques à reproduire des tendances observées dans la température de l'eau et des paramètres de stratification. Nous avons pris trois modèles lacustres (Simstrat, GOTM, GLM) et des données à haute-fréquence de trois lacs (Lough Feeagh-Irlande, Lac Erken – Suède, et Müggelsee – Allemagne), et pour chaque lac nous avons identifié dix tempêtes et dix vagues de chaleur pour tester les modèles. Les modèles ont bien reproduit la direction et la magnitude du changement pendant les tempêtes et les vagues de chaleur. Une sur- ou sous-estimation statistiquement significative n'a été observée que dans quelques cas. Les décalages temporels des changements simulés avaient tendance à être moins de 1 heure. Néanmoins, en comparaison avec des périodes de référence (i.e. non extrêmes), l'erreur du modèle pendant les événements extrêmes était 30-100% plus élevée (à l'exception des tempêtes dans le lac le moins profond). En conclusion, on peut utiliser des modèles unidimensionnels hydrodynamiques pour étudier les effets des événements météorologiques extrêmes aux lacs. Cependant, il faut prendre en compte que la précision des modèles est abaissée. Cette dernière pourrait être réalisée par exemple en adoptant une approche d'ensemble. Les deux premiers chapitres le cadre théorique et la méthodologie de la thèse. De plus, les deux études peuvent être utilisées comme soutiens pour les prochaines études sur les événements extrêmes.

La modélisation des ensembles est une étape prometteuse pour la communauté de la modélisation aquatique, spécialement quand on modélise des événements météorologiques extrêmes. Afin de faciliter l'usage des ensembles dans la communauté de modélisation des lacs, nous avons créé un package sur le logiciel de R, *LakeEnsemblR*, qui est présenté au Chapitre 3. Les utilisateurs du logiciel n'auront besoin que d'une seule collection de fichiers d'entrée et de configuration pour exécuter et calibrer cinq différents modèles unidimensionnels hydrodynamiques (FLake, GLM, GOTM, Simstrat, et MyLake) et pour sauvegarder les résultats dans un seul fichier de sortie. Le logiciel peut aussi être utilisé pour visualiser et analyser les résultats des modèles. Dans le manuscrit, nous avons aussi démontré l'usage du logiciel sur deux lacs, Lough Feeagh en Irlande et Langtjern en Norvège. L'avantage d'une approche d'ensemble était évident dans la génération d'une zone d'incertitude crédible autour de la prédiction moyenne, mais aussi dans le fait que le moyenne du ensemble parfois performait mieux que le meilleur résultat d'un des modèles individuels. Le potentiel de la modélisation d'ensemble était un des résultats du deuxième chapitre, mais était aussi largement reconnu par la communauté de modélisation lacustre. Un usage plus répandu de cette méthode pourrait conduire à des améliorations dans les études de prédiction, tant à courte qu'à longue terme.

Le dernier chapitre de cette thèse s'inscrit dans la continuité des deux premiers chapitres, et il concerne les effets de plusieurs facteurs causaux potentiels sur comment le phytoplancton réagit aux tempêtes. Les facteurs examinés sont la vitesse du vent, la profondeur de la couche mélangée, la température de l'eau de surface, le rayonnement solaire entrant, et la concentration en nutriments dans l'hypolimnion. Chaque facteur était varié indépendamment des autres dans un plan factoriel complet tout en induisant une perturbation du vent sur 24 heures. La vitesse du vent a eu un effet non-monotone, où des vitesses de vent modérées (c. 5-10 m/s) pouvaient augmenter les concentrations du phytoplancton après les tempêtes, mais des vitesses de vent élevées (> 10 m/s) avaient des effets moins forts ou même des effets négatifs. Lorsque la couche mélangée était plus profonde que ≈ 8 m, l'effet de la tempêtes était fortement réduit. Le rayonnement solaire, la température de l'eau de surface, et la concentration des nutriments dans l'hypolimnion ont aussi un effet sur l'influence des tempêtes sur le phytoplancton. Des niveaux plus élevés de rayonnement solaire et de nutriments causaient une augmentation du phytoplancton après les tempêtes. Des niveaux plus chauds d'eau de surface montraient un effet négatif sur la concentration de phytoplancton après une perturbation du vent. Enfin, l'effet du réchauffement climatique a été évalué en mettant à l'échelle les températures de l'air à un niveau prévu en 2040-2070, suivant le scénario d'émission RCP8.5. Même si le réchauffement influençait les moyennes d'été de plusieurs variables lacustres, la réponse du phytoplancton aux tempêtes ne changeait pas évidemment dans un climat plus chaud. Ce chapitre inclut la modélisation des écosystèmes lacustres, plutôt que seulement la

physique des lacs comme dans les chapitres 2 et 3. Il se concentre aussi sur l'étude de la résistance (i.e. magnitude de réponse) des lacs à un événement météorologique extrême, sous l'influence du réchauffement climatique. En même temps, un des résultats critiques ce ne sont pas seulement les extrêmes qui sont importants, mais plutôt la distribution totale des conditions météorologiques possibles. Les réponses divergentes de phytoplancton aux tempêtes, observées dans des autres études, sont causés par des caractéristiques de tempêtes et les conditions lacustre précédents, et notre approche de modélisation nous permettait d'étudier les effets des plusieurs facteurs individuels et de faire une prédiction pour des effets potentiels à l'avenir.

En conclusion, cette thèse a contribué à une plus grande compréhension des mécanismes de comment les événements extrêmes ont des effets sur la structure thermique et biogéochimique d'un lac. Une compréhension mécanistique est essentiel pour évaluer dans quels types des lacs certains réponses se produisent, et aussi pour construire des modèles prédictifs qui peuvent informer la gestion des lacs. La thèse montre également quelques interactions que peuvent avoir le réchauffement climatique à long terme et les événements météorologiques extrêmes à court terme. Ce sujet n'est pas souvent considéré, mais pourrait être important pour des efforts de prédiction. Finalement, les chapitres de cette thèse constituent une preuve supplémentaire que la modélisation mécanistique est une approche valable pour étudier les effets d'événements météorologiques extrêmes sur les lacs. De nouvelles voies d'investigation restent ouvertes, qui sont particulièrement importantes si l'on considère les tendances à la hausse des températures mondiales et le rôle croissant des phénomènes météorologiques extrêmes. Les lacs sont des écosystèmes importants, tant par leur biodiversité unique que par leur rôle pour l'humaine. Une meilleur compréhension des impacts des événements extrêmes sur les lacs nous aide à mieux gérer ces systèmes et à anticiper des conditions à l'avenir.

SAMMANFATTNING (PÅ SVENSKA)

Extremt väder kan ha stora och långvariga effekter på sjöar. Stormar blandar olika vattenlager och sätter sediment i rörelse. Höga temperaturer stimulerar stratifiering och kan orsaka värmestress för vattenorganismer, och hög nederbörd påverkar inflöden av näringsämnen till sjöar. Intensiteten och frekvensen av dessa händelser förändras med globala klimatförändringarna, men samtidigt påverkar de förändrade processerna i sjöar också hur extremt väder samverkar med sjöar. Tidigare och starkare stratifiering förändrar till exempel vertikala profiler av näringsämnen och ökar motståndet mot omblandning på grund av vind, vilket kan förändra kopplingen mellan stormar och växtplanktons produktion.

Begreppen "motstånd" och "resiliens" beskriver hur ett ekosystem reagerar på och återhämtar sig från en störning. Extremt väder består av naturliga störningar och i denna avhandling undersökte vi motståndet och resiliensen av sjöar mot sådana störningar, och hur de kan förändras med global uppvärmning. Huvudmetoden som används här är processbaserad modellering, vilket har använts i allt större utsträckning de senaste åren för att undersöka effekterna av extremt väder på sjöar. Det finns osäkerhet i simulationsmodeller, men en stor fördel är möjligheten att utforska många olika scenarier vid klimatförändringar och extremt väder. Denna avhandling är en liten del av ett större MANTEL projektet, vilket innehåller flera doktorsavhandlingar som också undersöker effekterna av extremt väder på sjöar.

Innan man börjar modellera, måste man utforska kopplingar mellan termisk stratifiering och sjöarnas biologi som extremt väder ska ha effekter på. Första kapitlet i denna avhandling består av en översikt om allmänna effekter av klimatuppvärmning på sjöars fysik, kemi, och biologi, med ett specifikt fokus på blandningsregimer, bestående av säsongsdynamik i sjöarnas stratifiering. Sedan fortsätter studien med att identifiera återkopplingscykler mellan processer i sjöar som kan orsaka en förändring till en ny blandningsregim eller som kan ge en blandningsregim som är motståndskraftig mot förändring. Tre skiften i blandningsregimer har undersökts: 1) från polymiktisk till stratifierad, 2) från dimiktisk till monomiktisk, och 3) från holomiktisk till oligo- eller meromiktisk. Polymiktiska sjöar blandas flera gånger om året, men om sådana sjöar är tillräckligt djupa (c. 3-10 m medeldjup), kan kortsiktiga stratifieringar uppstå på grund av minskningen av vattnets klarhet. Under vissa omständigheter kan en sån stratifiering leda till en ytterligare minskning av klarhet (på grund av mer löst kol eller växtplankton), och stratifieringen kan därmed stabilisera sig. Denna feedback kommer dock sannolikt inte att ge stabilitet över flera år, eftersom stratifieringen försvinner på vintern. Sjöar med istäcke på vintern (dimiktiska sjöar) övergår till ofrysta (monomiktiska) sjöar på grund av klimatuppvärmning, och is-albedo återkopplingen kan påskynda denna övergången i mycket djupa sjöar (mellandjup 50 m eller mer). Majoriteten av studierna kring detta ämne antyder dock att ett gradvist skifte är mer troligt. Holomiktiska sjöar blandas från vattenytan till botten på vintern varje år, oligomiktiska sjöar blandas oregelbundet fullständigt, och meromiktiska sjöar blandas aldrig från ytan till botten på grund av ett tyngre djupt vattenlager (på grund av ackumulerade lösta ämnen). Klimatuppvärmning orsakar en trend mot mindre frekvent fullständig omblandning. I vanliga fall säkerställer uppvärmningen av djupa vattenlager att fullständig blandning sker ibland, och därmed stimuleras oligomixis. Men om ökningen i vattendensitet på grund av ackumulering från lösta ämnen överstiger minskningen i vattendensitet på grund av uppvärmning, kan en meromiktisk regim uppstå. I slutet av kapitlet nämner vi modellering som ett möjligt sätt att studera några av dessa återkopplingscykler, särskilt de som relaterar till förlusten av polymixis och möjlig formationen av meromixis.

Det andra kapitlet utgjorde ett nödvändigt steg för att börja modellera kortlivade effekter från extremt väder. Modellkvalitet fastställs ofta under en kalibrerings- eller valideringsperiod, som sträcker sig över flera år. Modellkvalitet över korta perioder under extremt väder har dock i stort sett varit okänd. Här utvärderade vi modellkvalitet på en-dimensionella hydrodynamiska modeller med syftet att reproducera observerade trender i vattentemperatur och stratifiering. Vi använde tre sjömodeller (Simstrat, GOTM, GLM) och hög-frekvens data från tre sjöar (Lough Feeagh i Irland, Erkenjön i Sverige, och Müggelsee i Tyskland), och i varje sjö identifierade vi tio stormar och tio värmevågor på vilka vi testade våra modeller. Modellerna reproducerade bra riktningen och omfattningen av förändringar under både stormar och värmevågor. Statistiskt relevanta över- och

underskattningar observerades i bara få fall. Tidsfördröjningar av simulerade förändringar brukade vara mindre än en timme. Dock var felmarginalen under extremt väder 30-100% högre jämfört med referensperioder (i.e. normalfall), med ett undantag för stormar i den grundaste sjön. Vi konstaterar att vi kan använda 1D hydrodynamiska modeller för att utvärdera effekter av extremt väder på sjöar, men vi behöver ta hänsyn till en lägre precision av såna modeller. Detta kan till exempel göras genom att använda ett ensemble-tillvägagångssätt. Tillsammans bygger de två första kapitlen grunden av avhandlingen: det teoretiska ramverket och metodiken. Dessutom kan båda studierna användas som grund för ytterligare studier till extrema händelser.

Ensemble modellering är en lovande metodik för vattenmodellerare, särskilt för de som modellerar extremt väder. För att underlätta användningen av ensemble-modeller, har vi utvecklat ett mjukvarupaket i R, *LakeEnsemblR*, vilket presenteras i kapitel 3. Användare behöver bara en enda uppsättning av inmatningsfiler och en konfigurationsfil för att köra och kalibrera fem olika en-dimensionella hydrodynamiska modeller (FLake, GLM, GOTM, Simstrat, och MyLake) och även för att spara resultaten i en resultatfil. Paketet kan också användas för att visualisera och analysera modellresultatet. I studien använder vi paketet på två sjöar, Lough Feeagh i Irland och Langtjern i Norge. Fördelen med ensemblemodellering var uppenbar i skapandet av en trovärdig osäkerhetsmarginal kring medelprognosen, men också i det faktum att medelprognosen av ensemblen var ibland bättre än den bästa individuella modellprognosen. Användningspotentialen av ensemble modellering var ett av resultaten från andra kapitlet, men den är även allmänt erkänd bland sjömodellerare. En bredare användning av denna metod kan leda till förbättringar i förutsägelser, både under korta och långa perioder.

Avhandlingens sista kapitel bygger på de två första kapitlen, och fokuserar på potentiella drivkrafter för hur växtplankton reagerar på stormar. De undersökta drivkrafterna är vindhastighet, blandningslagerdjup, ytvattentemperatur, inkommande kortvågig strålning, och halter av näringsämne i hypolimnion. Varje variabel skalerades självständigt i en faktoriell design, medan vi inducerade en 24-timmars vindstörning. Vindhastighet hade en icke-monoton effekt, där måttliga vindhastigheter (c. 5-10 m/s) kunde öka växtplanktonkoncentrationer efter stormar, men höga vindhastigheter (> 10 m/s) hade svagare eller negativa effekter. När blandningslagret var djupare än ungefär 8 m, minskade stormens effekt kraftigt. Inkommande solstrålning, ytvattentemperatur, och hypolimnisk koncentration av näringsämnen hade också effekt på hur stormar påverkar växtplankton: högre strålning och näringsämnen främjade effekter av stormar, och högre ytvattentemperatur hade negativa effekter av stormar på växtplankton. Slutligen undersöktes effekten av klimatuppvärmning med en lufttemperatur beräknat för perioden 2040-2070 och enligt RCP8.5 klimatscenariot. Medan klimatuppvärmning hade en effekt på sommergenomsnitt av flera variabler i sjön, förändrades reaktionen av växtplankton till stormar inte mycket i ett varmare klimat. Det här kapitlet inkluderar modelleringen av sjöekosystem, inte endast av sjöfysik som i kapitel 2 och 3. Kapitlet fokuserar även på sjöars motstånd (i.e. storleken av reaktion) mot extremt väder, som ett resultat av klimatuppvärmning. Samtidigt är ett av de viktigaste resultaten inte bara att extrema händelser är viktiga, utan snarare hela fördelningen av möjliga väderförhållandena. Växtplanktons olika reaktioner av stormar, observerade i denna studie, orsakas av både stormens egenskaper och befintliga förhållanden av sjön, och vår modelleringsmetod kunde undersöka effekterna av flera variabler individuellt och skapa en uppskattning av möjliga framtida effekter.

Sammanfattningsvis har denna avhandling bidragit till en ytterligare processbaserad förståelse av hur extremt väder påverkar den termiska strukturen och biokemin i sjöar. Processbaserad förståelse är viktigt för att bedöma i vilka typer av sjöar vissa reaktioner kommer att uppstå, och också för att konstruera prediktiva modeller som kan bidra till sjöförvaltning. Avhandlingen visade dessutom på några av interaktionerna mellan klimatuppvärmning och kortsiktigt extremt väder. Detta ämne behandlas sällan och kan vara viktigt för att förutse det framtida klimatet. Avhandlingens kapitel visar ytterligare att modellering är en värdefull metod för att undersöka effekterna av extremt väder på sjöar. Det finns flera spännande och nya möjligheter för ytterligare forskning, som är särskilt viktiga med tanke på hur den globala temperaturen kommer att öka i framtiden, och den ökande betydelsen av extremt väder. Sjöar är viktiga ekosystem, både med tanke på deras unika biologiska

mångfald och också deras roll för människor. En bättre förståelse av effekterna av extremt väder på sjöar hjälper oss att förbättra förvaltningen av dessa ekosystem och att förutse deras framtid.

INTRODUCTION

LAKE RESPONSES TO EXTREME WEATHER EVENTS

Extreme weather events represent atmospheric conditions that are only rarely experienced. As many processes in the environment are nonlinear, environmental responses to extreme conditions might be more extreme still and can be hard to predict. Therefore, extreme events are periods of additional interest, and they can indeed affect ecosystems for a prolonged duration (Jennings et al. 2012). The focus in this thesis is on the effect of extreme weather events (Box 1) on lakes, and how the response of lakes to these events may change under a warming climate. Many physical lake conditions are directly influenced by atmospheric conditions, such as surface water temperature, ice cover, light availability, and mixing dynamics (e.g. Magnuson et al. 2000; Kirillin 2010; Woolway et al. 2021). These lake conditions again influence, and interact with, chemical and biological variables, for example oxygen, nutrient, and phytoplankton concentrations (Nowlin et al. 2005; Wilhelm and Adrian 2008; Mackay et al. 2014). Precipitation patterns additionally control catchment discharge and nutrient inflow into lakes (De Eyto et al. 2016; Carpenter et al. 2017).

Box 1. What is an extreme event?

Extreme events 1) represent occurrences near the ends of a probability distribution, above (or below) a certain threshold value, and 2) have a certain start and end date, which only describes a small part of the full period under consideration. The term “extreme event” does not specify what variable we are talking about. We often use an adjective to specify the nature of what type of event we consider, e.g. “extreme climatic events”, “extreme weather events”, or “extreme flooding events”. An extreme event (e.g. extreme weather) may not always have an extreme impact (Seneviratne et al. 2012). Definitions or thresholds can vary between studies (Seneviratne et al. 2012; Ummenhofer and Meehl 2017; Van de Pol et al. 2017) and may involve a level of arbitrariness; therefore they should be well-defined in each specific study.

There is not a clear difference between “extreme weather events” and “extreme climatic events”, although the former tends to focus more on short-term events (e.g. storms) and the latter more on seasonal-or-longer timescales (e.g. dry summers) (Seneviratne et al. 2012).

Four types of extreme weather events have received special attention from limnologists in the past decades: wind storms, heatwaves, rainfall events, and droughts. Extreme wind events mix water layers, and this causes upwelling of nutrients, deepening of the mixed layer, cooling of the surface water, and overall relocation of compounds and organisms (Crockford et al. 2015; Andersen et al. 2020; Mesman et al. 2020). Consequences of storms diverge strongly, but can include phytoplankton blooms (Soranno et al. 1997; Kasprzak et al. 2017). In shallow (parts of) lakes, wind storms can resuspend large amounts of sediment or uproot macrophytes (Havens et al. 2001). Heatwaves are the apparent opposite of storms, as they promote separation of water layers (i.e. increased stratification) and warmer surface layers (Wilhelm and Adrian 2008). The high water temperatures experienced by water bodies during heatwaves, often accompanied by oxygen shortages near the lake bottom, can be especially problematic for macrofauna and fish (Ficke et al. 2007; Kangur et al. 2013). High precipitation events can cause flushing of a lake, but also bring large amounts of dissolved organic matter and nutrients into the system, potentially making up a large percentage of the annual budget (Weyhenmeyer et al. 2004; Shrestha et al. 2020). Droughts can lower water levels in lakes, affect nutrient balances, and during droughts lakes may simultaneously exhibit similar patterns as during heatwaves (Zohary and Ostrovsky 2011; Tilahun and Kifle 2019). A quick visual summary of these main processes is provided in Figure 1.

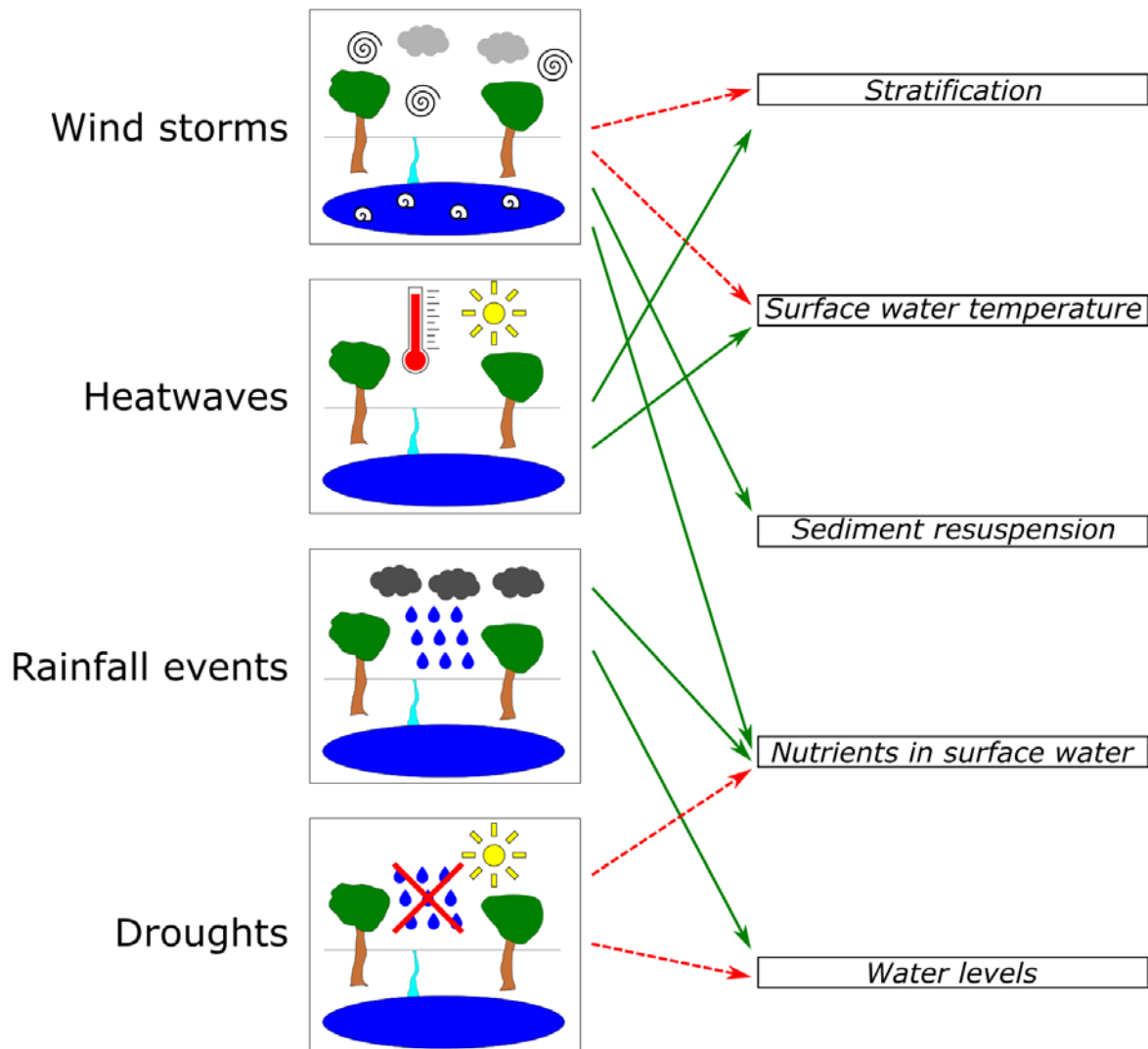


Figure 1. A graphical representation of some of the effects of four extreme weather events: wind storms, heatwaves, rainfall events, and droughts. Green and solid arrows indicate increasing effects and red and dashed arrows decreasing effects.

STORMS AHEAD: EXTREME EVENTS AND CLIMATE CHANGE

The above-mentioned examples and citations showcase some of the large impacts that extreme weather events can have on lake ecosystems, and this partially explains the scientific interest in the topic. However, studies on extreme events are increasing in number during the last years due to a rising awareness that climate change will include a change in frequency and intensity of extreme weather events. Both low and high precipitation extremes are becoming more frequent, albeit in different regions of the world (IPCC 2014). Increases in storm frequency and intensity also show a spatially-diverging pattern, but with clearly identifiable trends in storm occurrence in specific regions (Möller et al. 2016; Sainsbury et al. 2018). Cold extremes are decreasing as warm extremes increase (IPCC 2014), although there are indications that, at least in Europe, temperature extremes shift at similar rates as central temperature trends (Rey et al. 2020) – that is, the temperature probability distribution shifts towards warmer temperatures, but does not change its shape.

Shifting intensities and frequencies of extreme weather events in a future climate add additional relevance to studies on their impacts. Furthermore, long-term climatic trends in lakes will affect how extreme events influence lakes. For example, as atmospheric warming promotes stronger stratification (e.g. Kraemer et al. 2015), this increases resistance to (wind) mixing (Schmidt 1928). One could then expect less impact of

comparable storms under a warmer climate. However, this must also account for trends in mixed layer depth – a shallower mixed layer means a higher impact of a storm – but these trends are more uncertain (Pilla et al. 2020). Earlier onset of stratification (Woolway et al. 2021) means that hypolimnetic nutrients start building up earlier in the season, so that a similar amount of upwelling would bring up more nutrients in a future climate. And the list of potential interactions between extreme events and climate warming could go on further. Isolated effects of climate warming and, to a lesser extent, extreme events are well-studied, but this interaction is not too often considered (Gal et al. 2020).

PERTURBATIONS AND ECOLOGICAL STABILITY

Up to now, we have been talking about extreme events, yet the title of this thesis is centred around the term “resilience”. The relation between the two can be found in the topic of “ecological stability”. Ecological stability is a “multidimensional concept that tries to capture the different aspects of the dynamics of the system and its response to perturbations” (Donohue et al. 2016). Maybe more than many other fields, “ecological stability” (and connected terms such as resistance and resilience) has experienced a wide variety in naming conventions, hypothesis testing, and schools of thought (Pimm et al. 2019; Stelzer et al. 2021; Van Meerbeek et al. 2021). As such, I will avoid elaborating too much on the topic, but will stress that ecological stability is inherently connected with perturbations, and that “resilience” – one aspect of stability – has to do with how systems recover from a perturbation – either the degree of recovery (Thayne et al. 2021) or its rate (Donohue et al. 2016). “Resistance”, on the other hand, is another aspect of stability and measures the direct response of a system to a perturbation (Donohue et al. 2016; Thayne et al. 2021), i.e. before its recovery.

Extreme weather events are amongst the most common natural perturbations that ecosystems experience. Studying how ecosystems respond to such events is therefore a valuable way of furthering our understanding of ecosystems and ecosystem stability (Altwegg et al. 2017). But the stability of lake ecosystems to extreme events is not only relevant for ecologists; a large variety of ecosystem services provided by lakes (e.g. drinking water provisioning) are affected by extreme weather events (Khan et al. 2015), and therefore the resistance and resilience of a lake is also important from an anthropocentric point of view.

It is largely unavoidable that lakes experience extreme weather events, even without climate change, but if we better understand lake ecosystem stability in relation to extreme events, some action may be taken. For example, in the shallow-lake theory outlined by Scheffer (1998) it is shown that while a clear-water state may occur over a wide range of nutrient concentrations, the risk of a sudden shift to a turbid state (e.g. due to an extreme event) decreases when nutrient concentrations are lower (Scheffer et al. 2001). Moreover, if we understand enough about our system to make forecasts based on weather predictions, lake managers could take preventive measures before extreme events occur based on these forecasts (Carey et al. 2021).

MANAGEMENT OF CLIMATIC EXTREME EVENTS IN LAKES AND RESERVOIRS FOR THE PROTECTION OF ECOSYSTEM SERVICES – THE MANTEL PROJECT

The chosen approach of studying resilience from the perspective of extreme weather events also originated from the placement of this PhD project within the wider MANTEL project (Management of climatic extreme events in lakes and reservoirs for the protection of ecosystem services). MANTEL is a Marie Skłodowska-Curie Action European Joint Doctorate Innovative Training Network (MSCA EJD ITN), a project that oversees the training of 12 PhD students in multiple universities and institutes in Europe, funded by the European Union. The common focus of the PhD projects within MANTEL is to investigate the effects of extreme climatic events on lakes and reservoirs, from a multitude of angles. Foci of the individual MANTEL PhDs include mixing dynamics, calcite precipitation, greenhouse gas emissions, microbial dynamics, and ecosystem services. More information can be found on <https://www.mantel-itn.org/>.

Within MANTEL, this PhD project combines the topics of modelling, resilience, and climate change. Additionally, it assesses both physical and biological variables (more on this in the next section). As with all individual MANTEL

PhD project, this project is especially closely connected to a subset of other MANTEL projects. Ana Ayala is based in Uppsala and uses physical models to understand how climate change and extreme events affect lake heat fluxes and thermal structure. Michael Thayne, based in Berlin, Germany, assesses long-term, high-frequency ecological data to discover critical thresholds in how lake ecosystems respond to storms. Julio Stelzer, stationed in Geneva, performs perturbation experiments, on multiple scales of complexity, to investigate how resource availability modifies ecosystem stability in microbial communities. Collaboration with these PhDs was an integral part of this PhD project and placed the research done in this thesis in a broader perspective of perturbation ecology and climate forecasting.

ON THE TIGHTROPE BETWEEN PHYSICS AND BIOLOGY

Studying the effects of extreme weather events on lake ecosystems involves walking on a fine line between physics and biology. While the initial cause (i.e. the extreme weather event) is purely physical, effects work their way down to lake biogeochemistry, macrofauna, and the microbial community (e.g. MacIntyre and Jellison 2001; Jennings et al. 2012; Calderó-Pascual et al. 2020; Hoke et al. 2020). And sometimes the effects on biogeochemistry work their way back up to again affect the physical lake conditions, which is the central topic of the first chapter of this thesis (Mesman et al. 2021). To study extreme events in lakes therefore requires one to be knowledgeable both in physics and biology. Fortunately, the field of limnology almost by definition includes physics and biology and has in fact from its origins studied both aspects (Forel 1880; Forbes 1887). There is therefore a good amount of literature to start from, although as said before, the interest in extreme weather events is relatively recent and still developing.

Following the definition of an extreme weather event (Box 1), the event itself is short, at least with respect to the period one is assessing. Lake responses may prove to be short-term as well (or even hardly affected by the event), but many examples exist of extreme events that caused long-lasting changes in lakes. Effects of storms on lake physics may vary from hours to months (Andersen et al. 2020), and potentially longer if water transparency is affected, and Mi et al. (2018) showed in a modelling study that the timing of the event matters as well; during a critical timing window ($\approx$ June until mid-July in their study lake), physical changes may persist for the rest of the stratified season, whereas outside that window, effects subside quickly. When events alter vertical profiles of biogeochemical compounds, effects may last long as well, for example in the German Lake Stechlin, where a deep phytoplankton community was brought to the surface by a storm and this caused a bloom that lasted for weeks (Kasprzak et al. 2017). Another example is Lake Lugano, where two cold winters in a row caused complete turnover in this otherwise meromictic lake, which greatly affected the biogeochemistry of the lake (Lehmann et al. 2015). High precipitation events affect lake catchments, and this may affect inflow characteristics, lake levels, and lake chemistry for multiple months, such as in 2009 in the Irish Lough Feeagh (De Eyto et al. 2016), or in 2011-2012 in the German Gollinsee (Brothers et al. 2014). However, the most spectacular long-term effects of extreme weather events may be found in shallow lakes, where extreme wind events may affect lakes for multiple years due to uprooting of macrophytes and mobilisation of large amounts of sediment, such as in lakes Okeechobee and Apopka in Florida, USA (Bachmann et al. 2000; Ji et al. 2018).

Many of these examples clearly show the potential links and feedback loops between physics and biogeochemistry. Storm and precipitation events cause more homogenisation of the water column and may increase solute concentrations in the surface water, affecting light availability and primary production. Heatwaves and droughts may promote more spatial heterogeneity in the water column, and this may lead to anoxia and temperature stress. The energy and compound fluxes induced by extreme weather events act like a trigger, and basin morphometry, thermal structure, water chemistry, and community traits control how far the effects reach.

LEARNING FROM EXTREMES USING OBSERVATIONAL STUDIES AND EXPERIMENTS

Extreme events are rare by definition and often unexpected; therefore, we need a long data record and/or data from multiple sites to collect enough observations and to arrive at valid and coherent conclusions. For this, long-

term ecological monitoring is essential (Dodds et al. 2012; Lindenmayer et al. 2012; Wüest et al. 2021), while we also need to report on individual events, from which we can indeed learn a lot (Altwegg et al. 2017). As some extreme events act on short timescales (e.g. hours or days), high-frequency data collection may be crucial (Jennings et al. 2012).

Review or meta-analysis papers can combine the findings from multiple sites into an overview to deduce emergent patterns. As examples, Reichwaldt and Ghadouani (2012) published a meta-analysis of the influence of rainfall patterns on cyanobacterial blooms; Stockwell et al. (2020) compiled a synthesis on the effects of storms on phytoplankton; and Cann et al. (2013) reviewed the link between extreme water-related weather events and waterborne diseases. Alternatively, combining data from multiple sites adds a spatial dimension in studying continental or sub-continental events. This was done for example by Klug et al. (2012), who analysed the impact of Hurricane Irene on nine lakes in north-eastern North America, and by Woolway et al. (2020), who used satellite-data to validate their model results, studying the effects of the 2018 summer heatwave in Europe. We can get our most valuable data from observational studies, but it may take effort (long-term high-frequency monitoring, international research collaborations, etc.) to collect and analyse sufficient data.

As a way to avoid waiting for an extreme event to occur and simultaneously obtaining a “baseline” or “control” situation (insofar that is possible in nature), one can perform experiments to study extreme events. This yields real data where effects can be causally attributed to the occurrence of an event. A caveat here is that the level of complexity only rarely approaches that of a real lake, but advantages include a better possibility for detailed measurements, a more complete understanding of your study system, and an increased possibility to construct a causal pathway.

At the basis of this experimental approach are perturbation experiments where mortality events (mimicking the effects of an extreme weather event) are induced and the response of the aquatic community is assessed. Examples of such experiments include Veraart et al. (2011) and Stelzer et al. (in preparation). However, the nature of the induced perturbation can include more aspects of an extreme weather event, with effects on both physics and biology. Such an approach was used by Hansson et al. (2020) and Urrutia-Cordero et al. (2020) to study the effect of heatwaves on phytoplankton composition using oscillating temperature regimes in mesocosms. Zhan et al. (under review) also applied heatwave treatments to mesocosms to assess phosphorus release rates from the sediment, including treatments with phosphorus-binding clay. As one of the most impressive examples, Giling et al. (2017a) induced thermocline deepening – simulating extreme wind mixing – in 20 m deep mesocosms to study effects of mixing on phytoplankton and lake metabolism, in the LakeLab facility in Lake Stechlin, Germany.

NEW FRONTIERS: PROCESS-BASED MODELLING OF EXTREME EVENTS

This thesis mainly focuses on another approach to study extreme events, namely process-based modelling (but see Chapter 1). This approach has its own respective advantages and disadvantages compared to observational and experimental studies, but has been applied less frequently in limnology with regard to extreme events. One of the reasons for this is that process-based models (from now, models) are usually applied to test scenarios on seasonal or decadal time scales, such as in climate forecasting (e.g. Sahoo et al. 2013; Schwefel et al. 2016; Ayala et al. 2020; Woolway et al. 2021). Only in short-term forecasting we find significantly shorter time scales, from hours to days (Thomas et al. 2020). Lake models are known to be rather skilful at replicating at least the physical lake conditions at seasonal time scales, but we do not know how well models perform at shorter (e.g. hourly) time scales, particularly during extreme events. We tackle this issue in Chapter 2.

Regarding daily to monthly time scales, we do find several examples of lake modelling studies on extreme weather events, all from the last few years. Bueche et al. (2017) and Woolway et al. (2020) applied physical lake models to look at changes in thermal structure during heatwaves, while Chen et al. (2020) also assessed impacts on ecological variables. Soares et al. (2019) looked at the impact of droughts on the thermal structure of a

Brazilian drinking water reservoir, and explored withdrawal scenarios to minimise effects of droughts on drinking water provisioning. Mi et al. (2018) used a model to explore the effects of different timings and intensities of wind storms on lake thermal structure. Lastly, Perga et al. (2018) used a model to support their observations-based study on storm effects. The recency of these studies shows that the modelling of extreme weather events is a novel and emergent field of research.

As described above, the interactions between extreme weather events and lake ecology are manifold and complex, covering atmosphere-water interactions, turbulence, sediment dynamics, nutrient update dynamics, and phytoplankton traits. A model therefore also needs to be sufficiently complex to describe such processes. But a too complex model, with many parts that cannot be validated, may lead to a lower quality of simulations (Shimoda and Arhonditsis 2016; but see Hellweger 2017). In Chapter 4 we take an intermediate path by coupling a complex (yet one-dimensional) hydrodynamic model to a biogeochemical model of intermediate complexity. We used this combined model to investigate the different drivers that may control the effect of wind perturbations on phytoplankton dynamics. Using this approach, we could study how wind speed, thermal structure, nutrient concentration, and climate warming might affect how phytoplankton respond to storms. Although the model does not include some potentially relevant processes, such as varying nutrient ratios, it can give an indication of the global responses of phytoplankton concentration to changing in-lake and meteorological variables.

One way to estimate uncertainty in model output is by using ensembles. An “ensemble” means that multiple models and/or model parametrisations are used to generate a single simulation result. Ensembles have as main advantage that there is a quantification of the uncertainty connected to a forecast, but also the ensemble mean (weighted or otherwise) often outperforms the best individual member, as biased simulations are filtered out (e.g. Trolle et al. 2014). Moreover, valuable information can be extracted from all ensemble members, rather than only from the single “best” fit (Baker and Ellison 2008). In other fields, such as climatology and weather and flood forecasting, the use of ensembles is well-established (Leutbecher and Palmer 2008; Mu et al. 2017; Wu et al. 2020), but in limnology this is not so common. One of the reasons for this is the lack of a common framework; each model requires different file formats and inputs, making the creation of a multi-model ensemble a demanding task. In Chapter 3, we present a software package – “LakeEnsemblR” – that greatly facilitates the use of ensembles in lake modelling. For now, this package only works for physical lake models, but we are working on a similar project for water quality models as well (<https://gleon.org/research/projects/lakeensembl-r-wq>, last accessed: 2021-07-19). The connection to this thesis can be found in the fact that extreme weather events represent periods of additional model uncertainty, considering meteorological inputs into the model, model assumptions, and often a lack of relevant validation data. An ensemble approach may therefore be especially helpful in forecasts involving extreme events.

Figure 2 shows the overall coverage of the papers in this thesis along the short-term/long-term and physics/biology spectra.

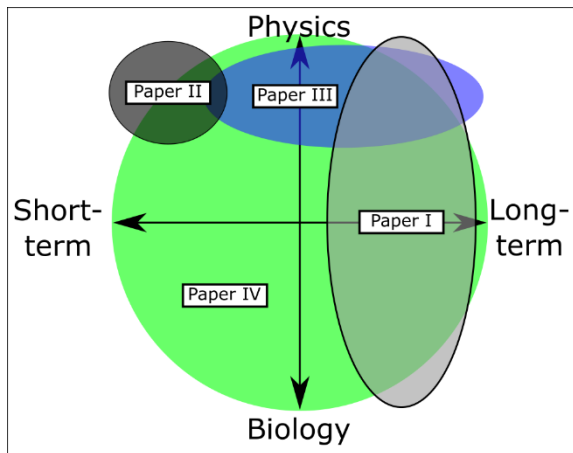


Figure 2. Diagram that shows what topics the papers in this thesis cover, considering short-term/long-term dynamics and physical/biological lake processes.

ADVANTAGES AND LIMITATIONS OF PROCESS-BASED MODELLING

The main advantage of a modelling approach lies in the possibility to test scenarios that would be impossible in an experimental setting, yet retaining a causal understanding, which may get lost in data-driven approaches (i.e. statistics or machine learning). Especially long-term climate warming scenarios, including realistic rates of warming and seasonal effects (such as earlier onset of stratification), are hard to assess in mesocosms. Also, the importance of thermal stratification in deep lakes is hard to replicate in an experimental setup, and requires costly facilities such as the one used by Giling et al. (2017a). Using process-based models, climate and wind perturbation scenarios can be explored with relative ease, and the physical constraints and clearly-defined structure of these models (compared to data-driven approaches) add to the confidence in such extrapolation scenarios.

Nevertheless, there are many obvious and important limitations to a modelling approach, and these should be taken into consideration when interpreting model outcomes. The primary disadvantage of the modelling approach is that we are not dealing with real data. Modellers try to increase the reliability of their models by validating their simulations on measured data, by building their models (as much as possible) on empirically-established relationships, and by choosing realistic estimates of parameter values (e.g. Jørgensen 1995). But we can never be sure that our model is accurate, especially when exploring imaginary scenarios, or forecasting the future. Additionally, any model, no matter its complexity, always simplifies the system it describes (Soetaert and Herman 2008). While this helps to make predictions and to understand the response of the model, there is always the risk that an important process is omitted, or described incompletely. While models may reveal important new information to us, we should always keep in mind the limitations of the models and be careful to not take our predictions for pure truth.

One particular problem that emerges from complex models is the concept of “equifinality”. This describes the mathematical possibility that multiple combinations of parameter value generate the same outcome (Beven 2006). For example, you can deepen your simulated mixed layer depth by increasing wind speed or by increasing transparency, and both could cause your model to fit your results better. But in reality, only one of these options may be true. In other words, models may give the right answers for the wrong reasons. This can be a problem, because these alternative model setups - equally correct from a calibration perspective - could diverge in their predictions when assessing certain scenarios. Equifinality is mostly unavoidable in complex models (Beven 2006), but can be mediated by having good data availability (e.g. in the above example, if you have accurate measurements of transparency, you do not have to vary them in your simulation), and also by using an ensemble approach.

Up to now, we used the following words to describe a model fit to data: “accurate”, “well”, “better”, “reliable”. But when is a fit “good” or “reliable”? We often calculate goodness-of-fit metrics, such as the Root Mean Square Error (RMSE), Mean Absolute Error (MAE), or the coefficient of determination (R^2) to describe our model fit to data. Nevertheless, these metrics can be deceiving; especially for spiky timeseries (e.g. discharge nutrient input), standard goodness-of-fit metrics are notoriously inaccurate and may give a pessimistic view of model performance (Elliott et al. 2000; Jachner et al. 2007). Conversely, if the data have strong seasonal cycles, such as for surface water temperature, one would probably not even need a model to reproduce the observed trend with an R^2 of above 0.8 (pers. comm. Rafael Marcé), which would be considered a good fit for most applications. Using a combination of metrics is a more promising approach to assess model fit (Elliott et al. 2000). However, to date we have no commonly agreed-upon guidelines or thresholds to approve or reject a model (Hipsey et al. 2020). While development of standardised thresholds may be an unobtainable goal, more critical assessments of model behaviour can lead to improvement, as outlined by Hipsey et al. (2020).

GOOD THINGS COME IN THREES: OBSERVATIONS, EXPERIMENTS, AND MODELLING

Modelling offers exciting new possibilities for scenario exploration and forecasting compared to other approaches, but has its limitations as well. Rather than promoting (or excluding) one method, we need to learn from observational studies, experiments, and modelling together to gain a better understanding of how extreme weather events influence lakes. Each approach has its specific strengths and should be valued for its merits. While this PhD thesis focuses mostly on the modelling aspect, the MANTEL project indeed focuses on all three facets. It is as part of MANTEL, and as a small part of a larger network of limnologists, that this thesis should be viewed, and hopefully it can contribute to a better understanding of the combined effects of extreme weather events and climate change on lakes.

AIMS OF THE THESIS

A process-based understanding of the impact of climate warming and extreme weather events on lakes is essential in order to make future predictions and to adapt lake management to changing conditions. Longer and higher-frequency records of lake variables make it possible to increase our insight in the physical, chemical, and biological consequences of extreme weather, while state-of-the-art models can be used to study a variety of scenarios regarding meteorological and lake conditions. The main aim of this thesis is to use these developments to better understand how climate warming and extreme weather events influence lake ecosystems, and how these two processes interact with each other.

The following research questions were addressed:

- How do extreme weather events influence lakes? (Chapters 2 and 4)
- How do effects of climate warming and extreme weather events interact? (Chapters 1 and 4)
- Is process-based modelling a viable approach to study effects of extreme weather events? (Chapters 2 and 3)

CHAPTER 1 - THE ROLE OF INTERNAL FEEDBACKS IN SHIFTING DEEP LAKE MIXING REGIMES UNDER A WARMING CLIMATE

Jorrit P. Mesman^{1,2,3*}, Julio A. A. Stelzer^{1,4,5}, Vasilis Dakos⁶, Stéphane Goyette², Ian D. Jones⁷, Jérôme Kasparian², Daniel F. McGinnis¹, Bas W. Ibelings¹

¹*Department F.A. Forel for Environmental and Aquatic Sciences and Institute for Environmental Sciences, University of Geneva, Geneva, Switzerland*

²*Group of Applied Physics and Institute for Environmental Sciences, University of Geneva, Geneva, Switzerland*

³*Department of Ecology and Genetics, Uppsala University, Uppsala, Sweden*

⁴*Department of Ecosystem Research, Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany*

⁵*Department of Biology, Chemistry, and Pharmacy, Freie Universität Berlin, Berlin, Germany*

⁶*Institut des Sciences de l'Evolution, University of Montpellier, Montpellier Cedex, France*

⁷*Faculty of Natural Sciences, Biological & Environmental Sciences, University of Stirling, Stirling, UK*

**Corresponding author: Jorrit.Mesman@unige.ch. Department F.A. Forel for Environmental and Aquatic Sciences and Institute for Environmental Sciences, University of Geneva, Boulevard Carl-Vogt 66, 1211 Geneva 4, Switzerland.*

ABSTRACT

1. Climate warming is causing changes in the physics of deep lakes, such as longer summer stratification, increased water column stability, reduced ice cover, and a shallower depth of winter overturns. An ultimate consequence of warming would be a transition to a different mixing regime. Here we investigate the role of physical, chemical, and biological feedback mechanisms that unfold during a shift in mixing regime, and whether these feedbacks could prompt and stabilise the new regime. Although climate, interannual temperature variation, and lake morphometry are the main determinants of a mixing regime, when climate change causes shifts in mixing regime, internal feedback mechanisms may gain in importance and modify lake ecosystem functioning.
2. We review the role of these feedbacks in three mixing regime shifts: from polymictic to seasonally stratified, from dimictic to monomictic, and from holomictic to oligomictic or meromictic.
3. Polymictic lakes of intermediate depth (c. 3-10 m mean depth) could experience seasonal stratification if a stratification event triggers phytoplankton blooms or dissolved organic matter release, reducing transparency and therefore further heating the surface layer. However, this feedback is only likely to have influence in small and clear lakes, it would be easily disturbed by weather conditions, and the resulting stratified state does not remain stable in the long term, as stratification is lost in winter.
4. The ice-albedo feedback might cause an accelerated shift from ice-covered (dimictic) to ice-free (monomictic) winters in sufficiently deep (mean depth 50 m or more) lakes, where temperature memory is carried over from one winter to the next. Nevertheless, there is an ongoing debate into whether this process can persist during natural weather variations and overcome self-stabilising mechanisms such as thermal insulation by snow. The majority of studies suggest that a gradual transition from dimictic to monomictic is more likely than an abrupt transition.
5. A shift from a holomictic to a meromictic regime can occur if anoxia is triggered by incomplete mixing and an increase in deep-water density - through the accumulation of solutes - exceeds a density decrease by hypolimnetic warming. A shift to meromixis would strongly alter the biology of a lake and

might be difficult to reverse. If solutes accumulate only minimally in the hypolimnion, an oligomictic regime is formed, in which years with complete and incomplete mixing alternate.

6. Understanding the importance of feedback mechanisms and the role of biogeochemistry when lakes shift in mixing regime could lead to a better understanding of how climate change affects lake ecosystems.

Keywords: climate change, meromixis, mixing regime, stratification, water transparency

INTRODUCTION

Temperatures in lakes all over the world have been rising over the past century as a consequence of global warming (O'Reilly et al. 2015). This warming has resulted in an overall increase in thermal stability, with longer periods of summer stratification and steeper thermoclines, restricting exchange of substances between the epi- and hypolimnion (Shimoda et al. 2011; Kraemer et al. 2015). Climatic trends driving the thermal stability in deep lakes have also had profound impacts on lake chemistry and biology. For instance, reduction of deep mixing can result in the depletion of oxygen (anoxia) in the hypolimnion (Schwefel et al. 2016). A longer duration of stratification and reduction of deep mixing can increase the heterogeneity of vertical nutrient profiles, with nutrient-rich deep waters and nutrient-poor surface waters (Winder and Sommer 2012; Schwefel et al. 2019). In turn, this altered vertical nutrient distribution affects lake biota such as phytoplankton and fish (O'Reilly et al. 2003; Winder and Sommer 2012). Moreover, observational studies of lake thermal structure and numerical climate simulations have pointed towards climate-induced shifts in mixing regime (Box 1), implying structural changes in lake ecosystems (Peeters et al. 2002; Ficker et al. 2017; Shatwell et al. 2019; Woolway and Merchant 2019).

In the present review paper, we look at the physical, chemical, and biological consequences of climate warming and increased density stratification in deep lakes, defined here as lakes that stratify during at least one season. We then identify internal feedbacks that can reinforce (positive feedbacks) or slow down (negative feedbacks) shifts between mixing regimes. The scope of this paper only includes regime shifts where such feedback loops were identified in the existing literature, or where they could be constructed using individual processes, and considers mixing regime shifts in the context of increasing atmospheric temperatures. The potential importance of feedbacks is well illustrated by the alternative macrophyte- (clear-water) and algae-dominated (turbid) states in shallow lakes (Ibelings et al. 2007). Regime shifts between these two states involve feedback loops between turbidity, nutrients, and trophic interactions that retain either state, also in the face of changing external processes such as eu-/oligotrophication or perturbations such as storms (Scheffer 1998; Scheffer et al. 2001).

In deep, stratified lakes the vertical distribution of oxygen, nutrients, and phytoplankton are strongly influenced by density stratification, which hints at the potential of mixing regimes to act as important drivers of ecosystem functioning. Mixing regimes are primarily driven by physical processes, and therefore under direct influence of climate change (Livingstone 2008; for definitions of mixing regimes, see Box 1). Mixing regimes in deep lakes differ from one another in several physical, chemical, and biological aspects (e.g. Boehrer and Schultze 2008; Adrian et al. 2009; North et al. 2014).

According to the classical view on mixing regimes (Hutchinson and Löffler 1956; Lewis Jr 1983), local climate and morphometry are the main factors determining the mixing regime of a lake. However, factors other than depth and climate, such as transparency (Brothers et al. 2014) and solute content (Boehrer and Schultze 2008), can also influence lake mixing. Conversely, mixing regimes might influence these factors. Thus, lake-internal feedbacks could stabilise and even determine the mixing regime, especially in situations where morphometry and climate can support multiple mixing regimes. It is in these situations that mixing regime shifts are to be expected, and already unfolding, in response to ongoing climate change. If self-sustaining feedback mechanisms hold the new regime in place, shifts in mixing regime may prove to be resilient.

Quantitative observations and numerical simulations specifically focusing on shifts in mixing regime by factors other than temperature are scarce, as long-term observations and detailed studies are needed to observe such shifts and identify the drivers. However, individual processes that could lead to feedback loops stabilising mixing regimes, are well described. In what follows, we review the literature on the physical trends related to increased duration and strength of density stratification, and the chemical and biological consequences thereof (Figure 1). Following this literature review, we derive processes at play during a transition in mixing regime and discuss their interaction in typical lake regime shifts. The observed feedbacks are brought together, visualised, and placed into the perspective of shifts in mixing regime under increasing temperatures. We also discuss the limitations of the relevance of each feedback and specify for what types of lakes these feedbacks may be considered. In this way, we believe our review provides new and pertinent information on how climate warming may affect lake ecosystems, extending beyond direct effects of temperature alone.

Box 1: Types of lake mixing regimes

Categorising lakes on the basis of their mixing regime is a well-established practice (Forel 1880; Hutchinson and Löffler 1956). Lakes are classified according to the number of mixing events per year and the degree of mixing. Depending on local climate, depth, salinity, and lake morphology, a lake mixes a certain number of times per year (never - amictic, once - monomictic, twice - dimictic, three or more times - polymictic), either completely – always from top to bottom (holomixis) –, only sometimes from top to bottom (oligomixis) or always partially (meromixis). Shallow lakes tend to be *polymictic*, i.e. they mix multiple times per year, although below what depth a lake is to be considered shallow has been the topic of discussion (see Padisák and Reynolds 2003). In most cases, the occurrence of polymixis is used to define a lake as shallow. Depending on lake fetch, transparency, and wind speeds, polymixis tends to occur below mean depths of 3 to 20 m (Padisák and Reynolds 2003; Kirillin and Shatwell 2016). This shallowness makes the lake prone to mixing events, either wind-induced or caused by convective cooling, although stratification events lasting multiple days or weeks are also possible (Mischke 2003; Wilhelm and Adrian 2008).

The presence of long-term, i.e. over at least a season, density stratification is used here to define what constitutes a deep lake. In deep lakes, seasonal temperature variation largely controls the mixing regime. Near the poles, lakes, for now, have permanent ice cover (*amictic lakes*) or only experience inverse stratification (i.e. cold above warmer water, as the maximum density of freshwater is achieved at 4°C) and these *cold monomictic* lakes only mix in summer. Moving to lower latitudes, winter temperatures are still low enough for inverse stratification and ice formation, but air temperatures in summer are high enough to allow formation of a warm epilimnion; these are *dimictic* lakes, that mix before and after a winter period with inverse stratification. Where winters are not cold enough for ice formation, stratification only occurs in summer and deep lakes only mix in winter: these are *warm monomictic* lakes (Lewis Jr 1983). The absence of strong seasonal temperature variation in tropical regions causes a different yearly pattern near the equator, with a more dynamic development of the epilimnion. However, mixing seasons often still exist as a result of seasonal patterns in radiation, rainfall, or wind, and tropical deep lakes are classified as warm monomictic, following Lewis Jr (1996). In the main text the term monomictic refers to warm monomictic lakes.

Winter mixing does not necessarily reach the deepest location of the lake. Complete mixing is called *holomixis* and incomplete mixing is termed *meromixis*. In permanent or “true” meromictic lakes, stratification is caused by an increased concentration of solutes that raises the density of the deep water, for example by sea water or saline groundwater influx (Hutchinson 1957; Gulati et al. 2017). The two chemically different layers do not mix for multiple years. However, in many temperate and tropical deep lakes, mixing depths vary year-to-year and complete winter mixing occurs at varying frequencies, ranging from on average once every year to once every 5 decades. These lakes are not holomictic, but no permanent chemical stratification is formed either. In this paper, we define these lakes as *oligomictic* (following Lewis Jr 1973). We reserve the term *meromictic* for

lakes with chemically different layers and stable density stratification due to the effect of solutes (following Gulati et al. 2017).

We therefore define the mixing regime of a lake both in terms of the frequency of mixing (poly-, di-, monomictic) and the extent of mixing (holo-, oligo-, meromictic). For a more complete description of mixing regimes and potential further subdivisions, we refer the reader to Boehrer and Schultze (2008).

PHYSICAL, CHEMICAL, AND BIOLOGICAL CONSEQUENCES OF ENHANCED STRATIFICATION

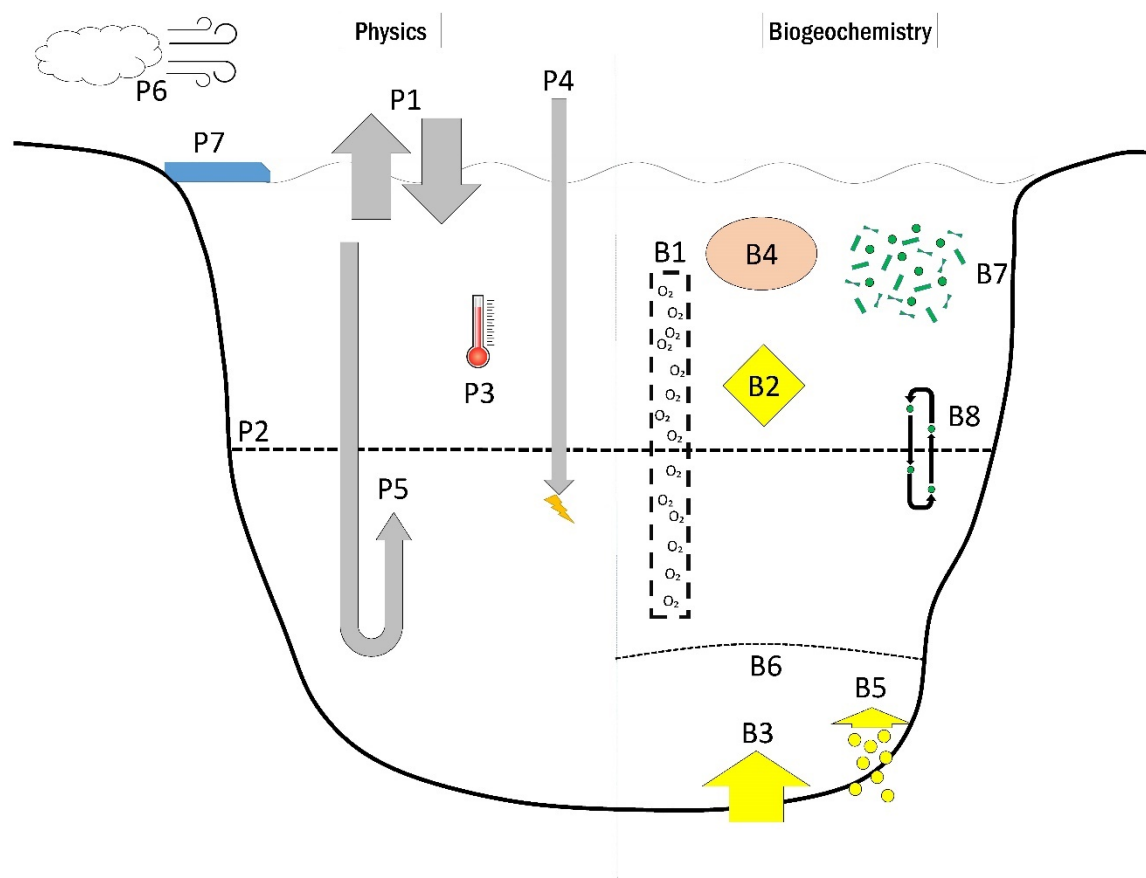


Figure 1: Overview of the physical and biogeochemical components and processes in deep lakes considered in the text. P denotes a physical and B a biogeochemical process. Energy fluxes at the air-water interface (P1) represent the interaction between climate and the lake. Thermal stratification (P2) is important for transport between water layers and is formed primarily by higher water temperatures (P3) in the surface layers compared to bottom layers. Light penetration (P4) causes heating of surface layers and is essential for phytoplankton growth. Deep-water mixing (P5) can occur as a result of strong convective cooling and marks the end of the stratified season. Wind stress (P6) also promotes mixing and deepening of the mixed layer. Ice cover (P7) affects surface heat fluxes and reduces effects of wind on the lake interior. Oxygen concentration (B1) is linked to many chemical and biological processes in the water column. Nutrient concentrations (B2) in the epilimnion are essential for the growth of phytoplankton. Nutrients and other type of solutes can be released from the sediment (B3). Coloured dissolved organic matter (CDOM, B4) reduces light penetration in the water column. Greenhouse gases can be emitted from the sediment (B5). If the deep-water layers of a lake are heavier than the overlying water due to solute content, meromixis is formed (B6). Phytoplankton biomass (B7) grows through consumption of resources such as nutrients and light in the photic zone of the lake. Some cyanobacteria have variable buoyancy (B8) that enables uptake of nutrients from below the thermocline, or they may use their buoyancy to form deep chlorophyll maxima in the metalimnion of the lake.

WATER TEMPERATURES AND STRATIFICATION

(Figure 1: P1, P2, P3) The increase in global surface air temperature (IPCC 2014) has an impact on lake temperature and water column stratification. Global surveys of surface water temperatures report an increase in epilimnetic temperatures with rates roughly between 0.2 and 1°C per decade (Shimoda et al. 2011; Kraemer et al. 2015; O'Reilly et al. 2015). The temperature difference between epi- and hypolimnion often increases, causing longer and stronger thermal stratification in summer (Fang and Stefan 1999; Foley et al. 2012; Kraemer et al. 2015). Even when temperature differences remain the same, the density difference becomes greater with warming, as the water density-temperature relation is steeper at higher temperatures (Wetzel 2001). As the density difference between epi- and hypolimnion increases, mixing of the two layers is reduced, which further heats the surface layer and increases density differences, as less heat is transported downwards. The stability of the water column is often expressed as the Schmidt stability (i.e. the potential energy stored in stratification per unit area) (Schmidt 1928; Idso 1973). Between 1970 and 2010, average Schmidt stability in lakes worldwide has increased by up to 25% (Kraemer et al. 2015).

(Figure 1: P2) A larger density difference between the epilimnion and hypolimnion increases the local stability of the water column. An increase in stability reduces the vertical turbulent diffusivity K_z , which indicates the rate of vertical mixing (Ravens et al. 2000; Wüest et al. 2000). Hence, a stronger stratification implies that dissolved substances less easily traverse the thermocline, promoting separation between surface and bottom waters.

OXYGEN DYNAMICS IN DEEP LAKES

(Figure 1: P2, P4, P5, B1) Oxygen sources (reaeration and photosynthesis) are mainly restricted to the epi- and metalimnion (Wetzel 2001; Obrador et al. 2014; Giling et al. 2017b), and in most lakes oxygen is constantly being depleted in the hypolimnion, especially near the sediment. Generally, deep convective mixing is often the major source of oxygen replenishment in the deep-water layers (Straile et al. 2003), although river intrusion can also notably affect hypolimnetic oxygen conditions (Fink et al. 2016). The extent of the oxygen-depleting processes in the water column and the sediment, the volume of the hypolimnion, and the sediment area to hypolimnion volume ratio define the rate at which oxygen concentrations fall after installation of the thermocline (Schwefel et al. 2018). Hypolimnia of highly productive systems have a higher oxygen depletion rate (Rippey and McSorley 2009; Müller et al. 2012). Deeper lakes contain more oxygen due to a thicker hypolimnion, and oxygen depletion rates tend to decrease with depth, so deeper lakes are less prone to become anoxic in one summer (Müller et al. 2012; Schwefel et al. 2018). However, they are less likely to experience complete vertical mixing, and climate warming further decreases this likelihood. In the case of incomplete mixing, the oxygen is only partially replenished and the hypolimnion will experience lower oxygen levels the following year. Therefore, a shift from holomictic to oligomictic behaviour implies a greater risk of anoxic conditions, for productive lakes in particular.

(Figure 1: P3, P5, B1) Numerous observations of hypolimnetic anoxia are attributed to shifts in the extent of mixing exist in both temperate (Foley et al. 2012; Ito and Momii 2015) and tropical regions (O'Reilly et al. 2003; Fukushima et al. 2017), and climate change is expected to amplify this trend (Peeters et al. 2002; Fang and Stefan 2009; Sahoo et al. 2013). While eutrophication is often seen as the main cause of anoxia, changes in deep-water mixing can be at least as important in deep lakes (Schwefel et al. 2016). Aside from the increase in stratification, climate change can affect hypolimnetic oxygen through increased temperatures as well, as mineralisation and metabolic rates are higher at higher temperatures, in the order of a 3%-6% increase per °C (Fang and Stefan 2009; Gudasz et al. 2010). In this way, hypolimnetic warming could increase the intensity of oxygen depletion in the hypolimnion and sediments (Straile et al. 2003).

INFLUENCE OF ANOXIA ON NUTRIENT DISTRIBUTION AND OTHER SUBSTANCES

(Figure 1: B1, B2, B3) Anoxia near the sediment can induce enhanced internal phosphorus loading through reduction of the benthic redox potential, so that iron-bound phosphate is released from the sediment (Søndergaard et al. 2003). While this enhanced release can be relevant on short time scales, on seasonal (or longer) time scales internal P budgets are mostly dependent on settling and mineralisation rates, as well as

sediment characteristics (Hupfer and Lewandowski 2008). During stratification, P tends to accumulate in the hypolimnion as nutrients are not mixed into the photic zone while mineralisation in the sediment and pelagic continues. When deep mixing occurs, large amounts of P can enter the photic zone, potentially boosting productivity (Lehmann et al. 2015; Lepori et al. 2018). Nitrogen can also be released from the sediment under anoxic conditions in the form of ammonium (Wetzel 2001). Denitrification occurs in anoxic hypolimnia and, especially, sediments (Wetzel 2001). It is a major loss term of nitrogen in lakes. When anoxia of the hypolimnion is ended by a mixing event, nitrogen, like phosphorus, can enter the photic zone and boost productivity. However, large losses of nitrogen to the atmosphere can occur through denitrification, as nitrate-rich water is brought in contact with the anoxic sediment (De Brabandere et al. 2015; Lehmann et al. 2015).

(Figure 1: P5, P6, B1, B2, B3) The stratification that is at the root of this build-up of nutrients in the hypolimnion, however, also prevents nutrients from entering the epilimnion, as increased stratification implies that dissolved substances are retained more in their respective layers. Reduced entrainment of deeper water layers and less intense winter mixing could cause decreased nutrient concentrations in the epilimnion, despite the higher nutrient concentrations in the hypolimnion (Yankova et al. 2017; Schwefel et al. 2019). As nutrients accumulate in the hypolimnion because of increased stratification with climate change, the amount of nutrients released to the epilimnion when complete mixing does occur goes up.

(Figure 1: B1, B3, B4, B5, B6) Apart from nitrogen and phosphorus, other substances are affected by hypolimnetic shortages of oxygen as well. Iron-oxide-bound carbon can be released as coloured dissolved organic matter (CDOM) under anoxia when iron is reduced (Hamilton-Taylor et al. 1996; Brothers et al. 2014). In the deep layers of meromictic lakes, the anoxic conditions enable the occurrence of reduction processes involving iron, manganese, and sulfide, which are often essential for creating and maintaining meromixis (Friedrich et al. 2014; Lehmann et al. 2015; Schultze et al. 2017). These elements can occur in dissolved form under anoxic conditions and accumulate in deep-water layers of meromictic lakes, where they increase deep-water density (Imboden and Wüest 1995; Gulati et al. 2017). Strong stratification and anoxia can also induce more methane emissions from lakes (Grasset et al. 2018; Vachon et al. 2019). Like dissolved solutes, dissolved methane and dissolved carbon dioxide can occur in high concentrations in deep, anoxic water layers, and affect density, with methane reducing and carbon dioxide increasing water density (Imboden and Wüest 1995; Schmid et al. 2002). The effect of dissolved gases on density can be especially important in lakes where there is a high influx of gases from the sediment, for example as a result of volcanic activity (Schmid et al. 2002).

INFLUENCE OF MIXING DYNAMICS ON LAKE PHYTOPLANKTON

(Figure 1: B2, B7) A change in nutrients in the epilimnion will strongly control phytoplankton development. As mentioned above, increased stratification might actually reduce nutrient levels in the surface water of lakes. Longer stratification in such a case means a longer period of nutrient limitation for phytoplankton (Yang et al. 2016a) and therefore a bigger advantage for species that efficiently use or store nutrients (Winder and Sommer 2012), and potentially for mixotrophic species, which have access to additional organic nutrient sources (Jansson et al. 1996). However, the effects of increased stratification and warming of surface waters differ between oligotrophic and eutrophic systems. In oligotrophic systems, a higher metabolic rate driven by higher temperatures in combination with nutrient shortage can lead to lower levels of biomass compared to colder temperatures, while in eutrophic systems, the higher temperature may boost growth and biomass (Jöhnk et al. 2008; Kraemer et al. 2017).

(Figure 1: P2, P4, B7, B8) Stratification also affects the phytoplankton's ability to remain near the surface and in the euphotic zone. Formation of a thermocline reduces the depth over which phytoplankton is mixed, effectively increasing their chance to remain in the photic zone (Huisman et al. 1999). At the same time, however, stratification reduces turbulence and vertical mixing deeper down in the water column, and sinking becomes a major loss term for many dense phytoplankton species (Diehl et al. 2002). A lower water viscosity at higher temperatures (Hutter and Jöhnk 2004) increases sinking rates and facilitates migration through buoyancy

regulation (Paerl and Huisman 2009). Stronger density stratification and suppression of turbulence thus may give an advantage to motile phytoplankton species (Huisman et al. 2004; Winder and Hunter 2008).

(Figure 1: P5, B2, B7, B8) Higher nutrient concentrations in the hypolimnion do not directly promote phytoplankton growth because of the lack of light at depth, with the exception of phytoplankton species that produce a deep chlorophyll maximum in the metalimnion (e.g. *Planktothrix rubescens*), or buoyancy regulators that are perceived to make excursions into the hypolimnion (e.g. *Microcystis*) (Fee 1976; Paerl and Huisman 2009). The strong vertical heterogeneity in nutrient levels induces the possibility that mixing events causing entrainment of hypolimnetic water into the epilimnion can lead to spikes of epilimnetic nutrient concentrations (Lehmann et al. 2015), stimulating phytoplankton blooms (Giling et al. 2017a). These events can be caused by extreme weather events such as storms, cold spells, or river floods (Jennings et al. 2012). With increased stratification in summer, the amount of energy needed for these deep mixing events increases, but the nutrient pulse after such an event tends to be stronger (Coats et al. 2006).

SHIFTS IN MIXING REGIME

In this section, we identify which processes could form positive or negative feedbacks that could lead to a shift in mixing regime. As these shifts are already unfolding and likely to continue into the future (Woolway and Merchant 2019), it is important to assess which changes to expect and if they are able to self-amplify under a given condition. The shifts in mixing regime that are treated here are: (1) from a polymictic to a seasonally stratified regime; (2) from a dimictic to a monomictic regime, where ice cover and inverse stratification in winter are disappearing; and (3) from a holomictic to an oligomictic or a meromictic regime. Here we investigate if and under what conditions feedback mechanisms can reinforce shifts in mixing regimes.

Two other shifts in mixing regime can also be expected with climate change, mediated through changes in hydrology. In lakes where water level is projected to decrease with climate change, a shift from stratified to polymictic can be expected if the water level falls below a critical value to sustain seasonal stratification (Zohary and Ostrovsky 2011; Kirillin and Shatwell 2016). Increase in water level could cause a shift in the opposite direction. Both temperature and water level can be a driver of a shift between polymictic and stratified regimes, and the feedbacks we discuss in the following section apply to both. In saline lakes, a reduction of freshwater inflow can cause a shift from meromictic to holomictic, as the freshwater layer on top of the heavier saline layer diminishes (Gertman and Hecht 2002; Kaden et al. 2010) and vice versa with an increase in precipitation (Melack and Jellison 1998). We are not aware of literature that describes feedbacks from the new mixing regime to the hydrological input, or changed biogeochemical conditions under the new regime that affect the vertical salt distribution in a way that affects the new regime's stability. Our view is therefore that such a response of the saline lake mixing regime is a direct function of the discharge and seasonality of the external inflow (although a threshold response is possible), and because of the lack of known internal feedbacks, we will not treat this regime shift further.

SHIFT FROM A POLYMICTIC TO A SEASONALLY STRATIFIED REGIME

Lakes of intermediate depth (c. 3–10 m mean depth, Kirillin and Shatwell 2016) can support both polymictic and seasonally stratified (dimictic or monomictic) regimes, based on morphometry, transparency, wind speed, and annual mean solar radiation flux (Kirillin and Shatwell 2016). A shift from polymixis to seasonal stratification might occur as a result of climate warming in these lakes (Kirillin 2010; Woolway and Merchant 2019). This trend can be amplified by reduced water transparency and lower wind speeds in summer (Shatwell et al. 2016). If transparency is reduced, less energy penetrates to deeper layers, as more solar radiation is absorbed near the surface. This can result in warming of the surface layer, cooling of the hypolimnion, and overall stronger stratification (Jones et al. 2005; Tanentzap et al. 2008), but the influence of transparency on stratification is significantly stronger in smaller lakes due to a lower contribution of wind mixing to turbulence formation (Fee et al. 1996). A decrease in transparency can be caused by phytoplankton growth or increased CDOM content, for example as a consequence of catchment-based inflow of nutrients or organic matter. CDOM loading from

peatlands or forests may increase as a function of climate change, for example through increased decomposition rates at higher temperatures (Jennings et al. 2010). Wind is a crucial factor in exchanging heat between atmosphere and lakes by inducing mixing (Imboden and Wüest 1995), and can be a decisive factor for hypolimnetic temperature trends. Indeed, decreasing wind speeds cause a cooling of the hypolimnion by reducing heat transfer to deep-water layers (Magee and Wu 2017). Regional trends in wind speed might have the potential to cause a shift in mixing regimes (Woolway et al. 2019). However, wind forcing is external to the lake system, and we are not aware of literature describing feedbacks between wind forcing and lake conditions that reinforce either the polymictic or stratified mixing regime.

Periods with warm and calm weather are promoted by climate change, and can induce stratification events in polymictic lakes, lasting multiple days or even weeks (Wilhelm and Adrian 2008). However, strong inter-annual variation in the duration of stratification within the same lake has been documented that cannot be explained by temperature changes alone (Riis and Sand-Jensen 1998; Brothers et al. 2014). Water transparency was determined to be a major factor of shifts in mixing regime in the studies of Riis and Sand-Jensen (1998), Brothers et al. (2014), and Shatwell et al. (2016), and is, as stated, influenced by phytoplankton growth and CDOM content.

In this paper, we are interested in feedbacks that would stabilise a newly established stratified regime, such as mechanisms that would perpetuate lower transparency. Brothers et al. (2014) described such a feedback in a eutrophic German lake with an average depth of 1.7 m (maximum 2.9 m) and a surface area of 3.3 ha. Strong rainfall flooded surrounding peatlands, leading to increased CDOM and nutrient concentrations and higher water levels (about 1 m) in the lake. Transparency was reduced due to a combination of increased CDOM and phytoplankton, which caused stratification and anoxia near the sediment, and promoted internal loading of CDOM and nutrients from the sediment, stabilising the stratified state. For a different lake, Riis and Sand-Jensen (1998) describe almost a doubling of the duration of stratification over a period of 40 years due to increased CDOM concentrations in an oligotrophic Danish lake of 8.1 m mean depth (maximum 12 m) and a surface area of 12 ha, but no stabilising feedbacks were identified. Model simulations of two eutrophic German lakes (maximum depths 8 and 9.5 m) by Shatwell et al. (2016) suggested that phytoplankton can have a decisive influence on mixing regimes in lakes of intermediate depth. The presence or absence of a clear-water phase in spring could change the mixing regime for that year. Again, no feedbacks are described. Still, in shallow lakes a heatwave or period of calm can trigger a period of stratification and potentially cause anoxia when oxygen depletion is sufficiently high, followed by nutrient release to the photic zone when stratification ends (Wilhelm and Adrian 2008). When the accumulated nutrients become available to phytoplankton during stratification, for example due to buoyancy regulation, the ensuing bloom could reduce transparency, leading to stronger heating of the upper water layers (Jones et al. 2005), and thus stabilise the stratified regime.

However, despite the crucial role of transparency in regulating thermal stratification and the study of Brothers et al. (2014) showing the potential of the transparency-reduction feedback in environmental data, this feedback might only apply to a select set of lakes. Below, we give three arguments why the likelihood that this feedback will cause bi-stability of polymixis and seasonal stratification might be limited: (1) the feedback can regularly be overridden by external perturbations unless a specific set of lake conditions, regarding morphometry and transparency, is present; (2) stratification hinders exchange between sediment and surface water, effectively weakening the feedback; and (3) there is a reset of lake conditions in winter and no carry-on of the feedback to the next year.

The feedback therefore requires a specific set of conditions to effectively influence lake mixing regime. Lakes that are too shallow cannot sustain seasonal stratification as commonly recurring convective or wind mixing events break down stratification completely. Conversely, deeper lakes often already have a stratified regime, thus restricting bi-stability to lakes with an intermediate depth range (c. 3-10 m, Kirillin and Shatwell 2016). In lakes larger than approximately 5 km², wind and convective mixing are the decisive factors to determine the

depth of stratification and transparency only has a minor effect (Fee et al. 1996), whereas Kirillin and Shatwell (2016) report a decreasing effect of transparency on mixing regime above a lake length of about 1-10 km based on an analysis of 379 lakes. Therefore, the feedback described above would only be relevant in small lakes of intermediate depth. Additionally, Persson and Jones (2008) show that in already turbid water, a change in transparency has little effect on thermal stability, which would suggest that the transparency-reduction feedback requires an initially low turbidity. If all light was already absorbed in the mixed layer before the reduction of transparency unfolds, a further drop in transparency would not make a large difference in heat distribution (Persson and Jones 2008). Along the same lines, a sensitivity analysis in the modelling study by Shatwell et al. (2019) indicated that the effect of varying transparency on stratification is strongest in small lakes with low to medium (up to c. 1.0 m^{-1}) extinction coefficients.

Stratification restricts exchange of dissolved materials between deep and shallow water layers. Therefore, sediment release of CDOM and nutrients would only marginally reach the epilimnion and affect light penetration. Nutrients would reach the surface layer after a mixing event, as is supported by findings of blooms after the end of stratification events (Wilhelm and Adrian 2008), but this would break the transparency-reduction feedback. Buoyant cyanobacteria could – potentially - use the nutrients in the hypolimnion and move across the thermocline into the light to grow (Paerl and Huisman 2009), keeping the feedback loop intact, although the reality of this remains under discussion (Bormans et al. 1999). In the study of Brothers et al. (2014), sediment release of substances did influence the pelagic despite consistent stratification, but the role of the thermocline was not discussed. The presence of a thermocline limits turbulence reaching the sediment, so stratification reduces resuspension of particles that sink to the bottom and promotes sedimentation losses. Formation of stratification can thus reduce particle-based turbidity. The reduced turbidity in turn decreases stratification, completing a negative feedback loop (Figure 2a). If the turbidity is caused by sinking particles (e.g. non-buoyant phytoplankton cells), this negative feedback inhibits sustenance of the stratified state.

Lastly, in winter, phytoplankton biomass is low and complete mixing occurs, so the feedback loop is broken. Therefore, there is no carry-over of mixing regime from year to year. Years with enhanced stratification could easily be followed by a year with polymictic behaviour since the occurrence of seasonal stratification in one year does not influence the likelihood of stratification in the next year. Stratification can be triggered by a period of warm and calm weather, which makes timing a relevant issue. A heatwave in spring/early summer can affect the mixing regime for the rest of the year, but a similar event at the end of summer has only a brief effect.

Summarising, in a polymictic lake of intermediate depth, a seasonally stratified regime can establish under lower wind speeds, decreased transparency, or a higher water level (Kirillin and Shatwell 2016). Changes in transparency can strongly influence thermal stability (Persson and Jones 2008; Tanentzap et al. 2008), and even shift mixing regimes (Brothers et al. 2014; Shatwell et al. 2016). Feedback loops could sustain the stratified state (Figure 2a), which might cause a sudden shift from a polymictic to a seasonally stratified regime for a particular year (Figure 2b). However, as discussed above, there is a suite of reasons why these feedbacks may not be dominant in most lakes.

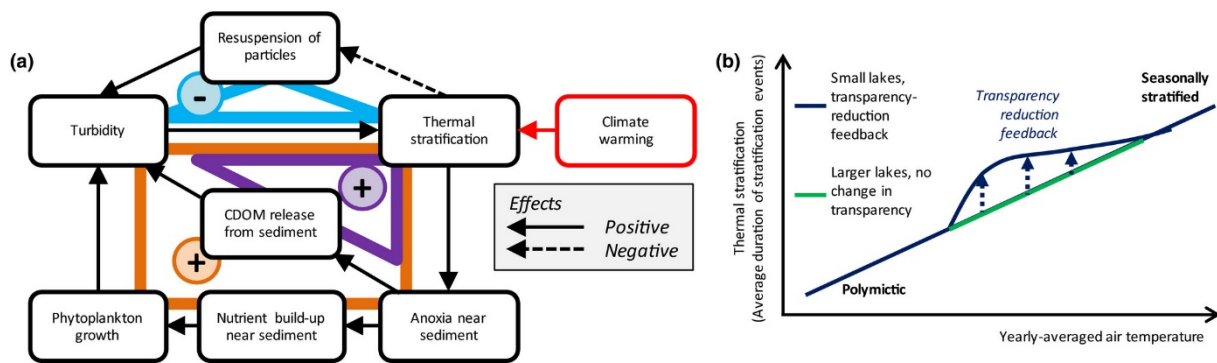


Figure 2: (a) The associated feedbacks for a shift from a polymictic to a seasonally stratified regime. Solid arrows denote a stimulating (positive) effect and dashed arrows a reducing (negative) effect. The effect of climate warming is shown in red. Three feedback loops are potentially formed. Both the purple and the orange feedback loops are positive (i.e. self-reinforcing). The blue, negative feedback loop is activated when the turbidity that supports the stratification is reduced because of sinking particles. **(b)** State diagram of a shift from a polymictic lake of intermediate depth to a seasonally stratified regime. Climate warming increases the duration of stratification events. When these periods become long enough to trigger a reduction in transparency, in some years there might be a sudden jump to a longer stratified period. This is most likely to occur in small lakes, where transparency has the strongest control on stratification patterns (blue line). If the turbidity is caused by sinking particles, sedimentation of these particles will result in clearer water and the breakdown of stratification. In larger lakes, or lakes where the positive feedbacks are only weak, the increase in duration of stratification will be more linear (green line). In a seasonally stratified regime, a reduction in transparency will not, or only marginally, increase the length of the stratified period.

SHIFT FROM A DIMICTIC TO A MONOMICTIC REGIME

Near the poles, loss of ice cover in deep lakes is likely to turn amictic lakes into cold monomictic lakes, and cold monomictic into dimictic lakes (Nöges et al. 2009). In temperate regions, it forces the two separate mixing events at the end of autumn and the end of spring into one period with a more-or-less uniform temperature profile; a shift from dimixis to monomixis (Ficker et al. 2017; Sharma et al. 2019).

For a freshwater lake of a given morphometry, weather conditions and water temperature determine whether ice forms or not (Leppäranta 2015). Climate change drives the atmosphere towards warmer conditions, but due to natural variation in weather, perpetuation of ice-free conditions after one ice-free winter is unlikely unless water temperatures express a memory of previous winters. Such a memory might be established due to the large thermal heat capacity of deep lakes and a dominant effect of ice-albedo. Ice has a higher albedo than water (i.e. ice reflects more shortwave radiation), reducing heating of an ice-covered lake. When ice disappears, the surface water warms faster through absorption of solar radiation (Austin and Colman 2007). A modelling study on the Laurentian Great Lakes under a prescribed weather cycle, atmospheric noise, and slow climatic forcing, showed that ice in deep lakes can prevent lake warming by its high albedo and promotes ice cover in following years (Sugiyama et al. 2017), which we define as a memory effect. Once ice disappeared, deep water layers warmed up to a larger degree, making it harder for water temperature to reach freezing levels in following years.

Only sufficiently deep lakes have the necessary thermal heat capacity to transfer the effect of ice cover to the next winter; Sugiyama et al. (2017) investigated lakes with an average depth of at least 50 m, but do not give a minimum depth required to generate a memory effect. Bi-stability occurred in ranges of annual mean air temperatures of c. 0.5°C (for lakes of 50 m depth) and c. 1.5°C (for lakes of 150 m depth). Outside of these ranges, the lakes were always ice-covered, or always ice-free, regardless of the ice cover in previous winter.

Apart from its higher albedo, ice insulates the lake from the atmosphere, limiting heat loss to the atmosphere in winter (Leppäranta 2015; Zhong et al. 2016). This insulation works in an opposite direction as the ice-albedo feedback (Figure 3a), and it weakens the memory effect. The relative importance of both processes is still disputed, but Sugiyama et al. (2017) find a dominant ice-albedo feedback with a one- to three-column model. In contrast, at a higher spatial resolution, Zhong et al. (2016) and Ye et al. (2019) did not find a dominant memory effect and state that the role of ice albedo is small, suggesting a smoother transition from dimictic to monomictic

with a warming climate. All three modelling studies were performed in a similar environment (the Great Lakes region) and actively investigated the role of ice-albedo in determining thermal structure. Similar to Zhong et al. (2016) and Ye et al. (2019), the modelling study of Shatwell et al. (2019) reported a gradual shift from ice-covered to ice-free winters in two lakes of 20-30 metres mean depth in Europe, rather than an abrupt shift. Other studies on the ice-albedo feedback and thermal memory in lakes are scarce. However, this topic has been addressed for sea ice; modelling studies suggest that the response of sea ice to atmospheric temperature changes might show lags, but is not truly bi-stable (Ridley et al. 2012; Li et al. 2013), and therefore a gradual loss of ice cover is to be expected.

In brief, although the role of ice albedo in lakes is still debated, it is generally considered that memory effects of ice cover in lakes have only a minor influence. In case of a dominant memory effect caused by a large thermal heat capacity and a dominant ice-albedo feedback, shifts in mixing regime between monomictic and dimictic lakes would have a sudden nature (Figure 3b, blue lines). If destabilising positive feedbacks are weak, a smoother transition from monomictic to dimictic is expected, with alternating dimictic and monomictic years (Figure 3b, green line). Both the ice-albedo feedback and the insulation effect could be relevant for the shifts from amictic to cold monomictic and from cold monomictic to dimictic as well. However, literature on these mixing regime shifts is limited.

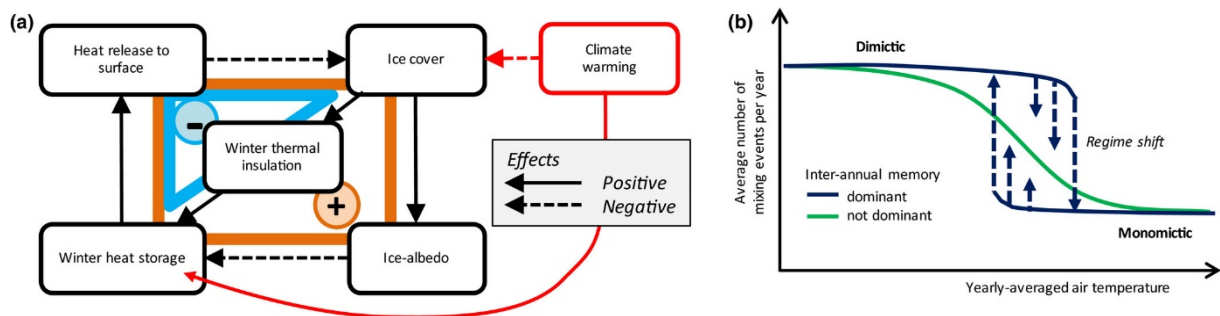


Figure 3: (a) The associated feedbacks for a shift from a dimictic to a monomictic regime. Solid arrows denote a stimulating (positive) effect and dashed arrows a reducing (negative) effect. The effect of climate warming is shown in red. Two feedback loops are formed. The blue feedback loop is negative (i.e. self-stabilising), while the orange loop is positive (self-reinforcing). (b) State diagram of a shift from a dimictic to a monomictic regime. Inter-annual thermal memory is supported by a large heat storage capacity and the positive feedback in (a). In case of a dominant memory effect, shifts in mixing regime would have a sudden nature (blue line and arrows), while if the memory effect is not dominant (green line), there is a smoother transition, with alternating dimictic and monomictic years. The length of the dotted arrows denotes the probability of a regime shift from one mixing regime to another.

SHIFT FROM A HOLOMICTIC TO AN OLIGO- OR MEROMICTIC REGIME

Some lakes that are (becoming) monomictic are experiencing less complete mixing events, and decreases in the maximum mixing depth as indicated by oxygen profiles (North et al. 2014; Saulnier-Talbot et al. 2014). Hydrodynamic models driven by climate scenarios predict this trend to continue, resulting in a progressively decreasing maximum mixing depth (Matzinger et al. 2007; Sahoo and Schladow 2008; Schwefel et al. 2016). Complete mixing – i.e. top to bottom - can even disappear entirely and maximum mixing depth could decrease by up to 80% (Matzinger et al. 2007; Sahoo and Schladow 2008). Perroud and Goyette (2010) predict a decrease in duration of fully mixed conditions for the peri-alpine Lake Geneva (Switzerland/France). These findings imply that complete mixing in monomictic lakes will decrease in the future and parts of the hypolimnion can stay isolated from the atmosphere for multiple years.

However, in oligomictic lakes there is an interplay between the increase in hypolimnetic temperature and the frequency of complete mixing events. The hypolimnion slowly heats over the year as a result of the geothermal heat flux and as warmer water from the epilimnion is gradually mixed into the deeper layers by turbulence. Incomplete winter mixing fails to cool the hypolimnion, resulting in a warming trend. This increase in hypolimnetic temperature facilitates complete mixing in subsequent years, as less cooling is required for an overturn. Additionally, the higher thermal expansivity of water at higher temperatures can increase the

likelihood of complete mixing in lakes with elevated salt concentrations in the hypolimnion (Matzinger et al. 2006). When deep mixing finally occurs during a colder winter, hypolimnetic temperatures show a sudden drop and the resistance to full mixing in subsequent years would increase again. This is why this process is referred to as a sawtooth pattern (Livingstone 1993; 1997). This pattern has been observed in several deep lakes (e.g. Stralle et al. 2003; Coats et al. 2006; Lepori and Roberts 2015), and might facilitate sporadic overturn events even under milder temperatures. Climate warming is predicted to lengthen the warming periods and reduce the frequency of turnovers and subsequent cooling (Livingstone 1997). In accordance with the sawtooth-pattern feedback, a decrease in the extent of winter mixing is expected during ongoing climate warming. However, if a new plateau in air temperatures is reached, the frequency of complete mixing is likely to return to its previous level as hypolimnetic temperatures catch up with winter temperatures, unless meromixis develops.

In both oligomictic and meromictic lakes, oxygen replenishment in the hypolimnion is strongly reliant on sporadically occurring winter mixing, and a reduced frequency of overturns means an increased likelihood of anoxia (Foley et al. 2012; Schwefel et al. 2016). As a secondary effect of the increased anoxia, internal nutrient loading and harmful effects for lake productivity and fish can be expected as a lake shifts from a holomictic to an oligomictic regime (O'Reilly et al. 2003). Internal loading in stratifying lakes changes the distribution of nutrients in the system, by increasing the concentration in the hypolimnion, but affecting the epilimnion only to a lesser extent. As eutrophication also increases oxygen depletion in the hypolimnion, eutrophication and climate warming both increase the risk of anoxia.

Model studies of deep-water mixing predict a reduced frequency of complete turnovers or even a complete disappearance, but as a gradual trend (Danis et al. 2004; Sahoo et al. 2013; Schwefel et al. 2016). The sawtooth pattern of hypolimnetic temperatures in oligomictic lakes facilitates deep mixing events after years with incomplete mixing (Livingstone 1993). However, most of the studies above did not include an effect of solutes (i.e. salinity) on water density - a decisive factor in the formation of meromixis (Boehrer and Schultze 2008; Camacho et al. 2017). Meromictic lakes have a denser, chemically different water layer below the hypolimnion, which is rarely mixed into the upper layers. Meromictic lakes can behave strikingly differently from thermally stratified lakes in terms of temperature profile, water renewal, chemistry, and ecology (Gulati et al. 2017; Lepori et al. 2018). The causes of meromixis are diverse (see Gulati et al. 2017), but a common characteristic is that the density difference is sustained. For example, in case of high iron concentrations below an oxic water layer, iron that is mixed into oxic water tends to precipitate and sink back into the anoxic water, where it dissolves again and maintains the density stratification (Boehrer and Schultze 2008). Internal processes like this make meromixis generally a very stable mixing regime.

Endogenic meromixis is a form of meromixis that is sustained by decomposition and increased concentrations of dissolved substances by biogeochemical cycles in the deep water layer (for full explanation, see Boehrer and Schultze 2008). This leads to the hypothesis of anoxia as a potential trigger for endogenic meromixis (Hutchinson 1957; Julià et al. 1998). In this situation, the onset of anoxia sets off the formation of a heavier water layer by an increased build-up of solutes in the hypolimnion and complete mixing becomes too infrequent to distribute these solutes through the water column. This build-up of solutes suppresses further mixing and could cause a more abrupt and permanent formation of meromixis. In Lake Lugano (Italy/Switzerland), a large (49 km²) and deep (maximum depth 288 m) per-alpine lake, endogenic meromixis might have formed as a result of anthropogenic eutrophication (Lepori et al. 2018). The possibility of meromixis caused by climate change has not been addressed often in scientific literature. Julià et al. (1998) mentioned climate-induced anoxia as a potential cause of meromixis in the Spanish Lake La Cruz. In a modelling study of the oligotrophic, monomictic Lake Ohrid (North Macedonia/Albania, maximum depth 289 m), Matzinger et al. (2007) found that above an atmospheric warming rate of 0.02°C/yr, hypolimnetic temperature increase would fall behind surface water warming rates. Additionally, solute accumulation in the hypolimnion would further increase the density of deep waters, preventing complete overturns in future scenarios (Matzinger et al. 2007). The increase in solute concentration must be strong enough to offset a reduction of density by hypolimnetic warming (Figure 4a).

Several physical lake processes can mix surface water into the hypolimnion, even when a chemical gradient is present, therefore reducing density differences. Wind-induced internal waves increase turbulence around the thermocline, and therefore mixing between both layers (Imboden and Wüest 1995). Differential cooling is the process where shallow areas experience fast convective cooling and this water mass moves downwards along the lake slopes in cases where morphology is suitable. This can lead to transport of water from the surface to deep water layers (Peeters et al. 2003; Ambrosetti et al. 2010). Intrusion of river inflow is another potentially important factor for deep-water renewal (Ambrosetti et al. 2010). Depth of river intrusion depends on inflow water temperature and lake thermal structure, amongst others (Fink et al. 2016). High sediment densities in the inflow can increase water density and allow penetration into the hypolimnion (Loizeau and Dominik 2000; Fink et al. 2016). In lakes where these processes cause significant deep-water renewal, a shift to meromixis is less probable. Formation of meromixis due to climate warming is also not likely in dimictic or polymictic lakes where complete mixing is frequent, but could occur in monomictic lakes in multiple climate zones.

It is difficult to determine in which lakes a shift towards meromixis is most likely to occur. Prime candidates are lakes that did not experience prolonged periods of anoxia and incomplete mixing until now, but are susceptible to experience these with the effects of climate change. Deeper lakes in particular seem to be vulnerable due to their tendency to mix incompletely (Danis et al. 2004). However, these are not the only factors, as also the chemical composition of the sediment and underlying bedrock determines the nature and quantity of compounds that can be released under anoxic conditions (Del Don et al. 2001; Boehrer and Schultze 2008). Additionally, Matzinger et al. (2007) suggest that meromixis is stimulated under a high rate of warming, which puts lakes at risk that lie in parts of the world that are experiencing rapid warming. Altogether, the likelihood of formation of meromixis with climate change is not obvious, and lake-specific approaches are necessary to evaluate this risk. Modelling efforts such as the one by Matzinger et al. (2007) are a promising approach, which should be supplemented by lake-specific information on sediment release rates of major density-affecting solutes.

In summary, as a holomictic lake warms, the likelihood of incomplete mixing increases, especially under rapid warming rates (Matzinger et al. 2007). This creates an oligomictic regime, where the sawtooth pattern (Livingstone 1997) may result in complete mixing in some years. This oligomictic regime increases the chance of anoxia and solute accumulation in the hypolimnion, potentially culminating in a sudden shift to meromixis (Figure 4b). Once a lake becomes meromictic, it might be difficult to reverse this change (Lepori et al. 2018). Lakes with the potential of strong solute release from the sediment and weak deep-water renewal are most susceptible to such a shift.

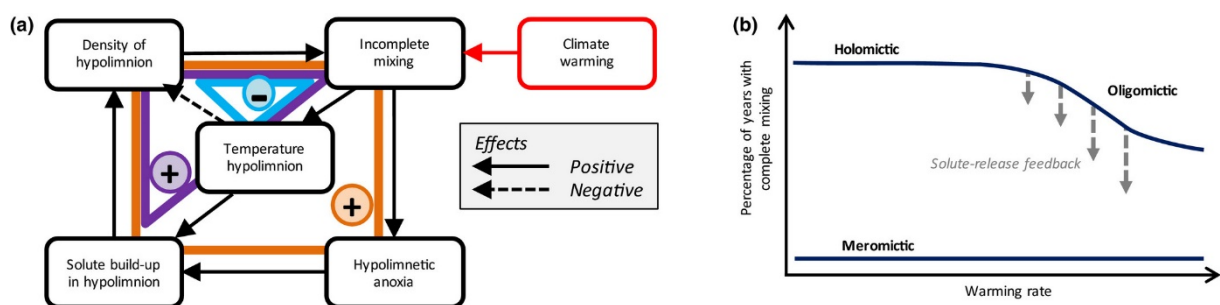


Figure 4: (a) The associated feedbacks for a shift from a holomictic to an oligo- or meromictic regime. Solid arrows denote a stimulating (positive) effect and dashed arrows a reducing (negative) effect. The effect of climate warming is shown in red. The negative (self-stabilising) feedback loop, in blue, causes a decrease in the density of the hypolimnion after incomplete mixing, while the positive (self-reinforcing) feedback loops, in purple and orange, stimulate a density increase. (b) State diagram of a shift from a holomictic to either an oligomictic or a meromictic regime. When incomplete mixing occurs as a result of warming, an oligomictic regime is formed. This increases the chances of forming anoxia and solute accumulation, potentially resulting in a meromictic regime if the density increase by solute build-up (positive feedbacks) exceeds the density decrease by hypolimnetic warming (negative feedback). The length of the dotted arrows denotes the probability of a regime shift from an oligomictic to a meromictic regime, but the possibility for this shift depends on lake-

specific characteristics. A shift is most likely to occur in lakes with little deep-water renewal, where large quantities of solutes can be released from the sediment.

CONCLUSION

Climate change can cause shifts in the mixing regime of deep lakes, which will change their behaviour in terms of physics, chemistry, and biology. In this study, we investigated whether certain feedbacks could affect these regime shifts. The investigated potential shifts are from polymictic to seasonally stratified, from dimictic to monomictic, and from holomictic to oligo- or meromictic. All these shifts in mixing regime display reinforcing feedback mechanisms, but these feedbacks are likely to be relevant under certain conditions only. In lakes of intermediate depth, polymixis and seasonal stratification can be alternative states, based on transparency and wind sheltering. If a period of stratification can trigger a strong reduction in transparency, for example due to phytoplankton bloom formation or release of CDOM, a stratified regime can form. However, this feedback is valid only under a narrow range of lake conditions, and the stratified state is not carried over from year to year, which is a full reset occurs each year. Dimictic lakes can become monomictic due to loss of ice cover. One study found that a shift from dimixis to monomixis could show bi-stability because of the ice-albedo feedback coupled to thermal heat capacity in sufficiently deep (at least 50 m average depth) lakes, but other studies in lakes and the sea suggest the opposite. The majority of studies would predict only a minor influence of memory effect of ice cover on lake dynamics, and therefore a gradual shift from mostly ice-covered to mostly ice-free winters. A climate-induced shift from holomixis to meromixis can occur if a density increase of the deep water layer by solute build-up outweighs a density decrease due to hypolimnetic warming. Such a shift would have profound influences on aquatic ecosystems, but more research is needed on this topic to assess where and when this can happen. If incomplete mixing does not result in a net density increase of the deep waters, an oligomictic regime is formed.

Although climate, interannual temperature variation, and morphometry are the main determinants of a mixing regime, transparency, water level, and internal feedbacks can facilitate and stabilise shifts between mixing regimes. Without denying the value of studies investigating mixing regime shifts driven by warming alone, we hope this paper places those findings in the perspective that several other components of lake ecosystems can influence mixing regimes as well. A change in mixing regime can mean a step-change in a physico-chemical parameter (e.g. anoxia) that can feed back to the vertical density distribution or heat budget. If we consider these processes as well, we may get a better understanding of how climate change affects lake mixing regimes. Given the great importance of mixing regime for functioning of lakes, more knowledge on the likelihood of transitions and the stability of such changes would be important for lake management. Observations of shifts in mixing regime due to internal lake processes are important, but may be hard to realise due to the long timescales and required data involved. For each of the three mixing regime shifts studied in this paper, modelling approaches have made important contributions. Inclusion of biogeochemistry in modelling could lead to further advances when investigating the shifts polymictic-stratified and holomictic-meromictic. The study of feedback loops in lake processes has so far been focussed mainly on shallow lakes (e.g. Scheffer 1998). Our review is one of the first studies to systematically explore the potential feedbacks occurring in deep lakes, as well as the climate dependency of these mechanisms.

ACKNOWLEDGEMENTS

J.P.M. and J.A.A.S. were funded by the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie grant agreement no. 722518 (MANTEL).

CHAPTER 2 - PERFORMANCE OF ONE-DIMENSIONAL HYDRODYNAMIC LAKE MODELS DURING SHORT-TERM EXTREME WEATHER EVENTS

Jorrit P. Mesman^{1,2*}, Ana I. Ayala^{1,2}, Rita Adrian^{3,4}, Elvira de Eyto⁵, Marieke A. Frassl⁶, Stéphane Goyette^{1,7}, Jérôme Kasparian^{1,7}, Marjorie Perroud¹, Julio A. A. Stelzer^{1,3,4}, Don C. Pierson², Bas W. Ibelings¹

¹*University of Geneva, Institute for Environmental Sciences, 1211 Geneva 4, Switzerland*

²*Uppsala University, Department of Ecology and Genetics, 75236 Uppsala, Sweden*

³*Leibniz Institute of Freshwater Ecology and Inland Fisheries, Department of Ecosystem Research, Berlin, Germany*

⁴*Freie Universität Berlin, Department of Biology, Chemistry, and Pharmacy, 14195 Berlin, Germany*

⁵*Marine Institute, Furnace, F28PF65 County Mayo, Ireland*

⁶*Griffith University, Australian Rivers Institute, Brisbane, Australia*

⁷*University of Geneva, Group of Applied Physics, 1211 Geneva 4, Switzerland*

**Corresponding author: Jorrit.Mesman@unige.ch, University of Geneva, Institute for Environmental Sciences, 1211, Geneva 4, Switzerland.*

ABSTRACT

Numerical lake models are useful tools to study hydrodynamics in lakes, and are increasingly applied to extreme weather events. However, little is known about the accuracy of such models during these short-term events. We used high-frequency data from three lakes to test the performance of three one-dimensional (1D) hydrodynamic models (Simstrat, GOTM, GLM) during storms and heatwaves. Models reproduced the overall direction and magnitude of changes during the extreme events, with accurate timing and little bias. Changes in volume-averaged and surface temperatures and Schmidt stability were simulated more accurately than changes in bottom temperature, maximum buoyancy frequency, or mixed layer depth. However, in most cases the model error was higher (30-100%) during extreme events compared to reference periods. As a consequence, while 1D lake models can be used to study effects of extreme weather events, the increased uncertainty in the simulations should be taken into account when interpreting results.

Keywords: Storm, heatwave, model validation, Simstrat, GOTM, General Lake Model

INTRODUCTION

Over the last few years, limnologists have devoted increased attention to extreme weather events (e.g. Bertani et al. 2016; Kasprzak et al. 2017; Andersen et al. 2020; Chen et al. 2020). These are predicted to become more frequent and intense with climate change (IPCC 2014; Bailey and Pol 2016), and can have profound effects on lake ecosystems. Extreme weather events, such as storms and heatwaves, have a direct effect on lake physics. Wind storms can induce mixing events, cooling of the surface layer, resuspension of sediments, and deepening of the thermocline (Jennings et al. 2012; Andersen et al. 2020). Heatwaves have effects that are largely opposite to storms, as these cause heating of the water column and strengthen thermal stratification (Jankowski et al. 2006; Huber et al. 2012). The disturbance in the thermal profile and inflow conditions caused by these events often mediates further changes in nutrients, oxygen, and phytoplankton community (Huber et al. 2010; Klug et al. 2012; Kasprzak et al. 2017). Physical disturbances in the water column due to an extreme event are often short-lived (Wilhelm and Adrian 2008; Jennings et al. 2012; Kuha et al. 2016; Stockwell et al. 2020), although they can also have a longer effect (Huber et al. 2012; Andersen et al. 2020), depending on the time of year when

they occur (Mi et al. 2018), or whether water transparency is affected as part of the event (e.g. dissolved organic carbon loading, or suspended particles) (Klug et al. 2012; De Eyto et al. 2016; Perga et al. 2018). Moreover, a short physical disturbance does not automatically imply a short-lived effect on biogeochemistry and ecology. For example, short-term mixing events can be a major factor affecting the transport of nutrients, stimulating phytoplankton growth (Soranno et al. 1997; Crockford et al. 2015).

Numerical lake models are useful tools for understanding aquatic processes, disentangling causal factors, and for estimating future trajectories of the system (forecasting, climate scenarios). Recently, several studies have applied one-dimensional (1D) lake models to study the effects of extreme weather conditions on lake thermal structure or lake ecology (Bueche et al. 2017; Mi et al. 2018; Perga et al. 2018; Soares et al. 2019; Chen et al. 2020). However, there is still a lack of understanding on how accurately lake models actually simulate observed conditions during these short-term events. It is common practice to assess models on the basis of their goodness-of-fit (e.g. root mean square error or mean absolute error) over the whole calibration and/or validation period, but these long timescales obscure any potential errors during disturbance by and recovery from short-term events. Evaluating event-specific errors will help to understand and minimise the uncertainty in model studies concerning ecosystem effects of extreme weather events. Showing that a model is capable to accurately simulate system changes caused by extreme weather events, will increase our confidence in their capability to provide reliable estimates for future effects of climate change. This advanced model testing is an important step in a multi-level model assessment (Hipsey et al. 2020).

In the present validation study, we used more than 10 years of hourly and sub-hourly in-situ measurements of meteorological variables and water temperature from three lakes of varying depths and mixing dynamics, to assess model performance during short-term extreme wind and temperature events. The analyses were done with three 1D hydrodynamic models - Simstrat (Goudsmit et al. 2002; Gaudard et al. 2019), GOTM (General Ocean Turbulence Model, Umlauf et al. 2005), and GLM (General Lake Model, Hipsey et al. 2019). These three models differ in turbulence schemes, calibration procedures, forcing variables, and parameterisations. Additionally, we report on observed changes in lake thermal metrics during storms and heatwaves in lakes with different morphology and mixing regimes. We focus our analysis on lake temperature (full profile, volume-averaged, surface, and bottom temperatures) and stratification metrics (Schmidt stability, maximum buoyancy frequency, and mixed layer depth), based on high-frequency temperature profile observations and simulations. Changes in these thermal metrics can translate into further changes in water transparency, and distribution and transport of oxygen and nutrients, with repercussions on biological processes.

We assessed whether the models could reproduce the direction, magnitude, and timing of change during an event, what the accuracy of the models was during extreme events compared to standard conditions, and if there was a consistent tendency of the models to over- or underestimate changes during an event. Following this, we draw conclusions on the implications of our findings for applying 1D hydrodynamic models to short-term extreme wind and temperature events in different types of studies.

METHODS

OBSERVATIONAL DATA

Meteorological and water temperature profile data from Lough Feeagh (Ireland), Lake Erken (Sweden), and Müggelsee (Germany) were used for this study. Long-term records of sub-hourly water temperature profile and surface meteorological data were available for the period 2004-2017 at Müggelsee and between 2005 and 2017 for Lough Feeagh and Lake Erken. Measurements of air temperature, wind speed and wind direction, relative humidity, incoming solar radiation, and air pressure were collected at each lake. Cloud cover was available at hourly intervals in the database generated by Moras et al. (2019) for Lake Erken and from the airport Berlin-Schönefeld for Müggelsee (10 km distance from the lake), and daily observations on-site were made for Lough Feeagh.

Lough Feeagh (53°56'21" N, 9°34'33" W; mean depth 14.5 m; maximum depth 46 m) is a monomictic lake, located on the west coast of Ireland. It experiences high rainfall and wind speeds, has no winter ice cover, and is rich in dissolved organic carbon (DOC) as a result of drainage from surrounding peatlands (De Eyto et al. 2016). Meteorological records and lake temperature profile data are available with measurement frequencies of 1 and 2 min, respectively. Meteorological data were collected on the shore of the lake (Met Éireann 2018). The water temperature profiles were measured by an automated monitoring buoy above the deepest point of the lake, with temperature sensors at 0.9, 2.5, 5, 8, 11, 14, 16, 18, 20, 22, 27, 32, and 42 m below the surface (De Eyto et al. 2020).

Lake Erken (59°50'37" N, 18°35'38" E; mean depth 9 m; maximum depth 21 m) is a dimictic lake in the eastern part of Sweden. It has a surface area of 24 km² and experiences ice cover in winter and stratification in summer (Persson and Jones 2008). High-frequency (30-min) lake temperature data from 2005 onwards were used for this study. Meteorological forcing data with a 5-min frequency are available from July 2008 onwards, and hourly forcing data were used before this point in time. Meteorological data were collected from a station on a small island 500 m off shore, while water temperature was measured at a monitoring buoy that was located a further 500 m from the island, at 15 m depth. Water temperature measurements were made at 0.5 m depth intervals prior to 2016, and at 0.25 m intervals after 2016.

Müggelsee (52°26'24" N, 13°38'58" E; mean depth 4.9 m; maximum depth 8 m), located in Berlin, Germany, is the shallowest lake in this study. It has a surface area of 7.3 km², is wind-exposed, and classifies as a polymictic lake (Wilhelm and Adrian 2008). It experiences ice cover in most winters and stratifies during summer at high air temperatures and moderate wind conditions. Lake temperature data were collected by a floating monitoring station anchored 300 m from the northern lake shore at a depth of 5.5 m. Water temperature at 2 m depth was measured every 5 min, and a profile with 0.5 m depth intervals from the surface up to 5 m depth was measured every hour. Meteorological data were available every 5 min, measured at the monitoring station (for more details on used sensors and methodology, see Wilhelm et al. 2006).

Precipitation and in- and outflows were not included in this study, and the water level was kept constant in the simulations. The reason for this is that these data were available at lower frequencies than the forcing and model time steps, and potentially at lower frequencies than the effects of the investigated events. Additionally, annual water level fluctuations are generally less than 1 m in Lough Feeagh and Lake Erken (Moras et al. 2019; Kelly et al. 2020), and only around 0.25 m in Müggelsee (Driescher et al. 1993), so water level was assumed to be of minor importance for thermal stratification patterns. Water transparency was also kept constant in all three models. The light attenuation coefficient was calculated from the average Secchi depth (S_d) observed over the simulated period with equations specific for the conditions in each lake; attenuation coefficient = $2.7 / S_d$ (Feeagh; Koenings and Edmundson 1991), $2.4 / S_d$ (Lake Erken; based on observed Secchi depths and light profiles, unpublished data), and $1.3611 * S_d^{-0.7105}$ (Müggelsee; Hilt et al. 2010).

For information on gap-filling procedures, see Suppl. Mat. A.

LAKE THERMAL METRICS

Model fit was assessed for the following thermal metrics: lake temperature (full profile), volume-averaged temperature, surface temperature (≤ 1 m depth), bottom temperature (deepest observation), Schmidt stability (Schmidt 1928; Idso 1973), maximum buoyancy frequency squared (N^2 , hereafter referred to as “maximum buoyancy frequency”), and mixed layer depth. The R package “rLakeAnalyzer” (Winslow et al. 2019) was used to calculate volume-averaged temperature, Schmidt stability, and maximum buoyancy frequency, see Read et al. (2011) for formulas. The mixed layer depth was defined using an absolute density difference from the surface (following De Boyer Montégut et al. 2004; Wilson et al. 2020). A threshold of 0.15 kg/m³ was chosen, which gave robust estimates of the depth of stratification for all three lakes. If the density of the deepest measured temperature was within this density threshold, the water column was assumed to be completely mixed and

mixed layer depth was set to the deepest measurement. The relation between water temperature and density by Martin and McCutcheon (1999) was used.

LAKE MODELS

Three 1D hydrodynamic lake models were used in this study: Simstrat, GOTM, and GLM. The models take into account lake morphology in turbulence equations, but otherwise assume horizontal homogeneity. These models all simulate the vertical thermal lake structure and are forced by the same meteorological input, but are different in their code structure, processes included (such as seiche-induced mixing, or different wavelengths of light), and parameterizations for surface fluxes and turbulence, so that each model could result in potentially different outcomes. A full description of the governing equations used by each of these open source models can be found in Goudsmit et al. (2002) for Simstrat, Umlauf et al. (2005) for GOTM, and Hipsey et al. (2019) for GLM, in addition to manuals and support on the respective websites (Simstrat: <https://github.com/Eawag-AppliedSystemAnalysis/Simstrat>, GOTM: <https://gotm.net/>, GLM: <http://aed.see.uwa.edu.au/research/models/GLM/>. Last access: 2021-08-13). Specific settings for each model used in this study are provided in the Suppl. Mat. B. The main differences between the models are mentioned below.

Simstrat and GOTM have a fixed layer structure, resolving turbulent kinetic energy production and diffusion between layers of fixed thickness. Layers in GLM can vary in thickness or merge depending on the degree of turbulent kinetic energy. Simstrat was forced with wind direction as an additional input variable; this is used to resolve mixing caused by seiches. Ice cover modules are present in Simstrat and GLM, while there is no ice module in the version of GOTM used in this study. Air pressure is a constant value in Simstrat and GLM, and the average value over the simulated period was used in this study, while measured air pressure was used as input in GOTM. Additionally, the used version of GLM could not be run with sub-hourly forcing due to the inherent structure of the code, while a forcing frequency of 10 min was used for Simstrat and GOTM. To account for this difference, additional runs with hourly forcing were performed for Simstrat and GOTM. Whenever these hourly forcing runs were used instead of the ones with 10-min forcing, this is specifically mentioned.

CALIBRATION

A period of one year was used for model spin-up and calibration. Automatic calibration procedures were applied to minimise the error in water temperature at all depths. The standard calibration procedures available for each model were different. Simstrat applied the PEST (model-independent Parameter ESTimation and uncertainty analysis) software to minimise the sum of squares of the error (Doherty 2015). The ParSAC python package was used for GOTM. It maximises the log-likelihood using a differential evolution method. GLM was calibrated with the “nloptr” R package (Johnson 2014), using the Nelder-Mead simplex algorithm (Nelder and Mead 1965) to minimise the root mean square error. Model parameters and calibration ranges can be found in Suppl. Mat. C. The remainder of the data series was used as validation period and to identify extreme events.

STORM AND HEATWAVE EVENTS

Model performance during extreme weather events was assessed on a selection of ten storms and ten heatwaves per lake.

The storm events were defined using 10-min wind speed observations. For the purpose of identifying storms missing data were not filled (Suppl. Mat. A) so that only actual measured data were used. The period April-October was used due to the frequent absence of winter profile data in Lake Erken and Müggelsee, due to ice cover. We chose to base the events on the turbulent wind energy flux at 10 m above the surface (P_{10} , $W m^{-2}$) instead of wind speed, because it is a more direct measure of the amount of energy transfer to the lake, and thus a more direct measure of the atmospheric impact on thermal stratification. P_{10} was calculated as $P_{10} = \rho_{air} C_D U_{10}^3$, using a fixed drag coefficient (C_D) of $0.9 \cdot 10^{-3}$ (Wüest et al. 2000), where ρ_{air} is air density ($kg m^{-3}$) and U_{10} is wind speed at 10 m above the surface ($m s^{-1}$). The top 5% of daily sums of P_{10} were selected, and days

within this selection were considered as a single event if they occurred within two days from each other. Events with less than 10 h of measured water temperature data, or no prior thermal stratification (Lough Feeagh and Lake Erken only), were excluded. The exact timing of the start and end of an event were defined when the 8-h moving average of wind speed passed the 75th percentile of all observed wind speed data. Lastly, P_{10} was recalculated for the whole duration of an event, but the 75th percentile of all P_{10} data was subtracted, to attach value only to the periods with extremely high wind speeds. The events were then ordered by the summed P_{10} and the top 10 events were selected.

The heatwave events were defined using air temperature data. To select warm spells relative to the time of the year, that is, also outside of the middle of summer, the two warmest three-day degree-day periods for each month in the period April-August were taken, always in two separate years. If the temperature on the days before and after this three-day period was above the 95th percentile of that month, these days were also included in the event. Events that had insufficient water temperature data, or that were within one week of another heatwave event, were excluded. In that case, the next warmest period was chosen, until an event with enough lake data was found. For Lake Erken, only one event of the four warmest degree-day periods in April had enough data. Instead of picking a colder period in April, an extra event in August was selected.

In order to compare the response of the models during extreme events with average weather conditions, ten “reference” wind and temperature periods were defined. The selection methods and time periods were identical to the methods and periods used for the extreme events, but instead of selecting events with the highest daily sums of P_{10} or highest three-day summed temperature, periods with values closest to the median were chosen. Reference events could not be within one week of an extreme event and the duration was fixed to 24 h for wind periods, and three days for temperature periods (Figure 1). For Lake Erken, reference temperature periods were shifted one month (May-September), due to frequently missing data in mid-April because of ice cover.

Simulations were initialised one week before each event. This initialisation was done to minimise model error and differences between models at the onset of an event, but at the same time to allow spin-up time of the simulation. Restricting the simulation period before the extreme event allowed for direct quantification of model performance during extreme weather conditions and isolation of the effects of the event, avoiding the effects of accumulated model error during pre-event normal weather conditions.

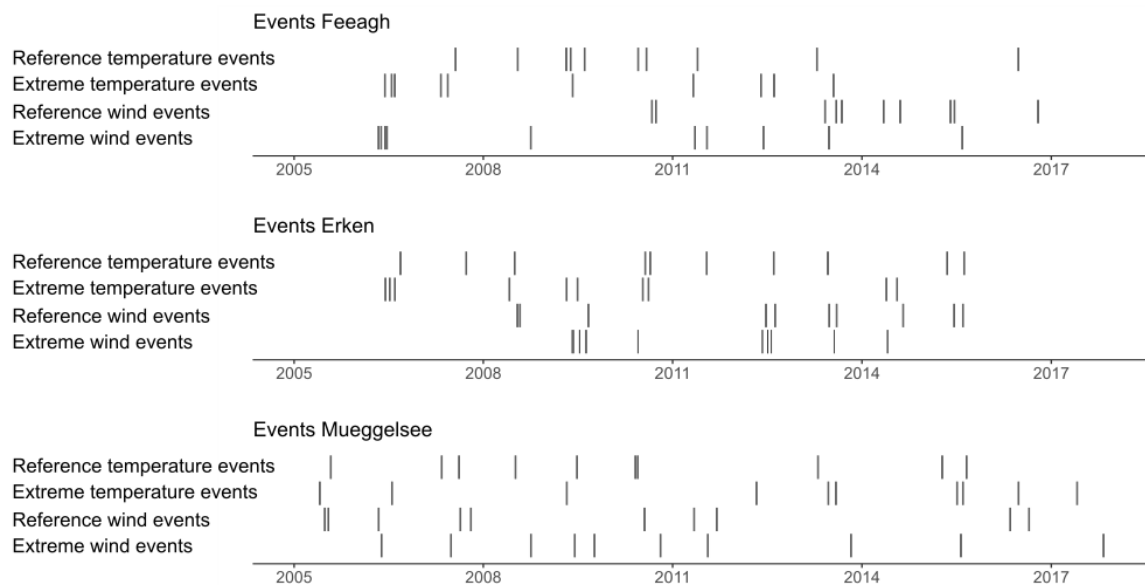


Figure 1. Timing of the extreme and reference events used in the analyses. The start and end dates of all events can be found in Suppl. Mat. D.

ASSESSMENT OF MODEL PERFORMANCE

Model performance was evaluated by comparing measured and simulated temperature profiles and the lake thermal metrics calculated from them, using Mean Absolute Error (*MAE*) as a measure for goodness of model fit. *MAE* was first calculated for the calibration and validation periods. Then, the *MAE* of the water temperature profile was compared between extreme and reference events with a *t*-test or a Wilcoxon rank-sum test (in case of non-normality or outliers) for each lake and storms and heatwaves separately. To see if different lakes and event types had a different effect on model fit, a two-way ANOVA on the *MAE* during extreme events only was performed. A post hoc Tukey test was done to compare lakes with each other. A one-way ANOVA on the *MAE* was done to compare the performance of the different models during extreme events, followed by a post hoc Tukey test.

In addition, the difference in thermal metrics between the two pre-event days and the two post-event days was defined as the change in a metric during an event. This change for each metric in observations was tested for significance with a *t*-test, or with a Wilcoxon sign test in case of non-normal data (assessed by QQ-plots and Shapiro-Wilk tests) or outliers. The performance of the models in simulating the change in a metric during events was assessed by inspecting plots and by calculating the Concordance Correlation Coefficient (CCC; Lin 1989) between the simulated and observed change in metric. The CCC is similar to Pearson's correlation coefficient, but penalises for a deviation from the 1:1 line and was therefore deemed a more accurate statistic for model comparison. To test for consistent bias in model simulations during events, a one-way ANOVA was performed on the change during an extreme event, for each lake, event type (storm/heatwave), and metric. A post hoc Tukey test was used to compare models with observations. In case the data was non-normally distributed (assessed by Shapiro-Wilk tests), a Kruskal-Wallis test and post hoc Dunn test were performed instead, using the "dunn.test" R package (Dinno 2017).

To evaluate model accuracy in simulating the timing of events, a temporal cross-correlation analysis was performed on the simulated and observed datasets for each event and each metric. The cross-correlation analysis temporally shifted the two datasets relative to each other, and the time lag with the highest cross-correlation coefficient was taken as the time lag in the simulation. Data gaps up to two h were linearly interpolated. Larger gaps were considered exclusion criteria for the cross-correlation analysis. Also, if the maximum cross-correlation coefficient between simulation and observations was below 0.3, the simulation was deemed too inaccurate to determine a time lag.

All analyses were done with the software R (version 3.6.2, R Core Team 2019). In those cases where the *p*-value of a statistical test was used to distinguish between significant and non-significant, an alpha of 0.05 was used.

RESULTS

MODEL PERFORMANCE FOR THE WHOLE SIMULATION PERIOD

The models successfully reproduced the seasonal cycles of temperature and stratification (Suppl. Mat. E). All models performed reasonably well, although GLM showed a poorer performance compared to the other two models, based on *MAE* during the calibration and validation periods (Figure 2).

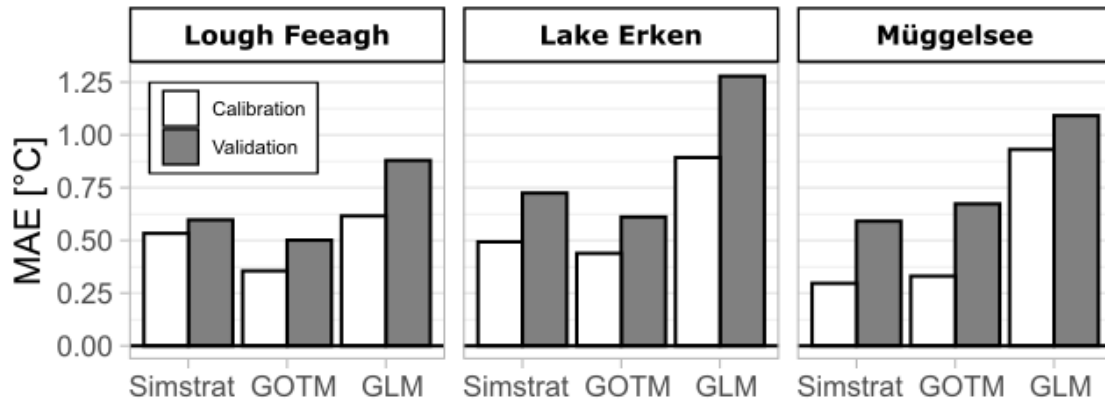


Figure 2. Bar graph of Mean Absolute Error (MAE) of lake temperature in °C for the calibration (first year) and validation period of each model and lake. For the exact values and other measures of goodness-of-fit, see Suppl. Mat. E.

OBSERVATIONS DURING EVENTS

The observed data confirmed the opposite effects of storms and heatwaves on surface temperature, volume-averaged temperature, Schmidt stability and maximum buoyancy frequency (Figure 3, Suppl. Mat. F). Differences between lakes could be observed. In the two deeper lakes of this study, Lough Feeagh and Lake Erken, Schmidt stability decreased and the mixed layer deepened during extreme wind events. Volume-averaged temperature was not strongly affected, but surface temperature decreased and bottom temperatures increased, indicating mixing between top and bottom waters. In Müggelsee, complete mixing occurred during all studied storm events, and the water column was often well-mixed already before the start of the actual event due to the lake's shallow depth (data not shown). For four out of the ten storms in Müggelsee, stratification formed again within a few days after the end of an event, which caused no change in Schmidt stability or mixed layer depth compared to before the event. Cooling of all water layers occurred during all ten storm events in Müggelsee.

During high temperature events, Schmidt stability tended to increase in Lough Feeagh and Lake Erken (Figure 3). There was no change in the mixed layer depth during these events. Water temperatures at all depths increased, but the increase was stronger near the surface than near the bottom. After heatwave events in Müggelsee, temperature in all water layers had increased to a similar extent, because effects of the heatwaves on stratification dissipated soon after the end of the events. Stratification occurred during nine of the ten events, but increases in Schmidt stability and mixed layer depth did not remain significant after the events.

In all lakes and during both storm and heatwave events, changes in maximum buoyancy frequency tended to follow the same trend as Schmidt stability, but were not significantly different from zero.

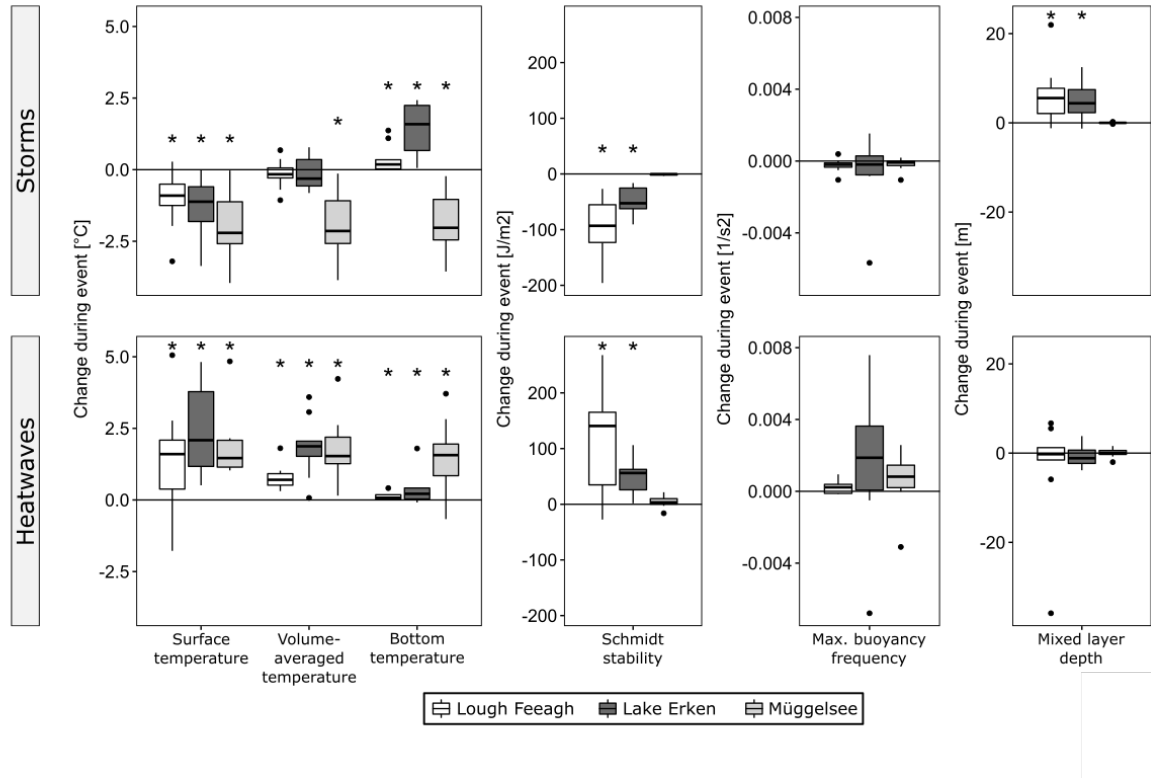


Figure 3. Boxplots showing the observed changes in temperature metrics, Schmidt stability, maximum buoyancy frequency, and mixed layer depth during the identified storms and heatwaves. Change during the event is calculated as the average over the two days after the event minus the average over the two days before the event. The boxplots show the median and first and third quartile. Whiskers extend to the smallest and largest value within 1.5 times the inter-quartile range from the nearest quartile (see `geom_boxplot` function in `ggplot2` R package, Wickham 2016). Values outside this range are defined as outliers (•). * indicates a significant difference from zero change (See Suppl. Mat. F).

MODEL PERFORMANCE DURING EVENTS

Generally, models performed better during the reference events compared to the extreme events. Only the simulations for Lough Feeagh had significantly higher *MAE* during storm events compared to reference wind events, while *MAE* during storm events in Müggelsee was significantly lower than the reference (Figure 4). In all lakes, the *MAE* of the water temperature profile was higher during the heatwave events compared to the *MAE* during the reference temperature events. A two-way ANOVA on the *MAE* during extreme events showed that different lakes ($F=18.58$, $p<0.001$), different event types (storm/heatwave, $F=6.54$, $p=0.01$) and the interaction between the two ($F=6.91$, $p=0.001$) had significant effects on *MAE*. Lough Feeagh had the lowest *MAE*'s during storm and heatwave events, compared to the other lakes (0.3-0.4 °C lower, Tukey test, $p<0.001$), and *MAE*'s were slightly higher during the heatwave events compared to the storm events (0.16 °C higher, Tukey test, $p=0.01$). During the extreme events, Simstrat and GOTM had a similar *MAE* (mean of 0.62 °C), while the *MAE* for GLM was 0.24 °C (39%) higher (One-way ANOVA, $F=5.32$, $p=0.005$, Tukey test, $p<0.05$, Suppl. Mat. G).

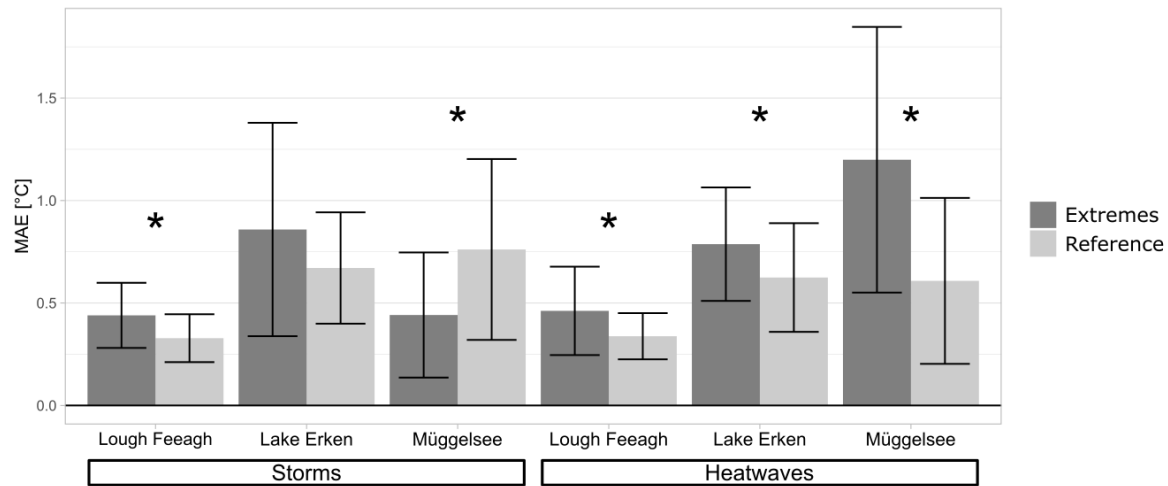
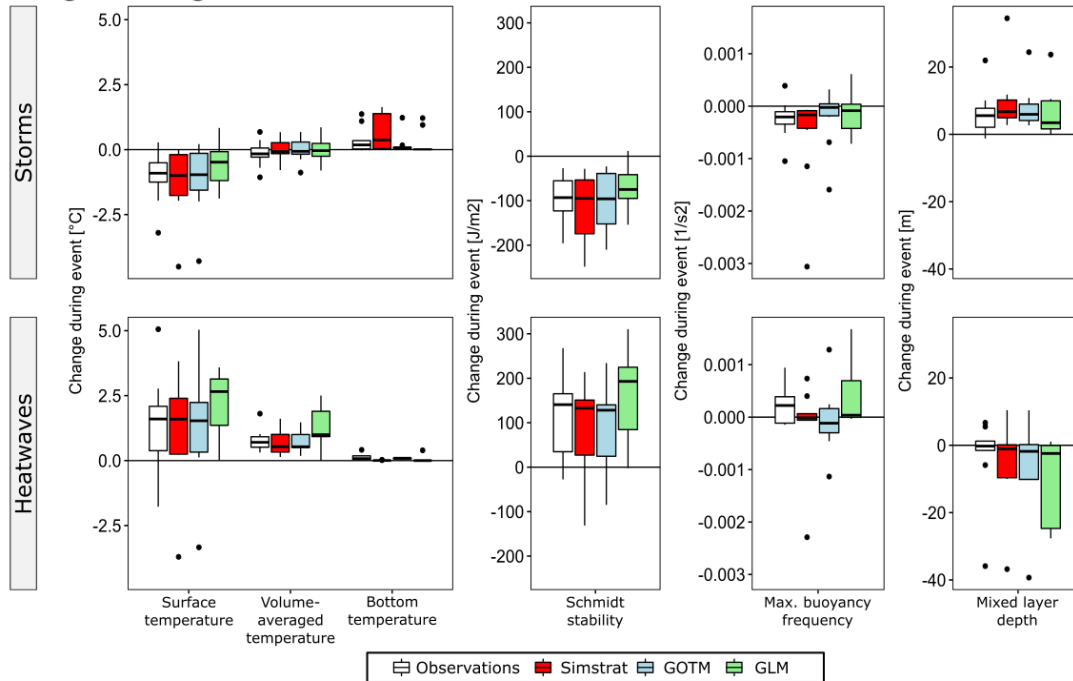


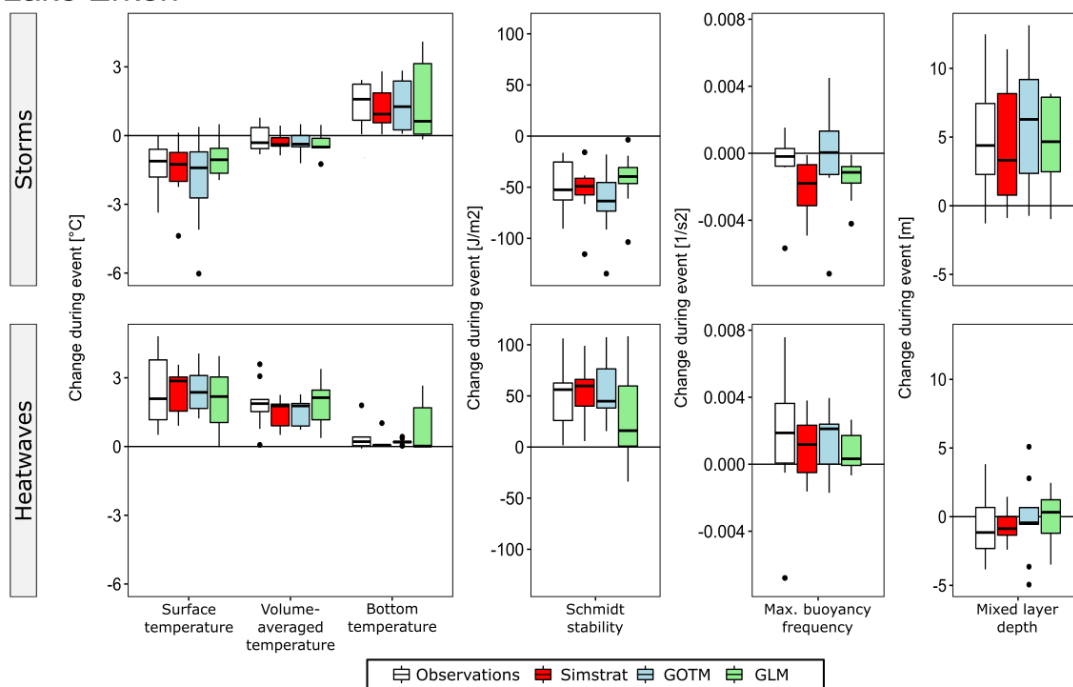
Figure 4. Mean Absolute Error (MAE) of the water temperature profile, comparison between extreme and reference events. The bars denote the average MAE during extreme or reference events, averaged over all models, and the error bars represent one standard deviation. Statistical differences in MAE were tested with t-tests, or Wilcoxon rank sum tests for Lough Feeagh storms and Müggelsee heatwaves due to non-normal distributions. Statistically significant results ($p < 0.05$) are indicated with a * (Suppl. Mat G).

Despite these increases in model error, the direction and magnitude of change during extreme events was often reproduced by the models (Figure 5, 6); during storms, the changes in surface- and volume-averaged temperature were accurately reproduced by all models (Concordance Correlation Coefficient, $CCC > 0.7$, Figure 6), while the bottom temperature was reproduced with less accuracy. Simstrat and GOTM reproduced changes in Schmidt stability and buoyancy frequency during storms better than GLM (Figure 6). The change in mixed layer depth during storms was reproduced with an average CCC of 0.5 for all models. The simulated changes during heatwaves had slightly lower performance for surface- and volume-averaged temperature than during storms (Figure 6). During the heatwaves, Simstrat and GOTM performed better than GLM for all metrics, except for bottom temperature, where GOTM and Simstrat performed poorly. Simstrat and GOTM simulated the change in mixed layer depth better during heatwaves compared to storm events. On average, changes in surface temperature, volume-average temperature, and Schmidt stability were simulated more accurately than bottom temperature, maximum buoyancy frequency, and mixed layer depth.

a) Lough Feeagh



b) Lake Erken



c) Müggelsee

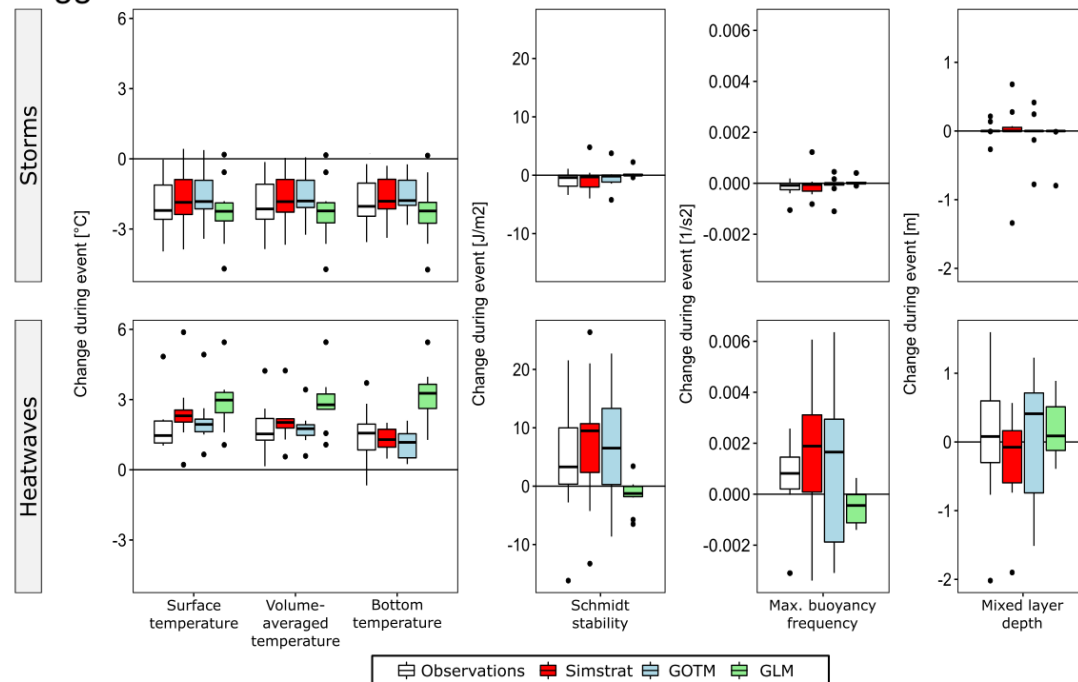


Figure 5. Boxplots showing the change in temperature metrics, Schmidt stability, maximum buoyancy frequency, and mixed layer depth during the identified storms and heatwaves. The change during the event is calculated as the average over the two days after the event minus the average over the two days before the event. The boxplots show the changes in the observations (white), Simstrat (red), GOTM (blue), and GLM (green) for a) Lough Feeagh, b) Lake Erken, and c) Müggelsee. The boxplots show the median and first and third quartile. Whiskers extend to the smallest and largest value within 1.5 times the inter-quartile range from the nearest quartile (see `geom_boxplot` function in `ggplot2` R package, Wickham 2016). Values outside this range are defined as outliers (•).

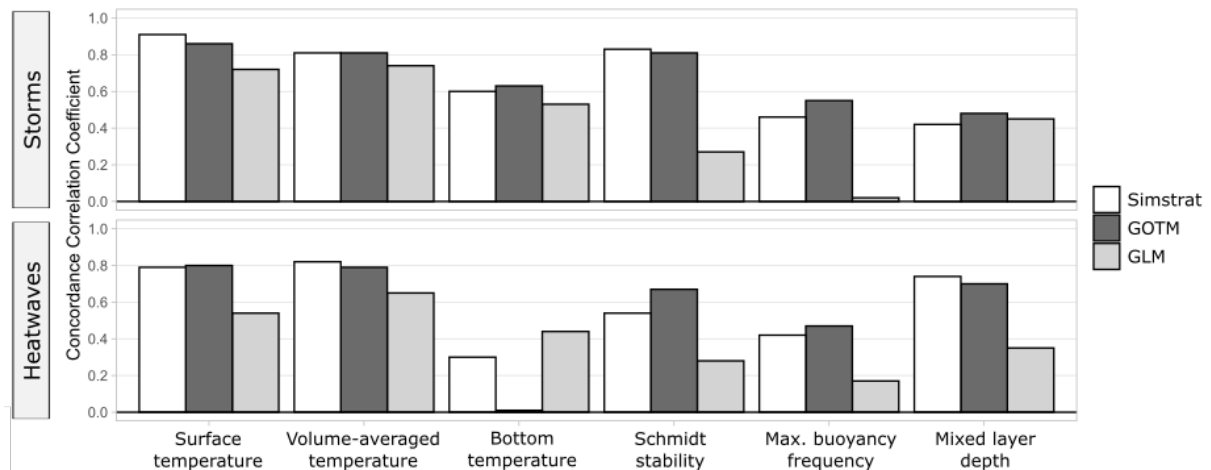


Figure 6. Average concordance correlation coefficient (CCC) between simulated and observed changes in temperature and stratification metrics, for each model and metric during storms and heatwaves. For the exact values and a comparison between CCC and Pearson's correlation coefficient, see Suppl. Mat. H.

Simstrat and GLM underestimated the increases in bottom temperature during heatwaves in Lough Feeagh (Kruskal-Wallis test, $Chi-sq=21.1$, $p<0.001$). GLM overestimated the increases in both surface (Kruskal-Wallis test, $Chi-sq=8.2$, $p=0.04$) and bottom temperatures (one-way ANOVA, $F=9.1$, $p<0.001$) during heatwaves in Müggelsee. None of the other extreme events showed a statistically significant difference in the mean change during the event between models and observations, for any metric. However, GLM underestimated the change in bottom temperature during reference wind events as well (Kruskal-Wallis test, $Chi-sq=15.5$, $p=0.001$). This was likely due to GLM showing very little heating of deep-water layers during the reference wind events in Lough

Feeagh, resulting in low variance and a significant difference with observations. Some heating of bottom layers is expected even under non-extreme conditions, for example as a result of vertical turbulent diffusion (Livingstone 1997).

Temporal cross-correlation could be performed for more than 80% of the events for Schmidt stability and volume-averaged and surface temperature, to calculate the simulation lag. Where the lags were calculated for these metrics, they were less than 1 h in more than 80% of the events (Suppl. Mat. I). For bottom temperature, maximum buoyancy frequency, and mixed layer depth, lags could only be calculated for about half of the events due to inaccurate simulations (see Material & Methods). About 70% (maximum buoyancy frequency) and 80% (bottom temperature and mixed layer depth) of the calculated lags were below 1 h. GLM was slightly worse in reproducing the timing of the simulations compared to the other models, but still had more than 50% (Schmidt stability, maximum buoyancy frequency, mixed layer depth) or more than 80% (temperature metrics) of the lags at or below 1 h. Differences between lakes varied per metric, but the timing of the simulations was not consistently better in any of the lakes.

In Suppl. Mat. J we show the temperature profiles and the corresponding detailed model simulations for three example events.

DISCUSSION

In the present study we tested the model performance of three 1D models to capture responses to two kinds of extreme weather events in three different lakes. Firstly, we assessed the model performance during the generic validation period. The model fit for the full validation period was comparable to other studies (RMSE ranging from 0.5 to 2.0 °C, e.g. Fang et al. 2012; Stepanenko et al. 2013; Bruce et al. 2018; Moras et al. 2019; Schwefel et al. 2019). All models performed within the margins commonly found in literature, although GOTM and Simstrat performed better than GLM. A potential reason for this could have been a consequence of forcing GLM with hourly data, as compared to 10-min data for GOTM and Simstrat. However, this was found not to be the reason for the lower performance of GLM, because when GOTM and Simstrat were calibrated and run with hourly data, model errors were still about 40% lower than for GLM (Suppl. Mat. E). Model validation studies like this are valuable to better understand in which systems the models perform well and where they may have limitations. It could be that the different layer structure is beneficial for GOTM and Simstrat in this case of short-term extreme events, whereas GLM with adaptive layers may perform better in water bodies with fluctuating water levels. The different calibration routines between the models might also have influenced the model fit. More studies of this type are required to understand structural uncertainty in lake models (Frassl et al. 2019).

In agreement with previous studies (Jennings et al. 2012; Kasprzak et al. 2017; Andersen et al. 2020), wind events caused reduced Schmidt stability, deepened mixed layers, and cooled surface waters while the bottom water warmed in the two deep lakes (Lough Feeagh and Lake Erken). The shallow Müggelsee was always completely mixed during the storm events. Heatwaves are associated with increased surface water temperatures and stronger stratification (Jankowski et al. 2006; Jöhnk et al. 2008). In this study, temperatures in all water layers increased during the high temperature events. In Lough Feeagh and Lake Erken, the surface temperature increase was stronger than near the bottom and stratification strengthened. In Müggelsee, stratification occurred during most of the heatwave events, in line with the findings of Wilhelm and Adrian (2008). However, within two days after the heatwave events, stratification had reached levels similar to before the event. This caused the temperature increase between two days before and two days after the events to be more or less uniform with depth.

In general, all models were able to reproduce the overall trends during either heating or wind events. Changes in surface and volume-averaged temperature and Schmidt stability were simulated most accurately, while changes in bottom temperatures especially during heatwaves were simulated less well. Also, the simulations of changes in maximum buoyancy frequency during storms and heatwaves, and of changes in mixed layer depth

during heatwaves, were less accurate. The present study is amongst the first to look at model performance during short-term events. In the scenario study by Mi et al. (2018), GLM also simulated credible changes in hypolimnetic temperature, mixed layer depth, and Schmidt stability after a wind perturbation, although a comparison with observations during wind events was not performed.

In addition to reproducing the general trends, only in a few cases did models consistently over- or underestimate a change during events. Increases in bottom temperatures were underestimated during heatwaves in Lough Feeagh by Simstrat and GLM, which suggests that these models fail to adequately simulate increases in bottom temperatures in deep lakes, at least over the short time intervals evaluated here. However, the increases in Lough Feeagh bottom temperatures during heatwaves were only around 0.2 °C. GLM overestimated temperature increase in the whole water column during heatwaves in Müggelsee, often by more than 1 °C, while not showing such a bias over the full validation period. We have not explored further why only GLM showed this overestimation during heatwaves. It may be related to the combination of GLM's flexible grid structure and the depth of the lake, with Müggelsee being a shallow lake. The positive bias to warmer temperatures during a heatwave was not observed in the GLM simulations of Lough Feeagh and Lake Erken. This aligns with a GLM simulation of Lake Ammersee (mean depth 38.6 m), where surface temperature was also not overestimated during a heatwave year (Bueche et al. 2017).

As with the overall model performance in this study, GLM displayed higher model errors than Simstrat and GOTM during extreme events. Like the performance during the calibration and validation periods, we found that even when Simstrat and GOTM were forced with hourly inputs, these models still showed lower errors than GLM (Suppl. Mat. G). The example results show that the surface heat fluxes had different values for each model (Suppl. Mat. J). This is partially the result of different calibration outcomes. The heat fluxes in the different models followed the same pattern, except for the longwave heat flux, which was notably different in GLM than in the other two models. This was likely due to a different parameterisation of the incoming longwave radiation. The behaviour of Simstrat and GOTM under extreme weather conditions was more similar to each other than to GLM (e.g. Suppl. Mat. J). This similarity is likely the result of a similar model structure, as both are k-epsilon turbulence models (Rodi 1980), while GLM calculates mixing based on energy and density gradients (see Hipsey et al. 2019). The reason for using multiple models in this study was to ascertain if certain models performed significantly better than others, but also to provide results that are representative of 1D models in general, rather than any one particular model. Because all three models, despite their differences, tended to simulate the same general trends, but showed a higher MAE during extreme weather events, we can assume that strengths and weakness in event simulations found here are likely to occur to a similar extent in other 1D hydrodynamic lake models as well.

Most simulations captured the observed timing of the extreme events, that is, most of the effects were simulated within 1 h of the observations, and more than 90% of the modelled events had lags of less than 4 h, for all metrics. It should be noted, however, that we could only determine the lag if a reasonable model fit after the cross-correlation analysis was obtained (cross-correlation coefficient of 0.3 or higher). So, there is a bias towards events that were simulated well. For Schmidt stability, volume-averaged, and surface temperature, lags could be determined in 80-90% of the cases, but for the other metrics only in 40-60% of the cases. To our knowledge, accuracy of timing of short-term events in hydrodynamic lake models has rarely been tested, yet it is a crucial aspect of model performance, especially for forecasting purposes. In studies aimed at forecasting phytoplankton blooms, timing is sometimes included in model assessment (Gurkan et al. 2006; Page et al. 2018), and changes in hydrodynamics can be an important driver in phytoplankton dynamics (Wilhelm and Adrian 2008; Kasprzak et al. 2017).

Despite the reproduction of the overall trends, the low degree of bias, and the accurate timing of simulations, model error increased during extreme events compared to the reference periods by roughly 30% during storm events in Lough Feeagh, and during heatwaves by 30% (Lough Feeagh, Lake Erken) to 100% (Müggelsee). This

lower performance shows that predictions made by hydrodynamic models during extreme weather events should be treated with additional caution. Notable exceptions were the storm events in Müggelsee, where the model error was 40% lower than during the reference periods. This likely has to do with the shallow depth of Müggelsee and might be systematic for shallow lakes in general; the selected storm events were some of the most extreme in a 14-year period and as a result this shallow lake mixed completely. This was correctly simulated by the models, and errors estimating these isothermal conditions tended to be lower than the errors than during the reference periods, when stratification sometimes occurred.

The larger errors during the storms in the deep lakes and during heatwaves can have multiple causes. Firstly, many of the models' parameterizations are nonlinear, and thus the magnitude of energy and turbulence fluxes might increase faster than linearly under more extreme conditions. By using high-frequency driving data, averaging errors relating to removing high frequency variation in meteorological forcing data were reduced. However, it is still possible that the values assigned to model coefficients during long-term calibration may not be appropriate for the extreme conditions of specific events and this would then automatically cause a larger error. Secondly, the assumption of one-dimensionality in the models holds less well during extreme events. During storms, the leeside of a lake and bays experience notably less wind forcing, internal waves can form, and wave breaking creates turbulence on underwater slopes (Wüest et al. 2000; MacIntyre and Jellison 2001). Shallow areas tend to stratify earlier and warm faster than deep areas (Woolway and Merchant 2018), potentially creating more horizontal heterogeneity during heatwaves. These three-dimensional processes are not included in 1D models, and these sources of error may be accentuated during extreme events. Lastly, extreme events could also increase the importance of processes that were not included or kept constant in this study, such as precipitation, inflow, or turbidity.

We found that extreme weather generally resulted in momentarily less accurate simulation of lake conditions, even with high-frequency forcing data collected on-site, and with all three models. But to what extent is this a problem? Numerical process-based lake models are still amongst the best tools we have to simulate thermal dynamics in lakes during extreme weather events and the fact that uncertainty increases during these conditions does not invalidate their usefulness. In flood and hurricane forecasting, it is acknowledged that numerical models have large uncertainty during extreme weather conditions (Todini 2004; Heming et al. 2019). The uncertainty connected to these forecasts is an important aspect of the output that is included when informing decision makers and the public. In the case of extreme events in lakes, uncertainty can be taken into account partially by simply being aware of it. For example, since the timing of event impacts was simulated accurately, for some purposes of modelling it might be sufficient to take the timing of the event as information and knowing that the magnitude of the impact could differ from the simulations. However, to quantify the uncertainty during extreme events, a potential pathway would be ensemble modelling with forcing scenarios of varying intensity. Because we found little consistent bias, model runs with higher and lower wind speeds or temperatures could provide an uncertainty band during extreme weather events. More research would be needed to determine what methods would be best suited to quantify uncertainty during extreme events.

The models in this study captured the overall trends, and the range of error during the extreme events (MAE 0.4 – 1.2 °C) is similar to the level of uncertainty found in other lake modelling studies during regular conditions (e.g. Soulignac et al. 2018; Moras et al. 2019). Larger model uncertainty during extreme events is, to a certain extent, expected because of greater spatial variations in lake thermal structure, larger energy fluxes, and more rapid changes in thermal gradients in the water column at small temporal scale, compared to non-extreme circumstances. It depends on the objective of the modeller if this reduced accuracy poses a problem. Larger error during extreme events might not pose a problem for long-term climate forecasting, as model fit during these short periods is generally not of interest for this type of studies. An exception to this statement would be if there are long-term consequences of extreme events, as in the case of tipping points (Scheffer et al. 2001). For short-term forecasting, however, extreme events are amongst the most important events to capture. This study shows that 1D lake models can be used to simulate these events, but the short-term predictions may be

less precise than would occur under more normal conditions. This should be kept in mind when interpreting the forecasts. The results in the present study suggest that forecasts for temperature data and Schmidt stability will be more precise than for maximum buoyancy frequency and mixed layer depth. For scenario studies (as in Mi et al. 2018), the increased uncertainty during events is likely not a major issue. The absolute magnitude of the effect of an event might differ from observations, but the overall response is simulated. Coupling of physical models and biogeochemical models involves a risk of error propagation; a wrong estimation of water temperature could lead to wrong growth rates, or a too shallow mixing event results in less nutrient upwelling than in reality. Because of this, it is likely that uncertainty during extreme events also increases for biogeochemical models.

CONCLUSION

Extreme weather events are projected to increase in magnitude and frequency and can have large and diverse effects on lake ecosystems. One-dimensional hydrodynamic lake models could help in elucidating their impacts on lakes, but so far no studies have investigated how well these models perform during such events. In this study, Simstrat, GOTM, and GLM were run during multiple selected storms and heatwaves in three lakes in order to assess model performance. The overall effects of extreme weather on lake temperature and stratification metrics were captured by the models with correct timing and little bias, but the precision of the model output was reduced compared to non-extreme conditions. As with the model fit during calibration and validation, Simstrat and GOTM performed better during extreme events than GLM.

The implications of these findings ultimately depend on a modeller's objectives, but we are convinced that the findings in this paper can help to elucidate the uncertainty of model predictions during extreme weather events. This would lead to a more responsible use of 1D lake models, as uncertainty is an important part of model simulations. We propose that 1D lake models can be adequate tools to evaluate changes in hydrodynamics during extreme weather events, provided that the increased uncertainty during these events is kept in mind when interpreting the results.

DECLARATION OF COMPETING INTEREST

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

ACKNOWLEDGEMENTS

The authors express their thanks to the Marine Institute, the Swedish Infrastructure for Ecosystem Science (SITES) and Uppsala University, and the Leibniz-Institute of Freshwater Ecology and Inland Fisheries (IGB) for collecting and sharing the water temperature data of Lough Feeagh, Lake Erken, and Müggelsee.

J.P.M, A.I.A, and J.A.A.S. were funded by the MANTEL ITN (Management of climatic extreme events in lakes and reservoirs for the protection of ecosystem services) through the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie grant agreement no. 722518. R.A. acknowledges support by the "LimnoSCenES" project (AD 91/22-1) within the BiodivERsA and the Belmont Forum programme.

APPENDIX A. SUPPLEMENTARY DATA

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.envsoft.2020.104852>

SOFTWARE AVAILABILITY

Instructions to download and install the models used in this study can be found at:

- Simstrat (version 2.1): <https://github.com/Eawag-AppliedSystemAnalysis/Simstrat/tree/v2.1>
- GOTM, (version 5.1): <https://gotm.net/>
- GLM, (version 3.0.4): <https://aed.see.uwa.edu.au/research/models/GLM/index.html>

Last access: 2021-08-13

CHAPTER 3 - LAKEENSEMBLR: AN R PACKAGE THAT FACILITATES ENSEMBLE MODELLING OF LAKES

Tadhg N. Moore^{1a*}, Jorrit P. Mesman^{2,3*}, Robert Ladwig^{4*}, Johannes Feldbauer^{5*}, Freya Olsson⁶, Rachel M. Pilla⁷, Tom Shatwell⁸, Jason J. Venkiteswaran⁹, Austin D. Delany⁴, Hilary Dugan⁴, Kevin C. Rose¹⁰, Jordan S. Read¹¹

*Shared co-first authorships

¹*Dundalk Institute of Technology, Centre for Freshwater and Environmental Studies, Dundalk, Co. Louth, Ireland*

²*University of Geneva, Department F.A. Forel for Environmental and Aquatic Sciences, Geneva, Switzerland*

³*Uppsala University, Department of Ecology and Genetics, Uppsala, Sweden*

⁴*University of Wisconsin – Madison, Center for Limnology, Madison, Wisconsin, USA*

⁵*Technische Universität Dresden, Institute of Hydrobiology, Dresden, Germany*

⁶*UK Centre for Ecology & Hydrology, Lancaster Environment Centre, Bailrigg, Lancaster, UK*

⁷*Miami University, Department of Biology, Oxford, Ohio, USA*

⁸*Helmholtz Centre for Environmental Research (UFZ), Department of Lake Research, Magdeburg, Germany*

⁹*Wilfrid Laurier University, Department of Geography and Environmental Studies, Waterloo, Ontario, Canada*

¹⁰*Rensselaer Polytechnic Institute, Department of Biological Sciences, Troy, New York, USA*

¹¹*U.S. Geological Survey, Middleton, Wisconsin, USA*

^a*Present address: Virginia Tech, Department of Biological Sciences, Blacksburg, VA, United States*

Correspondence: tadhgm@vt.edu (T.N. Moore), jorrit.mesman@unige.ch (J.P. Mesman), rladwig2@wisc.edu (R. Ladwig), johannes.feldbauer@tu-dresden.de (J. Feldbauer)

ABSTRACT

Model ensembles have several benefits compared to single-model applications but are not frequently used within the lake modelling community. Setting up and running multiple lake models can be challenging and time consuming, despite the many similarities between the existing models (forcing data, hypsograph, etc.). Here we present an R package, LakeEnsemblR, that facilitates running ensembles of five different vertical one-dimensional hydrodynamic lake models (FLake, GLM, GOTM, Simstrat, MyLake). The package requires input in a standardised format and a single configuration file. LakeEnsemblR formats these files to the input required by each model, and provides functions to run and calibrate the models. The outputs of the different models are compiled into a single file, and several post-processing operations are supported. LakeEnsemblR's workflow standardisation can simplify model benchmarking and uncertainty quantification, and improve collaborations between scientists. We showcase the successful application of LakeEnsemblR for two different lakes.

Keywords: Ensemble modeling, Vertical one-dimensional lake model, R package, Calibration, Thermal structure, Hydrodynamics

1. INTRODUCTION

Numerical process-based lake models are powerful tools to simulate processes occurring in aquatic ecosystems. These models enable the users to investigate scientific and engineering hypotheses or scenarios, which would

otherwise not be feasible (or even possible) to field-test for physical, logistical, political or financial reasons. Over recent decades, the understanding of fluid dynamics and physical transport processes in lakes has improved thanks to enhanced field monitoring and intensive laboratory studies (Kitaigorodskii and Miropolsky 1970; Imboden 1973; Csanady 1975; Spigel and Imberger 1980; Imberger and Hamblin 1982; Imberger 1985; Spigel et al. 1986). With better empirical relationships and physical understanding of processes, the pioneer lake models that emerged from these studies were essential to addressing emerging water quality issues like eutrophication (French and Imberger 1984).

Today, one-dimensional (1D) lake models are frequently used to characterise lake hydrodynamics. These models assume complete and instantaneous horizontal mixing. In many systems this is a reasonable assumption, because vertical thermal gradients are typically much larger than horizontal thermal gradients. The assumption holds for lakes with a small to moderate surface area that are not affected by Coriolis acceleration or other significant horizontal transport processes (Patterson et al. 1984). To model water column thermal dynamics resulting from atmospheric exchange processes, inflow entrainment and turbulence, different theoretical approaches have been developed and applied in lake models, e.g., bulk models, energy-balance approach models, and models that use a pure turbulence approach to account for mixing (Goudsmit et al. 2002). Alternative approaches apply simpler schemes to solve advection-diffusion equations or use constants for transport processes.

Since the 1980s, there has been a rapid expansion in the publication of process-based aquatic ecosystem models. However, the aquatic ecosystem community has not fully exploited the diversity of available models by comparing the performance of models against one another, which affords both the opportunity to identify technical improvements but also improve overall model predictions (Janssen et al. 2015). Critical voices still highlight the problem that modelling teams tend to ‘reinvent the wheel’ (Mooij et al. 2010) instead of building on existing software. The Lake Model Intercomparison Project (LakeMIP) had several key findings regarding the current state of lake modelling: (1) the majority of lake models replicate surface temperature dynamics coherently well (Stepanenko et al. 2013), (2) individual lake models clearly outperform others for specific lake sites (Thiery et al. 2014), and (3) models that explicitly incorporate sediment heating and resolve turbulence over lake depth are better suited to represent lakes in numerical meteorological studies and to research hydrodynamic processes for deep lakes (Stepanenko et al. 2013; Thiery et al. 2014). Most authors agree that open community approaches as well as publishing the model as open-source code are the best steps for sustainable development and to ensure future technical improvements (Janssen et al. 2015; Read et al. 2018; Frassl et al. 2019). Still, a lack of common community framework for model calibration, validation, and processing has resulted in few studies that quantify model performance (benchmarking) and minimal progress in improving code and applications (Arhonditsis et al. 2014; Hipsey et al. 2020).

In the 1990s, atmospheric researchers popularised the use of ensemble modeling in operational forecasting and uncertainty predictions (Parker 2013). Ensemble modeling involves either running the same model multiple times with different settings or running multiple models on the same study site. One of the main advantages of model ensembles is that the uncertainty in the model predictions can be estimated (Trolle et al. 2014; Wu et al. 2020). This allows the modeller to assess the likelihood of occurrence of certain model predictions. Connected to this, ensemble runs of an individual model are a means of taking into account nonuniqueness (i.e. equifinality - see Beven 2006) in parameter sets (Gal et al. 2014; Nielsen et al. 2014). The average of individual model runs from different models can be a more robust predictor than any of the individual model runs (Trolle et al. 2014 and sources therein; Kobler and Schmid 2019). If only the “best” model is retained, valuable information in other model fits is disregarded (Baker and Ellison 2008). An ensemble of multiple models supports the identification of methodological and technical differences and shortcomings between the different models, and covers a wide set of different parameterisations of processes. This can improve the understanding of model performance and guide future model development (Janssen et al. 2015; Frassl et al. 2019).

Model ensembles are now widely used in meteorological forecasting (Gneiting and Raftery 2005; Leutbecher and Palmer 2008), flood forecasting (Wu et al. 2020), and climate studies (Parker 2010; Mu et al. 2017). Ensemble models have gained momentum in large-scale water quality studies (van Vliet et al. 2019), but their adoption in limnology has been slow. We believe the limnology community recognises the benefits of using ensembles and multi-model simulations (Stepanenko et al. 2010; Nielsen et al. 2014), but lacks scientific software to facilitate lake ensemble modelling. Past efforts to apply multiple lake models to the same study systems (Stepanenko et al. 2010 (LakeMIP); Nielsen et al. 2014; Trolle et al. 2014; Yao et al. 2014; Frieler et al. 2017 (ISIMIP); Kobler and Schmid 2019; Gal et al. 2020) have often been the result of large international collaborations. While these initiatives have revealed pertinent new information, the labour required to build these networks is a barrier to broader implementation.

To remove these barriers and facilitate running ensembles of lake models, we developed LakeEnsemblR. Here, we describe the package version 1.0.0 and apply it to predict temperature and ice cover in two lakes. LakeEnsemblR is a numerical framework to run five 1D hydrodynamic lake models simultaneously (see Supplement - Table C1), using the same configuration and driver data, in the form of a package in the R software environment (R Core Team 2020). The model source codes are open-source and the model executables can be run on Windows, MacOS, and Linux platforms. The two main objectives of LakeEnsemblR are a) to improve the accessibility of different hydrodynamic models for new users and b) to allow experienced users to utilise the powerful approach of running an ensemble of lake models in a consistent and coherent framework. These two aims are achieved through six key aspects of its functionality: 1) facilitating easy setup and configuration of model files; 2) running all models with standardised input files; 3) standardising model output; 4) providing tools for convenient post-processing; 5) standardising calibration routines; and 6) aggregating and enabling for ensemble averaging to account for different sources of uncertainty between the models. The structure of the package allows future development and addition of more models, and the code is freely accessible under a GNU General Public License v2.0.

2. METHODS

2.1 MODEL DESCRIPTIONS

2.1.1 FLAKE

FLake (Freshwater Lake model, see Supplement - Table C1) is a bulk model that was developed primarily for fast lake-to-atmosphere coupling within numerical weather prediction models (Mironov 2005; Mironov 2008). FLake simulates lake systems using a two-layer parametric representation focusing on the heat budget. The upper, well-mixed layer is considered thermally homogeneous, whereas the temperature in the lower, stably stratified layer is approximated by a self-similar (dimensionless shape) profile. FLake also uses self-similarity to model ice and sediment temperatures. Due to its computational efficiency, FLake has been widely used in numerical weather prediction models (Mironov et al. 2010; Šeparović et al. 2013) and lake studies on both global and local scale (Vörös et al. 2010; Thiery et al. 2014; Woolway et al. 2019). LakeEnsemblR version 1.0.0 uses a version of FLake that has been adapted to include heat input through inflows (pers. comm. Georgiy Kirillin). The default FLake model option implemented in LakeEnsemblR simulates the vertical temperature dynamics up to the mean depth of the lake, as FLake assumes a rectangular shape of the basin and does not incorporate the lake's specific hypsography. The assumptions of FLake match best when using the mean depth of the lake, therefore the FLake simulations extend to a shallower depth than the other hydrodynamic models.

2.1.2 GLM

The General Lake Model (GLM, see Supplement - Table C1) is a vertical 1D hydrodynamic lake model developed by the University of Western Australia (Hipsey et al. 2019). GLM applies a flexible Lagrangian structure to replicate mixing dynamics. Here, neighboring layers either split or merge depending on the density of the layers. Surface mixing dynamics are calculated via an energy balance approach, where the available kinetic energy is compared to the potential energy of the water column. The model has been widely applied, for example to

simulate seasonal dynamics of temperature and ice cover (Bueche et al. 2017; Fenocchi et al. 2018), project impacts of water management measures on lake ecosystems (Weber et al. 2017; Ladwig et al. 2018; Feldbauer et al. 2020), and to assess scenarios regarding extreme events (Mi et al. 2018; Soares et al. 2019). It has also been rigorously tested in a large number of lakes (Bruce et al. 2018). In the version 1.0.0 of LakeEnsemblR, version 3.1.0 of GLM is used.

2.1.3 GOTM

The General Ocean Turbulence model (GOTM, see Supplement - Table C1) was developed by Burchard et al. (1999). It is a vertical 1D hydrodynamic water column model that includes important hydrodynamic and thermodynamic processes related to vertical mixing in natural waters (Umlauf et al. 2005). It was initially developed for modelling turbulence in the ocean (Burchard et al. 2006), but it has been adapted for use in hydrodynamic modelling in lakes (Sachse et al. 2014). GOTM has been used to model the dissolution of CO₂ in lakes (Enstad et al. 2008), extreme events in a eutrophic marine system (Ciglenečki et al. 2015), impact of macrophytes on water quality (Sachse et al. 2014) and hindcasting and future climate change projections of the thermal structure of a lake (Moras et al. 2019; Ayala et al. 2020). LakeEnsemblR version 1.0.0 uses version 5.4.0 of the lake branch of GOTM.

2.1.4 SIMSTRAT

Simstrat is a vertical 1D hydrodynamic lake model (see Supplement - Table C1), combining a buoyancy-extended k-epsilon model with seiche parameterisation, and was originally developed by Goudsmit et al. (2002). Simulated variables include surface energy fluxes, and vertical profiles of turbulent diffusivity and water temperature. Multiple options for external forcing are available, as well as variable wind drag coefficients, inflow settings, and ice and snow formation (Gaudard et al. 2019). Simstrat has been successfully applied in lakes and reservoirs of varying morphometry in different climate zones, and in scenarios regarding climate warming (Stepanenko et al. 2013; Thiery et al. 2014; Schwefel et al. 2016; Kobler and Schmid 2019). The model is currently maintained by the “Surface Waters - Research and Management” Department of EAWAG (Switzerland) and version 2.4.1 is currently used in LakeEnsemblR.

2.1.5 MYLAKE

MyLake (Multi-year Lake simulation model, see Supplement - Table C1) is a vertical 1D lake model developed and hosted by the Norwegian Institute for Water Research (NIVA), the University of Helsinki (Finland), and Université Laval (Canada) (Saloranta and Andersen 2007). MyLake simulates daily vertical profiles of lake water temperature, density stratification, seasonal ice and snow cover, sediment-water dynamics, and phosphorus-phytoplankton interactions (Saloranta and Andersen 2007). The model has been used to simulate water temperature, ice and phytoplankton dynamics in mostly Northern and alpine regions (Saloranta et al. 2009; Couture et al. 2018; Kobler and Schmid 2019). The version used in LakeEnsemblR version 1.0.0 is written in R and corresponds to the MyLake Matlab version 1.2.

2.2 R PACKAGE DESCRIPTION

R is an open-source and freely available statistical program that is widely used in the limnological community and has previously been used for community-developed tools, such as rLakeAnalyzer (Read et al. 2011; Winslow et al. 2019) and LakeMetabolizer (Winslow et al. 2016). All core functions in LakeEnsemblR version 1.0.0 have associated documentation with replicable examples all of which can be accessed through help functions within R (tested with versions 3.6.2 and 4.0.2, R Core Team 2020).

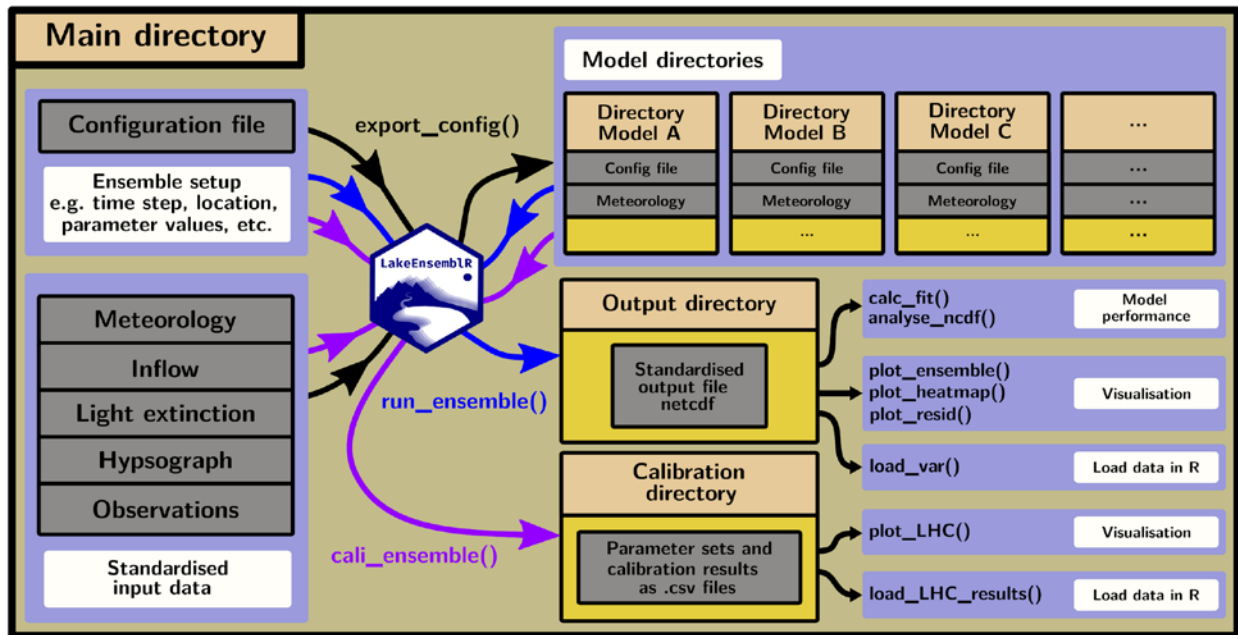


Figure 1. Conceptual overview of the LakeEnsemblR package showing the main folder structure and important functions.

2.2.1 MAIN WORKFLOW

The package works with one centralised configuration file, in which the user defines the settings of the model run and provides the locations of the standardised input files (see Box 1). The package exports the settings in the configuration file and the standardised input files to the requirements of each individual model (*export_config()* function), after which the models can be run (*run_ensemble()* function). The resulting water temperatures, densities, and ice cover thickness of the individual models are then compiled into a netcdf file and can be extracted or plotted in R (Figure 1). If observations are provided, these are added to the netcdf file as well. Optionally, this process can be repeated with different forcing files or different parameter sets, to add multiple ensemble members to the netcdf (*run_ensemble()* function, *add=TRUE* argument). This supports multi-model ensembles as well as simulations of multiple parameterisations of the same model(s). The combined model output can either be stored in text or netcdf format. In case observations are provided, parameter values of the different models can be calibrated (*cali_ensemble()* function), see section “Calibration algorithms” (Figure 1).

Box 1. Settings controlled by the LakeEnsemblR configuration file. Whenever it is stated “Link to ... file”, the file path to the LakeEnsemblR standardised file should be given. The configuration file is written in yaml text format and is easily readable in any text editor. Comments are provided in the example configuration file to explain what each parameter does and what the input options are.

- Location
 - o Coordinates
 - o Elevation
 - o Depth
 - o Hypsograph
- Time
 - o Start and end date of simulation
 - o Model integration time step
- Config files
 - o Links to model-specific configuration files
- Observations

- o Links to observational data (water temperature, ice thickness)
- Input
 - o Link to meteorological forcing
 - o Link to initial temperature profile
 - o Light extinction coefficient (constant or varying over time)
 - o Switch ice models on or off
- Inflows
 - o Switch on or off
 - o Link to inflow file
- Output settings
 - o File format
 - o Depth resolution
 - o Output time step
 - o Variables to generate output for
- Meteorological scaling factors (optional)
- Model-specific parameter values
 - o In this section, the user can change values in the model-specific configuration files
- Calibration settings
 - o Initial value, lower and upper boundaries for calibration of either model-specific parameters or scaling factors for the meteorological forcing.

2.2.2 DATA REQUIREMENTS

The minimum data requirements to run LakeEnsemblR are a hypsographic file, a light extinction coefficient, an initial temperature profile, and a time-series of meteorological forcing variables. In the LakeEnsemblR configuration file, the user needs to provide the location of the files. The files should have specific headings, so the program can identify what information is provided (see Supplement A).

In the hypsographic file, the surface area (m^2) per depth (m) of the lake is given. The light extinction coefficient (m^{-1}) can be either given as a single value or varying over time. An initial temperature profile is needed if temperature observations are not provided for the simulation starting date. The meteorological forcing must have a constant time step and not contain missing values. Required meteorological forcing data include air temperature ($^{\circ}\text{C}$) and downwelling shortwave radiation (W/m^2). Wind speed (m/s) needs to be given as well, either as a scalar or a vector (including wind direction). Either relative humidity (%) or dewpoint temperature ($^{\circ}\text{C}$) needs to be provided, and if relative humidity is not provided, it is calculated from dewpoint temperature and air temperature according to the weathermetrics package (Anderson et al. 2013). Downwelling longwave radiation (W/m^2) can either be provided directly to the models, or if it is not, will be calculated internally from cloud cover (-), air temperature ($^{\circ}\text{C}$), and humidity (relative humidity or dewpoint temperature), according to Konzelmann et al. (1994). Air pressure at lake surface level is also needed to run the models, but air pressure at sea level can be provided instead, in which case air pressure at lake surface level is estimated using the barometric formula, assuming a sea level temperature of 15°C (Berberan-Santos et al. 1997). Lastly, providing precipitation (mm/h or mm/d) is optional, but omitting it will cause the models that require precipitation (GOTM and GLM) to be run with a precipitation of 0, which may result in issues with the water balance. The influence of direct precipitation on the heat budget tends to be minimal (Imboden and Wüest 1995).

Optional data that can be provided are discharge (m^3/s), temperature ($^{\circ}\text{C}$) and salinity (PSU) of inflows, as well as water temperature and ice thickness observations. In the present version of LakeEnsemblR, outflow discharges can only be set to be identical to inflows, due to the many differences between the models in water balance calculations. Varying water levels are therefore not yet supported, although users can change model-specific settings related to the water balance. Observations are used for initialising temperature profiles, calibration, and plotting. If provided, observations are added to the output netcdf file.

2.2.3 GETTING STARTED

The LakeEnsemblR code is available on GitHub (<https://github.com/aemon-j/LakeEnsemblR>) and needs to be installed into the R environment, following instructions on the GitHub page. LakeEnsemblR itself cannot run the models, but instead this is done through supporting R packages (FLakeR, GLM3r, GOTMr, SimstratR, MyLakeR), which contain ways of running each model on the platforms Windows, MacOS, or Linux, through executables contained in the packages or having the model code in R.

After LakeEnsemblR is installed, a folder containing the setup for the ensemble run should be created. This can be done by editing the template folder provided within the package or by copying a setup from https://github.com/aemon-j/LER_examples. The LakeEnsemblR configuration file (in yaml format) contains all modifiable settings and input file paths. The input files themselves (e.g. for meteorology or inflows) need to be in comma-delimited format and need to have the correct column headers. Templates for any file can be generated through the `get_template()` function. Once the configuration file and the input files have been set up, the `export_config()` function can be run. This function exports the settings in the LakeEnsemblR configuration file and the LakeEnsemblR input files as required by each individual model. This means that for some models, units are converted, model parameters are changed, or input files are saved in a different format. The setup for each individual model is placed in its own directory.

After running `export_config()`, the ensemble can be run through the `run_ensemble()` function. In each model folder, the model-specific output is generated, which is then compiled into a netcdf file or text files (user choice) in a shared “output” folder. `run_ensemble()` runs the models without calibration. The `cali_ensemble()` function runs the calibration, following the specifications in the calibration section of the LakeEnsemblR configuration file, and stores the results of the calibration in the folder specified by the `out_f` argument. If netcdf output is chosen, several functions are available in the package to visualise the output (`plot_heatmap()`, `plot_ensemble()`, `plot_resid()`), load the data into R (`load_var()`), determine start and end of stratification and ice cover (`analyse_ncdf()`), or calculate goodness-of-fit (`calc_fit()`). Each function has documentation that can be loaded in R by typing `?name_function`.

While the running and calibration of the models is controlled by the R code, both the input and output files are in formats that are accessible by a wide array of software. Therefore, it is possible for users to do the pre- and post-processing with different software. A vignette is available on the LakeEnsemblR GitHub repository, which describes step-by-step how to run an ensemble, with multiple code examples. A wiki is available with additional information and frequently asked questions.

2.2.4 CALIBRATION ALGORITHMS

The LakeEnsemblR package provides functionality for automated parameter estimation using one of three methods. A simple calibration method based on Latin hypercube sampling, a Markov Chain Monte Carlo approach (MCMC), and a method for constrained fitting of the models to data using one of several available standard optimisation algorithms. The last two methods are implementations of the R package FME (Soetaert and Petzoldt 2010) using the functions `modMCMC()` and `modFit()`, respectively. Details about the MCMC and constrained fitting can be obtained from Soetaert and Petzoldt (2010) and the sources given therein. The Latin hypercube sampling method uses upper and lower bounds for all parameters that are to be calibrated and then samples evenly within the parameter space given by these bounds (e.g. McKay et al. 2000). Then the models are run and evaluated for all sampled parameters sets. By default, six measures of model performance are calculated: root mean square error (RMSE), Nash–Sutcliffe efficiency (NSE), Pearson correlation coefficient (r), mean error (bias), mean absolute error (MAE), and normalised mean absolute error (NMAE) (see Table C2 in the supplement). The user can also supply their own quality function which calculates measures of fit from modeled and observed data. Each of the three calibration methods can be run in parallel computation, where the models are distributed over the available cores. The parameters which are to be estimated, and their upper and lower bounds (if applicable) are specified in the master configuration file.

Scaling factors of meteorological forcing are parameters that are often calibrated in models (e.g. Gaudard et al. 2019; Ayala et al. 2020). Some models within LakeEnsemblR have internal parameters that scale the (meteorological) forcing, but not all. In order to be able to use the same scaling factors for all five models, the calibration section of the master configuration file distinguishes between model-specific parameters and meteorological (scaling) parameters. All three calibration methods can be used to obtain parameters that optimise the chosen model performance measure for the individual models. If common optimum scaling factors for all models in the ensemble are wanted, the user needs to apply their own method to aggregate the scaling factors of the models.

2.2.5 COMBINING MULTIPLE ENSEMBLE RUNS

Uncertainty of lake model output comes from different sources that are related to: forcing data, initial conditions, model parameter values, or structural reasons like process description and numerical methods (Thomas et al. 2020). LakeEnsemblR foremost tackles the uncertainties related to structural differences between different models. But, LakeEnsemblR can also be used to address other sources of uncertainties; the *run_ensemble()* function allows to add different model runs to a single netcdf file. Using this functionality, model runs with different parameterisations, forcing data, or initial conditions can be run and compared. Many diagnostic functions like *calc_fit()* or *plot_ensemble()* have two additional arguments *dim* and *dim_index* to select which dimension should be used.

3. EXAMPLE APPLICATION OF LAKEENSEMBLR

We applied the LakeEnsemblR package to two lake case studies: Lough Feeagh (IE) and Langtjern (NO). Lough Feeagh is a temperate monomictic lake with a maximum depth of 46 m and a surface area of 3.9 km². Langtjern is a shallow dimictic lake with a maximum depth of 12 m and a surface area of 0.23 km². Langtjern is separated into three distinct basins and our modelling efforts concentrated in the north basin with a maximum depth of 9 m and surface area of 0.06 km². A detailed description of Lough Feeagh can be found in Allott et al. (2005), or De Eyto et al. (2016), and a detailed description of Langtjern can be found in Couture et al. (2015), Henriksen and Wright (1977), and Wright (1983).

The Latin hypercube sampling method with 500 parameter sets was applied to both study cases. For each model, the parameter set with the lowest RMSE was selected. One full year was used to calibrate the models (2013 for Lough Feeagh, May 2014 to May 2015 for Langtjern), and the following year was reserved for validation of the simulated temperatures. Scaling factors for wind speed and shortwave radiation were calibrated for all five models, and in addition model-specific parameters *k_min* (GOTM), *coef_mix_hyp* (GLM), *c_relax_C* (FLake), *a_seiche* (Simstrat), and *C_shelter* (MyLake) were calibrated as well. These parameters were selected from parameters used for calibration in previous studies (see Supplement - Table C3). The inflows and outflows were omitted in all simulations. For the Langtjern simulation, hourly meteorological forcing was used to explore water temperature and ice dynamics, whereas for Lough Feeagh, the models were calibrated and validated using both hourly and daily averaged values to compare performance of water temperature, except for MyLake which only operates at the daily time scale.

In this section, we provide an example of how LakeEnsemblR can be used to partition and quantify different sources of uncertainty; boundary conditions, initial conditions, parameter and structure uncertainty. In order to do this, the Lough Feeagh ensemble was run a total of 300 times over a period of 16 days during the stratified period (June 12th to June 27th 2013), while different factors were varied to estimate their impact on the simulation output. To isolate the effect of initial conditions, the models were run using 100 different initial temperature profiles, that were drawn from a normal distribution around the observed value with a standard deviation of 0.1 °C. For boundary conditions the models were forced with 100 different versions of the meteorological data, where random noise was added to air temperature and wind speed from normal distributions with a mean of 0 °C and a standard deviation of 0.5 °C, and a mean of 0 m/s and a standard deviation of 0.5 m/s, respectively. For parameter uncertainty, 100 parameter values were drawn for each calibrated

parameter using either a normal or lognormal distribution (Table C4). To quantify and compare the variation of the different model runs between the different sources of uncertainty, the standard deviation of the water temperature for each time step at two depths (0.9 m and 16 m) of the output was calculated across the 100 ensembles, for each model separately.

For Lough Feeagh, we additionally ran an ensemble with different parameterisation of the five models to compare the uncertainty related to the chosen model with the uncertainty related to the calibrated parameters and scaling factors for each individual model. Starting from the Latin hypercube calibration (using daily forcing data), we first selected the best 10% parameter sets in terms of their RMSE for each model. From these sets, we extracted the range of the calibrated parameter and scaling factors and then sampled 20 parameter sets for each model within this range using Latin hypercube sampling. Then we ran the ensemble using these parameter sets and combined all ensemble runs in one netcdf file.

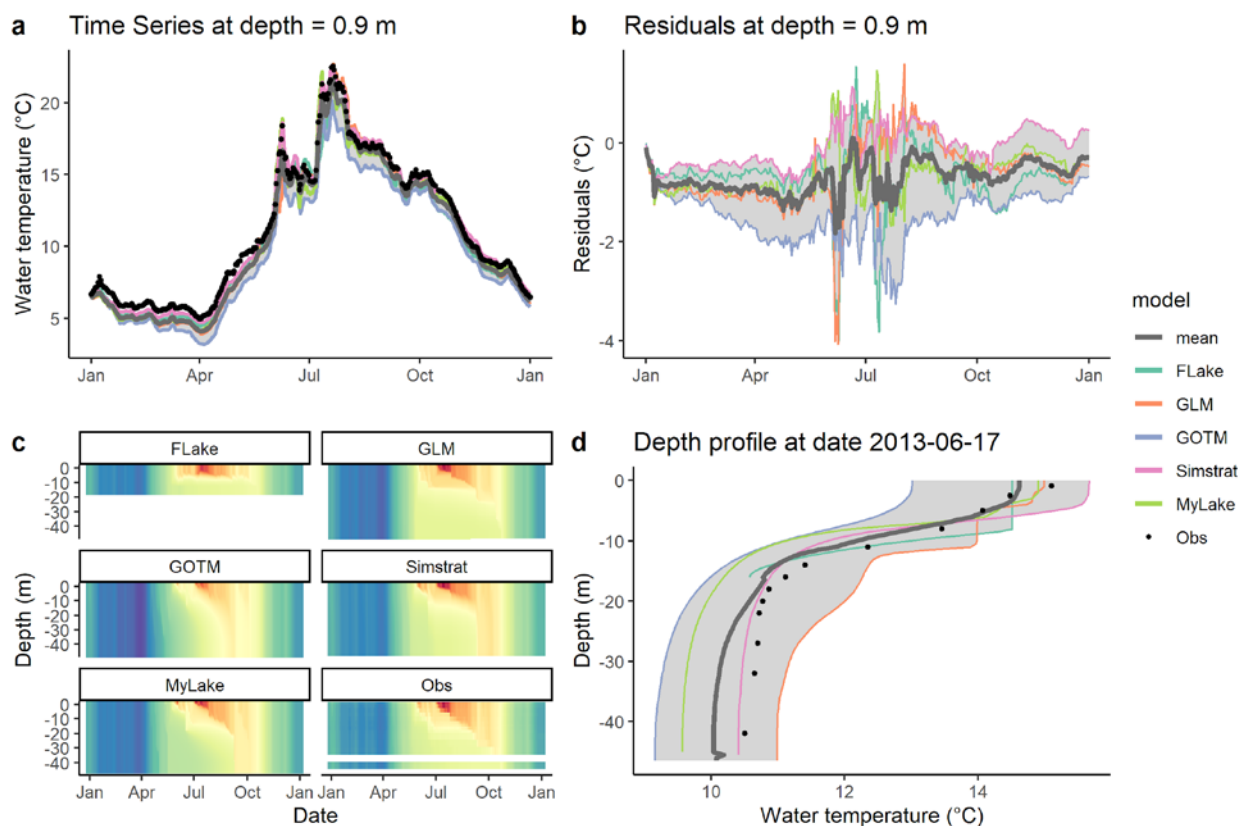


Figure 2. Calibrated ensemble output for simulated water temperature in 2013 for Lough Feeagh using daily forcing data, showing: a time series of model output at 0.9 m depth for all models, b residuals for the time series at 0.9 m depth, c filled contour maps from each of the models and observations, and d the ensemble modelled depth profile for 17 June 2013.

3.1 LOUGH FEEAGH: WATER TEMPERATURE DYNAMICS

Both simulations in Lough Feeagh using daily and hourly meteorological forcing generally produced satisfactory results of simulated temperature in the calibration period, compared to other simulations (e.g. Arhonditsis and Brett 2004; or Arhonditsis et al. 2006) with $RMSE < 1.3^{\circ}C$ for daily forcing (Table 1, Figure 2) and $RMSE < 0.9^{\circ}C$ for hourly forcing (Table 2). Except for FLake, even the uncalibrated model runs had satisfactory model performance, and calibration improved the model fits further. Compared to the calibration period, most models performed worse during the validation period (Table 1 for daily data and Table 2 for hourly data). Except for Simstrat, during the calibration phase all models tended to underestimate water temperatures over all depths

and throughout the year (Figure 3), on average ranging from about 0.1 °C (GLM, hourly forcing, Table 2) to 1 °C (GOTM, daily forcing, Table 1).

In general, the calibrated model performance was better using hourly forcing data compared to daily forcing data. Of the five models, FLake performed poorest when using daily forcing data and GLM performed poorest when using hourly forcing data. The best performing model differed between hourly and daily forcing data with GOTM performing best when using hourly data (calibration phase), and Simstrat performing best when using daily data (calibration and validation phase). In all models the largest residuals were seen at observed temperatures of 10 to 15 °C, during the time of the onset and end of summer stratification, and around the depth of the thermocline (Figure 3). Using daily average forcing data, the ensemble average was amongst the best performing fits and when using hourly forcing data the ensemble mean outperformed the individual models in most of the calculated performance measures, due to errors of individual models cancelling each other out in the ensemble mean (Table 1 and 2).

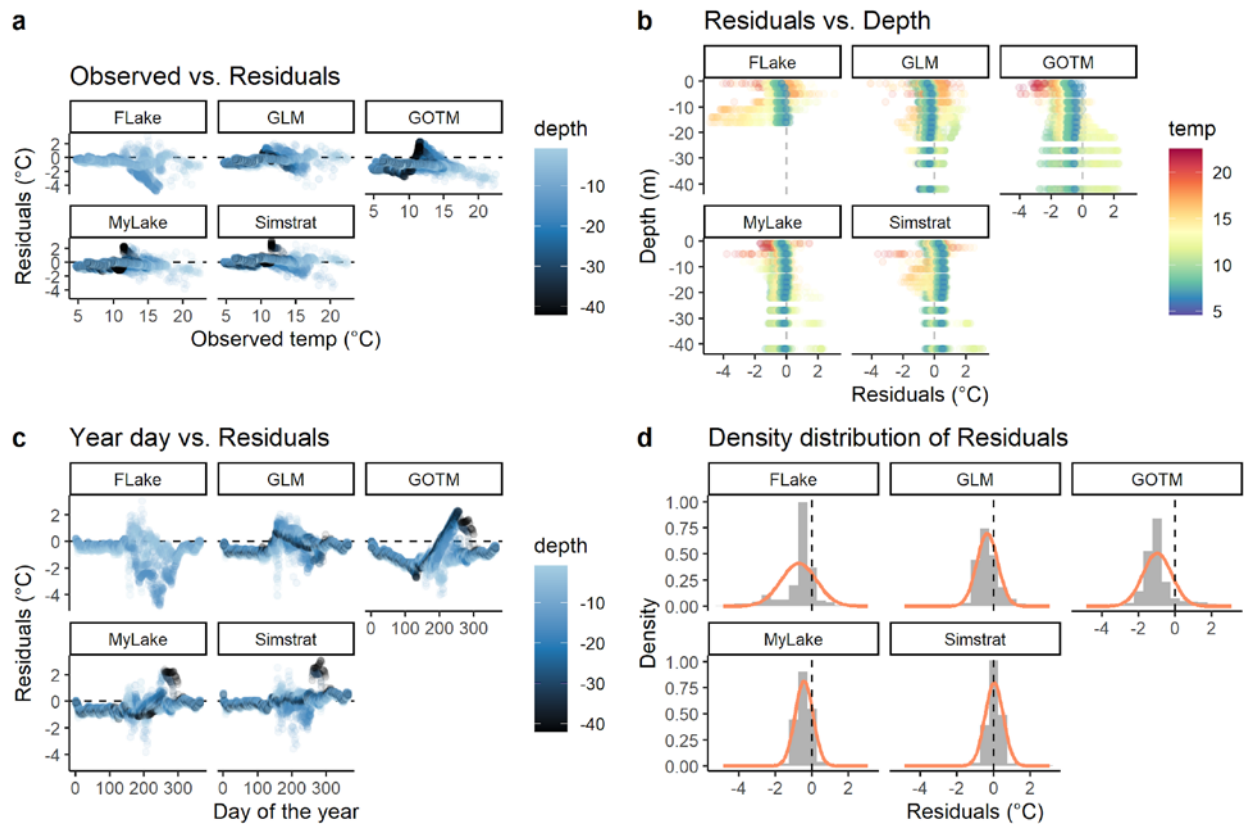


Figure 3. Water temperature residual diagnostic outputs from the calibrated ensemble run for Lough Feeagh in the year 2013 using daily forcing data. (a) Observed water temperature vs. residuals; (b) residuals vs depth, with the absolute simulated temperature in °C; (c) day of the year vs residuals and (d) distribution of the residuals.

Table 1. Model results or goodness-of-fit - uncal(ibrated), cal(ibrated), and val(idated) - for water temperature (°C) in Lough Feeagh using daily forcing data. Calibration was done for the year 2013 and validation for the year 2014. The best model performances are marked in bold. Shown are Root Mean Square Error (RMSE), Pearson's r (r), Nash-Sutcliffe Efficiency (NSE), Normalised Mean Absolute Error (NMAE), Mean Absolute Error (MAE), and Bias (or mean error).

measure	period	FLake	GLM	GOTM	Simstrat	MyLake	Ensemble mean
RMSE	uncal	3.057	0.846	1.698	0.625	1.719	1.189
	cal	1.210	0.670	1.261	0.502	0.656	0.629
	val	2.297	0.847	1.425	0.693	0.780	0.916
R	uncal	0.682	0.979	0.965	0.977	0.946	0.974
	cal	0.804	0.983	0.969	0.983	0.983	0.985

	val	0.756	0.981	0.964	0.986	0.988	0.984
NSE	uncal	0.631	0.948	0.788	0.971	0.783	0.896
	cal	0.942	0.967	0.883	0.982	0.968	0.971
	val	0.776	0.944	0.840	0.962	0.952	0.934
NMAE	uncal	0.175	0.082	0.165	0.044	0.131	0.101
	cal	0.072	0.070	0.133	0.035	0.065	0.064
	val	0.132	0.081	0.132	0.045	0.067	0.079
MAE	uncal	2.011	0.691	1.501	0.438	1.318	0.962
	cal	0.812	0.558	1.152	0.337	0.533	0.534
	val	1.610	0.720	1.286	0.467	0.628	0.760
Bias	uncal	-1.909	-0.575	-1.484	0.038	-1.308	-0.955
	cal	-0.720	-0.347	-0.986	0.028	-0.436	-0.458
	val	-1.560	-0.362	-1.048	-0.352	-0.526	-0.664

Table 2. Model results or goodness-of-fit - uncal(ibrated), cal(ibrated), and val(idated) - for water temperature (°C) in Lough Feeagh using hourly forcing data. MyLake cannot be run with hourly time steps and was therefore not included in this table. Calibration was done for the year 2013 and validation for the year 2014. The best model performances are marked in bold. Shown are Root Mean Square Error (RMSE), Pearson's r (r), Nash-Sutcliffe Efficiency (NSE), Normalised Mean Absolute Error (NMAE), Mean Absolute Error (MAE), and Bias (or mean error).

measure	period	FLake	GLM	GOTM	Simstrat	Ensemble mean
RMSE	uncal	2.957	0.943	0.801	1.107	0.726
	cal	0.617	0.819	0.594	0.599	0.469
	val	0.607	1.174	0.855	0.701	0.570
R	uncal	0.682	0.971	0.977	0.966	0.976
	cal	0.816	0.977	0.983	0.979	0.985
	val	0.824	0.972	0.984	0.985	0.992
NSE	uncal	0.655	0.935	0.953	0.910	0.961
	cal	0.985	0.951	0.974	0.974	0.984
	val	0.984	0.891	0.942	0.961	0.974
NMAE	uncal	0.157	0.081	0.074	0.072	0.063
	cal	0.040	0.066	0.058	0.046	0.045
	val	0.044	0.087	0.070	0.047	0.051
MAE	uncal	1.909	0.718	0.634	0.756	0.581
	cal	0.413	0.600	0.477	0.445	0.378
	val	0.461	0.874	0.672	0.496	0.466
Bias	uncal	-1.749	-0.340	-0.489	0.567	-0.305
	cal	-0.191	-0.091	-0.318	0.074	-0.126
	val	-0.300	0.096	-0.548	-0.345	-0.272

3.2 LANGTJERN: LAKE ICE DYNAMICS

The models FLake, GOTM, MyLake and Simstrat accurately captured the onset of ice cover on Langtjern (-5 to +9 days) while GLM had larger errors (+10 to +17 days) (Figure 4). The ensemble mean, which was calculated by taking the average of the day of year when ice onset and ice-off occurred, was also relatively accurate (+3 to +6 days). For capturing the disappearance of ice cover, there was larger variability between the models compared to ice onset. In both years, GOTM and Simstrat predicted ice-off too early (-44 to -16 days). GLM overestimated ice-off in 2015 and 2016 by 27 to 19 days, respectively, whereas FLake and MyLake predicted ice-off relatively accurately both years (-1 to +8 days).

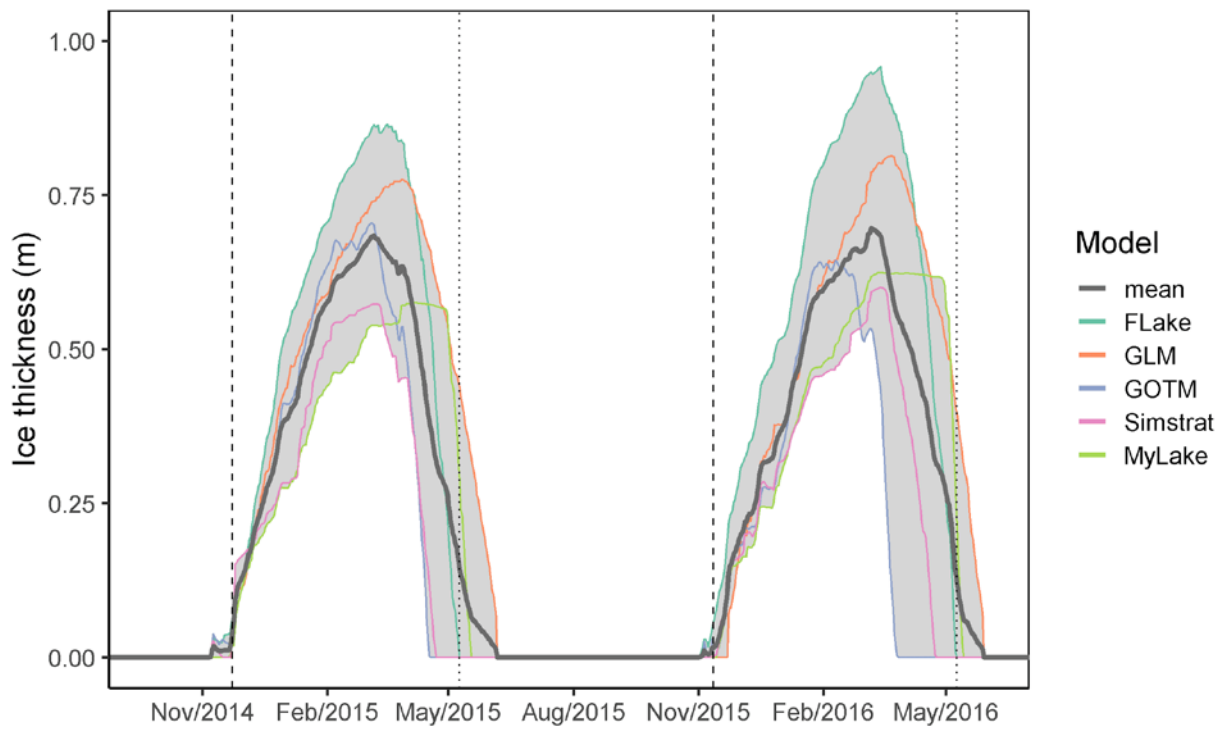


Figure 4. Calibrated ensemble model time series output for ice thickness for Langtjern, Norway. Dashed lines indicate the observed onset of ice and dotted lines indicate observed ice-off.

The temperature profiles had a larger RMSE for the calibration and validation period in general for Langtjern compared to Lough Feeagh, particularly MyLake (3.62 to 4.24 °C) and GOTM (3.36 to 4.70 °C) (Table 3). These models failed to accurately simulate the stratification structure with increased mixing during the summer months leading to larger errors. FLake had the lowest uncalibrated RMSE (2.02 °C), which was further reduced following calibration (1.08 °C). For summary plots of Langtjern of the model ensemble and residuals see Figure B1 and B2.

Table 3. Model results or goodness-of-fit - uncal(ibrated), cal(ibrated), and val(idated) - for water temperature (°C) in Langtjern using hourly forcing data (as MyLake requires daily input, LakeEnsemblR averages sub-daily input to daily time steps for MyLake simulations). Calibration was done for the year 2014-15 and validation for the year 2015-16. The best model performances are marked in bold. Shown are Root Mean Square Error (RMSE), Pearson's r (r), Nash-Sutcliffe Efficiency (NSE), Normalised Mean Absolute Error (NMAE), Mean Absolute Error (MAE), and Bias (or mean error).

Measure	Period	FLake	GLM	GOTM	Simstrat	MyLake	Ensemble Mean
RMSE	uncal	2.020	2.394	4.696	3.437	4.416	2.838
	cal	1.084	2.164	3.364	2.568	3.626	3.013
	val	1.135	1.764	4.045	4.171	4.242	3.699
R	uncal	0.887	0.868	0.786	0.833	0.807	0.874
	cal	0.983	0.906	0.865	0.913	0.845	0.881
	val	0.983	0.938	0.818	0.755	0.786	0.824
NSE	uncal	0.895	0.760	0.074	0.504	0.181	0.662
	cal	0.963	0.794	0.501	0.709	0.420	0.622
	val	0.962	0.862	0.275	0.229	0.203	0.433
NMAE	uncal	0.453	0.530	0.910	0.632	0.659	0.492
	cal	0.450	0.433	0.817	0.569	0.599	0.587
	val	0.454	0.362	0.828	0.677	0.636	0.602
MAE	uncal	1.260	1.601	3.515	2.637	3.126	1.929

	cal	0.830	1.469	2.686	2.211	2.818	2.189
	val	0.863	1.022	3.017	3.059	2.880	2.361
Bias	uncal	0.985	-0.298	1.076	-0.515	0.409	0.344
	cal	0.274	-0.575	0.313	-0.834	-0.615	0.019
	val	0.399	-0.104	0.823	-1.062	0.160	0.328

3.3 UNCERTAINTY PARTITIONING

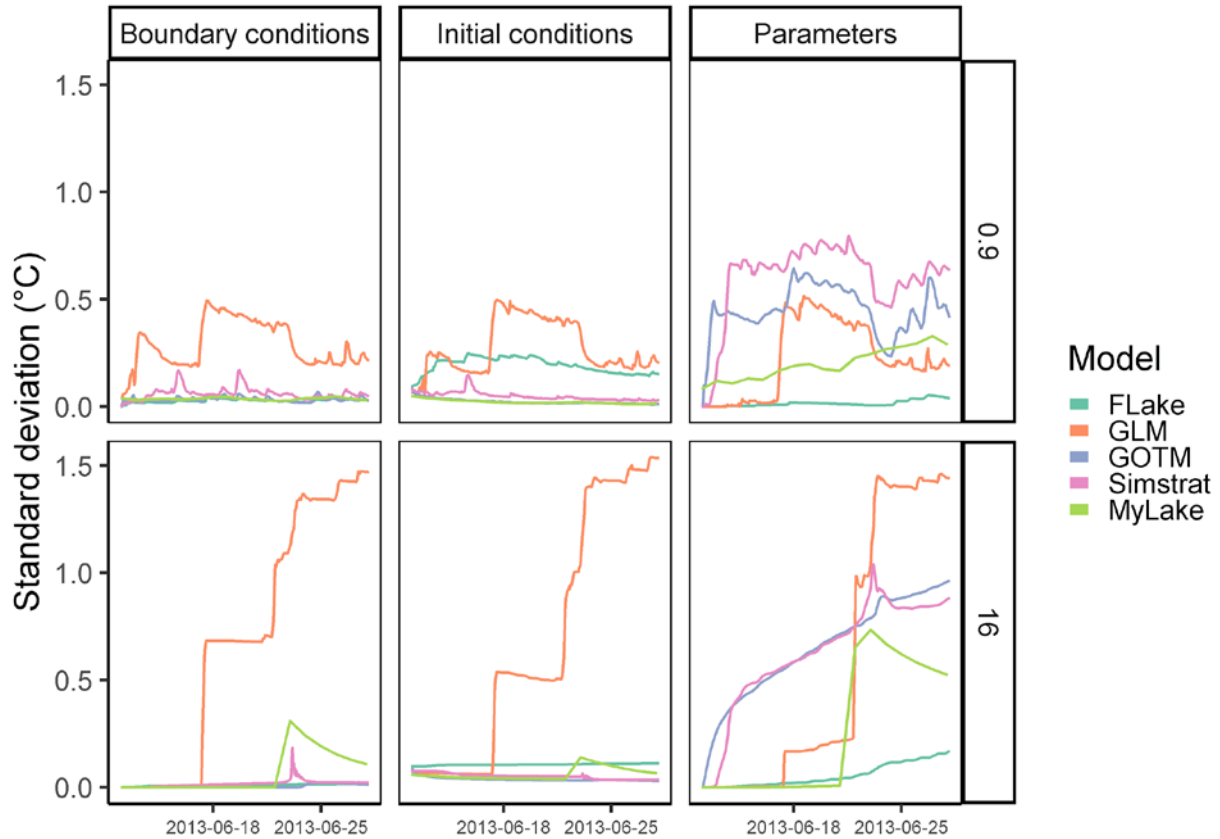


Figure 5. Partitioning of the different sources of uncertainty for ensemble simulations in Lough Feeagh; boundary conditions, initial conditions and parameters between models at depths of 0.9 m and 16 m. Each model was simulated 100 times for 16 days with adjustments to the boundary conditions, initial conditions, and model parameters accordingly. Standard deviation was calculated across all 100 simulations for each day.

Parameter uncertainty had the largest effect on the standard deviation of water temperatures at the depth of 0.9 m compared to initial conditions and boundary conditions for all the models except FLake in Lough Feeagh (Figure 5). Each of the parameters chosen were to account for mixing within the water column but their implementation in each model is different due to the different formulation of mixing equations in each model. Also, the distributions of these parameters were not comparable between models with some being normally distributed while others were log-normal distributed (Table C4). As such, parameter-uncertainty cannot accurately be compared between models, but it can be accounted for when using a one-model ensemble. Across the different models, boundary conditions were more sensitive for GLM than for the other models, at both 0.9 m and 16 m depth. With regards to uncertainty in the initial conditions, FLake and GLM had higher standard deviation at 0.9 m compared with GOTM, Simstrat and MyLake. GLM had a much higher standard deviation at 16 m for initial conditions, boundary conditions and parameter uncertainty. This is partly due to the strong stratification which is seen in GLM (Figure B3). For parameter uncertainty, GOTM, Simstrat and GLM had a high standard deviation at 0.9 m and 16 m, while it was lower for MyLake and FLake had the lowest uncertainty.

3.4 MULTI-PARAMETER ENSEMBLE

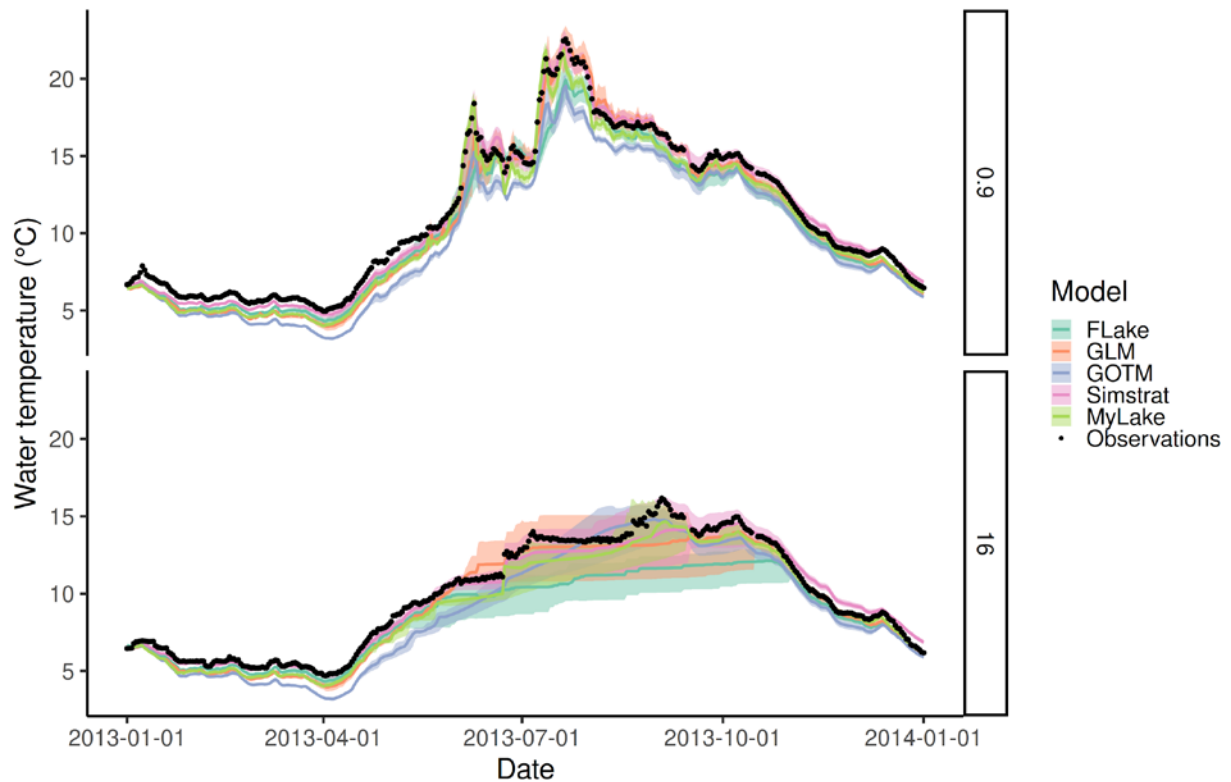


Figure 6. Uncertainty of the simulated water temperature due to the calibrated model parameter and scaling factors for the five models in Lough Feeagh, at 0.9 m depth and 16 m depth. The shaded areas give the range of values of an ensemble of 20 model runs with different parameterisation.

The model-specific parameters and scaling factors that resulted in good model performance had a broad distribution (see Figure B4 in the Supplement as an example). For the model-specific parameters of FLake, GLM, and Simstrat as well as for the shortwave radiation scaling factor for FLake and Simstrat this distribution spanned more than 75% of the range given in the calibration process. This suggests that the chosen parameters are interrelated and there might not be a single best parameter set, that the parameters were non-sensitive, or that the parameter range in the calibration was too narrow. The application of a multi-parameter ensemble is showing the uncertainty related to not being able to clearly identify a single best parameter set (Figure 6). The uncertainty of the simulated water temperature was larger during summer months and at greater depths for all models. For the water temperature close to the surface (0.9 m depth) the uncertainty due to the chosen model was slightly larger than the one related to the calibrated parameters throughout the year, for all models. At 16 m depth the uncertainty due to the calibrated parameter was about the same as the one related to the used model.

3.5 DISCUSSION

As the simulations with hourly time step in Lough Feeagh show, the ensemble mean can outperform individual lake models, which is in line with the findings of Kobler and Schmid (2019) and Trolle et al. (2014). For the Lough Feeagh simulations with a daily time step, the Simstrat model performed best, followed by the ensemble mean and MyLake. Using hourly time steps, GOTM performed best of the four models individually, albeit not as good as the ensemble mean. In Langtjern, FLake simulated water temperature profiles best, while Simstrat and MyLake performed the worst, although these two models simulated ice-on and ice-off well. In both Lough Feeagh and Langtjern, most models performed worse in the validation period than in the calibration period, which is to be expected due to the short (1 year) calibration period.

As shown in this study, and also observed while testing LakeEnsemblR in multiple other lakes (unpublished results), the best-performing model could vary per study case, and no single model consistently outperformed others. This shows an advantage of using ensembles compared to single model simulations, which are not likely to provide an optimal fit in every circumstance, while ensembles can incorporate individual strengths of multiple models. Similarly, ensemble modelling can highlight weaknesses of individual models compared to others which can further aid in model selection or refinement.

Ensemble predictions also give an indication of the uncertainty due to a different process description or parameterisation. This uncertainty may vary over depth or time (e.g. Figure 2 and Figure 5). An increased uncertainty in ensemble predictions represents diverging behaviour of different ensemble members. It might be important to interpret model predictions during periods with increased uncertainty with additional caution, and ensembles are a way to identify these periods. For a single set of parameters, the investigation of model-specific residuals in particular (e.g. Figure 3) supports the quantification of uncertainty and the identification of better suited models for specific case studies. In the Lough Feeagh case study, the models GOTM, MyLake and Simstrat had a bias for simulated water temperatures near the lake bottom and during fall mixing (Figure 3 a and Figure 3 b). By looking at the depth-discrete residual dynamics (Figure 3 c) as well as the density distribution of residuals (Figure 3 d), the model with the lowest overall bias for Lough Feeagh was GLM (scattering over the whole vertical axis) and Simstrat (negative bias at surface and positive bias at bottom). Running a calibrated model ensemble allows the user to quantify these model-specific biases and uncertainties, making scenario projections or forecastings more robust. Additionally, running ensembles with different parameterisations, initial conditions, or different boundary conditions can help to quantify the uncertainties related to the respective source.

Similarly to Kobler and Schmid (2019) and Yao et al. (2014), there was large variation between the different models in predicting ice cover phenology (Figure 4). However, most models captured the overall timing of ice-on and ice-off, which play a key role in the subsequent timing of stratification and several ecological processes in a lake. The ensemble represents the large uncertainty that is inherent in modelling lake ice cover (Sharma et al. 2019), which is important to account for when modelling lakes with periodic ice cover. It has recently been shown that the ensemble mean of ice timing and thickness can perform better than the individual models (Kobler and Schmid 2019), which was supported here.

A key part of modeling is being able to identify and quantify the different sources of uncertainty. This is especially important if the model is to be used in a forecasting framework. Thomas et al. (2020) used a single one-dimensional hydrodynamic model and partitioned out the sources of uncertainty over a 16-day forecast of water temperature profiles in a reservoir. Using the LakeEnsemblR framework, this can be explored and quantified further, using multiple models. The brief examples that are shown in Figure 5 and Figure 6 are a way in which such an analysis can be conducted and the information gained from this exploration can inform decisions on model and parameter selection.

4. SUMMARY

4.1 FRAMEWORK

LakeEnsemblR facilitates the pre-processing of data that is needed to run multiple 1D models and combines the results into a single, standardised output file. Each model in the package requires a different format and structure of its configuration and input files. This has been standardised in LakeEnsemblR by requiring only one set of input and configuration files and by using the same format for all input files. By having to specify a specific header for each column of an input file, mistakes involving column order and units are avoided, and in the configuration file only a reference to the file location needs to be given, instead of having to specify which column contains what information.

LakeEnsemblR relies on R packages for each model, hosted on GitHub and archived in Zenodo (see Software Availability). These packages contain pre-compiled model executables for the platforms Windows, MacOS, and

Linux, or the model code in R. This greatly facilitates user access to the models, as the ability to run the models is gained fully within the R environment. Some models provide pre-compiled executables on their respective websites, but often for only one platform, which regularly requires users to compile the model themselves. LakeEnsemblR removes this initial hurdle for modellers who want to apply one or multiple models.

The calibration methods provided in LakeEnsemblR can all be applied to the models without requiring the user to write custom calibration scripts. The ability to use the same calibration method for multiple models increases the comparability of the simulations. Results in the present study confirm that LakeEnsemblR's calibration methods can markedly improve model fit.

Like the input, each model generates its own specific output, often in different file types and consisting of different variables and units. LakeEnsemblR combines these outputs into one standardised format, either in text or netcdf. This allows quick application of the post-processing functions provided in LakeEnsemblR (e.g. *analyse_ncdf()* and *plot_heatmap()*), but also makes it easier for users to extract output and process the results in their preferred way. The standardised output is only generated for variables that are shared between the models. However, the full model-specific output is still available in the model output folders and can be accessed by the users.

By facilitating pre-processing, running, calibration, and post-processing, LakeEnsemblR supports accessible model ensemble applications by aquatic modellers new to the field. However, because all files required to run the models are present in the model folders, it in no way restricts more experienced users from using the full functionality of each of the different models. The "model parameters" section of the LakeEnsemblR configuration file allows the user to change any parameter in the model-specific configuration files, and files generated by LakeEnsemblR's *export_config()* function can be manually altered before starting the ensemble run.

4.2 RECOMMENDATIONS FOR USE

LakeEnsemblR eases the configuration, running and processing of a hydrodynamic lake model ensemble, and allows the user to explore the results in various ways. However, by making it easier to apply multiple models, there is the risk that less attention will be paid to individual model setup and that models may be applied to situations beyond what they were designed and tested for. For example, by considering five models at once, the overall number of parameters increases markedly and the user might be tempted to only use default parameter settings without critical consideration of the consequences.

In order to properly calibrate a model and avoid problems such as nonuniqueness of calibrated parameter sets (i.e. equifinality - see Beven 2006) it is important to make deliberate decisions and employ rigorous model validation. In addition to looking at single performance metrics for the simulated state variables, it is advisable to assess the model's capability to reproduce fluxes and emerging properties, patterns, and relationships (Hipsey et al. 2020). In order to find and select the right parameters to calibrate, the best practice approach would be to apply a sensitivity analysis (e.g. Andersen et al. 2021). Many methods for sensitivity analysis are available, but the Latin hypercube sampling method included in LakeEnsemblR can be used as an initial approach to quantify sensitivity. Where a complete sensitivity analysis is not feasible, expert or a priori knowledge on the models should be used to select the calibration parameters. In the present study, we aimed at demonstrating the possibility of calibration with LakeEnsemblR rather than exploring the parameter sensitivity of each model, and we chose model parameters based on the parameter selection done in previous studies (see Table C3 in the Supplement for parameters that were calibrated in previous studies).

However, the possibility to combine runs with multiple models and parameterisations also is an opportunity to tackle issues regarding sources of uncertainty. LakeEnsemblR can be used to quantify different sources of uncertainty (boundary conditions, initial conditions, parameter, model structure), increase understanding about what model works best under different circumstances, and also within-model comparisons can be made.

Although not applied in the present study, post-processing techniques applied in other research fields, such as blending (Vannitsem et al. 2021), can be applied to the ensemble result so that ensemble members are weighted and more information is retrieved from the ensemble. However, we advocate the use of LakeEnsemblR within established modelling practices (e.g. Arhonditsis and Brett 2004; Hipsey et al. 2020), rather than as a replacement.

4.3 OUTLOOK

The simulations in Lough Feeagh and Langtjern showcase the main functionalities of the package. However, LakeEnsemblR can be applied to a wider range of locations and scenarios. In long-term climate simulations, lake model ensembles have been applied as part of the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP) (Frieler et al. 2017; Vanderkelen et al. 2020), and LakeEnsemblR can facilitate similar efforts. Ensembles offer several possibilities for weekly or seasonal forecasting efforts (e.g. Krishnamurti et al. 2000; Thomas et al. 2020), and LakeEnsemblR can be run not only with multiple models, but also forced with several different weather forecasts. Studies of processes in lake physics that are difficult to model, such as consequences of extreme weather events (Mesman et al. 2020) or lake ice phenology (Yao et al. 2014), can especially benefit from an ensemble approach. While LakeEnsemblR currently only covers hydrodynamic models, its predictions can also serve as input for water quality models. Such a water quality ensemble can ultimately serve to assess and qualify the performance of multiple aquatic ecosystem models (Hipsey et al. 2020), while also giving uncertainty to the ecological impacts of management scenarios on ecosystems. More applications are possible, and the modular structure of the LakeEnsemblR code allows for the addition of new models and continued development.

Although the advantages of ensemble modelling have been acknowledged by the lake modelling community, until now no software to run multiple lake models for a single study site was available. LakeEnsemblR provides the necessary tools to widely apply ensembles of 1D lake models. Additionally to facilitating pre-processing of data, running of an ensemble of models, and standardising output, LakeEnsemblR allows the aquatic science community to start rigorous intra-model comparison studies of alternative process-based vertical 1D hydrodynamic lake models. Prior to the development of LakeEnsemblR, having an ensemble of models bound together with a consistent application programming interface, rigorous tests and comparison of alternative model codes were rare. We sincerely hope that LakeEnsemblR can provide a consistent framework for lake ensemble studies, uncertainty partitioning investigations, and intra-comparison modelling studies.

ACKNOWLEDGEMENTS

We thank the Global Lakes Ecological Observatory Network (GLEON) and the Aquatic Ecosystem Modellers Network Junior (AEMON-J) for bringing this group of researchers together. AEMON-J is a global, early-career network for aquatic ecosystem modellers that strives to advance the scientific field of numerical modelling in aquatic ecosystems as well as to build a welcoming community for novice and advanced modellers. Projects like this require a wide range of expertise, and this large group made the creation of this R package and the writing of this manuscript possible.

We also express our gratitude to the research institutes and the individuals that made changes to the models that allowed us to incorporate them into LakeEnsemblR, or provided assistance with bug fixing and compiling, most notably IGB Berlin, Germany, and Helmholtz Centre for Environmental Research UFZ, Germany (FLake), the University of Western Australia, Australia, and Virginia Tech, USA (GLM), EAWAG, Switzerland (Simstrat), Aarhus University, Denmark and Bolding & Bruggeman (GOTM), and Université Laval, Canada (MyLake). We thank the Marine Institute, Ireland and NIVA, Norway for collecting and sharing the data used in this study. Lastly, we thank Kaelin Cawley and other GLEON members for their participation in discussions in the early stage of the project. Reference to trade names does not imply endorsement by the U. S. government.

Author contributions: T.N.M., J.P.M., R.L., and J.F. conceptualised the study. T.N.M., J.P.M., R.L., and J.F. wrote most of the package code, with contributions of R.P., T.S., and J.R. T.N.M., J.P.M., R.L., J.F., F.O., R.P., J.J.V., and

J.R. tested the package during development. T.N.M., J.P.M., R.L., and J.F. wrote the manuscript, with input from the other authors. All authors participated in discussions during package development and the publication process.

Funding

T.N.M. was funded by: the WATExR project which is part of ERA4CS, an ERA-NET initiated by JPI Climate, and funded by MINECO (ES), FORMAS (SE), BMBF (DE), EPA (IE), RCN (NO), and IFD (DK), with co-funding by the European Union (Grant number: 690462) and also by NSF grants DEB-1926050 and DBI-1933016. J.P.M. was funded by the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie grant agreement no. 722518 (MANTEL ITN). R.L. was funded through a National Science Foundation ABI development grant (#DBI 1759865). J.F. was funded by the European Social Fund and co-financed by tax funds based on the budget approved by the members of the Saxon State Parliament. R.M.P. was funded by Sentinel North Research Internship Scholarship program for foreign students at Université Laval and student travel award support from GLEON. T.S. was supported by German Science Foundation grants DFG KI 853/13-1 and CDZ 1259. J.J.V. was supported by a Natural Sciences and Engineering Research Council of Canada Discovery Grant (RGPIN-2018-06389). K.C.R. was funded by National Science Foundation grants 1754265, 1638704, and 1761805.

SOFTWARE AND DATA AVAILABILITY

The LakeEnsemblR code is available at <https://github.com/aemon-j/LakeEnsemblR>. LakeEnsemblR and the packages it relies upon (FLakeR, GLM3r, GOTMr, SimstratR, MyLakeR, glmtools, gotmtools) can be installed in R following the instructions on the GitHub page, using the `install_github()` function of the devtools package (Wickham et al. 2020). The packages to run the models do not contain the source code of each model, only the executables for Windows, MacOS, and Linux. Links to the websites of the respective models are provided on GitHub. Example set-ups of LakeEnsemblR are provided at https://github.com/aemon-j/LER_examples. For further instructions on how to run LakeEnsemblR, we refer the reader to the AEMON-J GitHub page (<https://github.com/aemon-j/LakeEnsemblR>), where a vignette and a Wiki are available with detailed instructions and code examples.

LakeEnsemblR version 1.0.0 and the model packages have been archived in Zenodo under the following DOIs:

LakeEnsemblR: 10.5281/zenodo.4146899

FLakeR: 10.5281/zenodo.4139807

GLM3r: 10.5281/zenodo.4146848

GOTMr: 10.5281/zenodo.4139780

SimstratR: 10.5281/zenodo.4139731

MyLakeR: 10.5281/zenodo.4067998

When using LakeEnsemblR for a publication, please also cite the sources of the respective models that you are including in your ensemble (see `citation("LakeEnsemblR")`).

CHAPTER 4 - DRIVERS OF PHYTOPLANKTON RESPONSES TO SUMMER STORMS IN A STRATIFIED LAKE: A MODELLING STUDY

Jorrit P. Mesman^{1,2,3*}, Ana I. Ayala^{2,3}, Stéphane Goyette², Jérôme Kasparian², Rafael Marcé^{4,5}, Hampus Markensten⁶, Julio A.A. Stelzer^{1,7,8}, Michael W. Thayne^{1,7,8}, Mridul K. Thomas¹, Don C. Pierson³, Bas W. Ibelings¹

¹*University of Geneva, Department F.-A. Forel for Environmental and Aquatic Sciences & Institute for Environmental Sciences, 1211, Geneva 4, Switzerland*

²*University of Geneva, Group of Applied Physics & Institute for Environmental Sciences, 1211, Geneva 4, Switzerland*

³*Uppsala University, Department of Ecology and Genetics, 75236, Uppsala, Sweden*

⁴*Catalan Institute for Water Research (ICRA), 17003 Girona, Spain*

⁵*Universitat de Girona, 17003 Girona, Spain*

⁶*Swedish University of Agricultural Sciences, Department of Aquatic Sciences and Assessment, 75007, Uppsala, Sweden*

⁷*Leibniz Institute of Freshwater Ecology and Inland Fisheries, Department of Ecosystem Research, Berlin, Germany*

⁸*Freie Universität Berlin, Department of Biology, Chemistry, and Pharmacy, 14195, Berlin, Germany*

*Correspondence: Jorrit.Mesman@unige.ch

ABSTRACT

Extreme wind events affect lake phytoplankton amongst others by deepening the mixed layer and increasing internal nutrient loading. Both increases and decreases of phytoplankton biomass after storms have been observed, but the precise mechanisms driving these responses remain poorly understood or quantified. In this study, we coupled a one-dimensional physical model to a biogeochemical model to investigate the factors regulating short-term phytoplankton responses to summer storms, now and under expected warmer future conditions. We simulated physical, chemical and biological dynamics in Lake Erken, Sweden, and found that wind storms could increase or decrease the phytoplankton concentration one week after the storm, depending on antecedent lake physical and chemical conditions. Storms had little effect on phytoplankton biomass if the mixed layer was deep prior to storm exposure. Higher incoming shortwave radiation and hypolimnetic nutrient concentration boosted growth, whereas higher surface water temperatures decreased phytoplankton concentration after storms. Medium-intensity wind speeds resulted in more phytoplankton biomass after storms than high-intensity wind. Simulations under a future climate scenario did not show marked differences in the way wind affects phytoplankton growth following storms. Our study shows that storm impacts on lake phytoplankton are complex and likely to vary as a function of local environmental conditions.

Keywords: *Stratification, Storms, Extreme events, Modelling, Phytoplankton, Climate change, Nutrient entrainment, Mixing*

INTRODUCTION

High wind speeds during storms reshape the lake physical and chemical environment in ways that alter phytoplankton biomass and growth. At the start of a chain of processes, wind stress at the lake surface induces internal mixing and this deepens the thermocline (Andersen et al. 2020). These processes affect the vertical distributions of oxygen and nutrients, and in turn phytoplankton growth and vertical distribution. Upwelling of

nutrient-rich water occurs during mixing events and can alleviate nutrient limitation, potentially causing phytoplankton blooms (Soranno et al. 1997; Kasprzak et al. 2017; Whitt et al. 2019). At the same time, surface temperature tends to decrease during storms (Kuha et al. 2016; Mesman et al. 2020), potentially reducing light-saturated phytoplankton growth rates (Trombetta et al. 2019). Additionally, a deeper mixed layer can increase light limitation for growth (Diehl et al. 2002) and deepening dilutes concentrations by mixing phytoplankton over a larger volume of water (Kuha et al. 2016). Sediment resuspension due to shear stress in shallower parts of the lake may simultaneously release nutrients and limit light availability (Ji et al. 2018). As such, there are conflicting effects of storms on nutrient and light availability (Stockwell et al. 2020), and the net effect of a storm on phytoplankton concentrations may depend on lake physiography and lake state prior to the event.

Changes in storm characteristics and lake thermal structure will affect phytoplankton responses to storms. As a result of climate change, extreme wind events will likely shift in frequency and intensity, with different parts of the globe experiencing increases or decreases (Möller et al. 2016; Sainsbury et al. 2018). Concurrent with these changes in meteorological conditions, as surface water temperatures increase and stratification strengthens (O'Reilly et al. 2015; Pilla et al. 2020), more energy is needed to mix the water column (Schmidt 1928), so that in a warmer climate a wind event of a given magnitude and duration may cause less mixing. The depth of the mixed layer, at the time when a storm hits, also determines the degree of lake mixing; a deeper pre-storm mixed layer reduces entrainment of hypolimnetic water by surface waves (Imboden and Wüest 1995). Long-term climate effects on mixed layer depth (MLD) are still ambiguous; both shoaling and deepening mixed layers have been observed, in addition to non-significant trends (e.g. Kraemer et al. 2015; Pilla et al. 2020) and it is likely that local trends in transparency or wind speed are at least equally important as trends in warming to determine changes in MLD (Persson and Jones 2008; Woolway et al. 2019). Lastly, stratification is expected to occur earlier in the year as the climate warms (Woolway et al. 2021), and this will lead to a longer separation of epilimnion and hypolimnion. Therefore, there will be a greater build-up of nutrients in the hypolimnion during the stratified period (Pettersson et al. 2003; Nowlin et al. 2005), which could be entrained into the mixed layer during a storm and become available for phytoplankton growth.

Understanding mechanistically how complex lake ecosystems are reshaped by storm events under present and projected future conditions is a challenging task. Process-based models have the advantage of allowing a quantitative comparison between different scenarios and identifying clear causal pathways even in complex systems and in conditions yet to be observed. Also, experiments that incorporate deep-water mixing and different scenarios regarding stratification, nutrient concentrations and climate warming are very demanding to set up (but see Giling et al. 2017a), whereas models can relatively easily explore such a wide range of scenarios. Another issue involving the study of extreme events, is that such events are rare by definition and hard to predict. Moreover, storms act on short timescales (hours to days), while lake monitoring programs often include only weekly or monthly samples. Therefore, biogeochemical data describing responses to storm events are scarce. In the present study, we use the General Ocean Turbulence Model (GOTM) model coupled to a biogeochemical model to study the impact of storms on phytoplankton dynamics. In Mesman et al. (2020), one-dimensional process-based models (including GOTM) were shown to simulate physical effects of storms with reasonable accuracy. This means that we can have some confidence that processes related to the transport and mixing of biogeochemical particles and solutes during storms are accurately simulated. Our approach allows us to draw conclusions about potential regulating factors for the response of phytoplankton to storms, and how climate warming may affect this response.

The main process under investigation here is the effect of storms on the redistribution of biogeochemical compounds between the epi- and hypolimnion. We use Lake Erken, a Swedish mesotrophic dimictic lake, as a case study, because of the available long-term time series of physical and biological variables that we used to calibrate the model. However, the findings in this study increase our understanding of the processes regulating phytoplankton responses to storms across stratifying lakes in general. Phytoplankton communities in these lakes are shaped by their need for both nutrients and light, which show opposing gradients in availability. Shallow

polymictic lakes are likely to react differently to storms, with more emphasis on sediment resuspension and uprooting of macrophytes (Ji et al. 2018), and our model results are not applicable there. We assess scenarios covering a broad range of atmospheric and lake conditions, that reflect conditions present in many temperate, stratifying lakes.

Here, we investigate 1) how storm intensity, thermal structure, light availability, and nutrient availability control phytoplankton response to storms during summer stratification, and 2) how climate warming may influence the response of phytoplankton to storms. To answer these questions, we performed two numerical experiments. In the first experiment, we repeatedly simulate a storm event while changing storm intensity, incoming shortwave radiation, and pre-event mixed layer depth, surface water temperature, and hypolimnetic nutrient concentration in a full factorial design. In the second numerical experiment, we compare the response of phytoplankton to wind perturbations between present-day and future-climate air temperatures, at different times of the year and at different storm intensities. These simulations help us to disentangle and better understand the dynamic response of primary producers to storms in a changing world.

METHODOLOGY

SITE DESCRIPTION

Lake Erken is a mesotrophic lake in Sweden (59°50'37" N, 18°35'38" E), with a mean depth of 9 m and a maximum depth of 21 m. The lake has a surface area of 24 km² and its retention time is 7 years (Blenckner et al. 2002). Lake Erken is dimictic, meaning that it experiences both winter ice cover and summer stratification, although short-term partial or complete mixing events are possible in summer in response to wind-induced mixing (Yang et al. 2016a). During summer stratification, both nitrogen (N) and phosphorus (P) can limit phytoplankton growth in the lake (Vrede et al. 1999), whereas during deep mixing or fully mixed conditions, light availability is the main limiting factor (Yang et al. 2016a). During summer, nutrient concentrations build up in the hypolimnion, and these nutrients are circulated through the complete water column after the autumn turnover (Pettersson et al. 2003).

In most years, Lake Erken experiences a distinct spring bloom followed by a clear water phase, and then a second phytoplankton biomass peak in summer/autumn (Yang et al. 2016b), a pattern followed by many monomictic and dimictic lakes across the globe (e.g. Sommer et al. 2012). The spring bloom in Lake Erken is dominated by diatoms such as *Aulacoseira spp.*, *Stephanodiscus spp.*, and *Asterionella formosa* (Weyhenmeyer et al. 1999; Yang et al. 2016b). In summer, a major bloom-forming species is the cyanobacterium *Gloeotrichia echinulata* (Karlsson-Elfgren et al. 2003; Yang et al. 2016b).

DATA COLLECTION

In this study, we used meteorological, water temperature, and biogeochemical data for the period 1999 to 2020. Meteorological data (wind speed, air temperature, air pressure, relative humidity, shortwave radiation, cloud cover, and precipitation) were collected using a weather station on a small island in the lake at hourly frequency. Moras et al. (2019) replaced missing meteorological data from nearby stations, selected by artificial neural network analysis, and we continued to use this dataset, supplemented by data until the end of 2020.

Discharge into Lake Erken was calculated by the HYPE model (Lindström et al. 2010), and validated using measured data from the main tributary of the lake. In this main tributary, discharge and temperature data were automatically monitored and summarised to daily values, while phosphate, total phosphorus, nitrate, and particulate organic matter concentrations in the inflow were measured once or twice per month. These data were collected only from 2004 onwards, and the first 5 years of the recorded nutrient loadings were recycled for 1999-2003, which was the spin-up period of the model (see below).

In the lake, hourly water temperature data were collected during the ice-free season with a thermocouple chain above the deepest point of the lake, every 0.5 m down to 15 m depth. Starting in 2017, these data were collected

year-round. Schmidt stability (Schmidt 1928; Idso 1973) and mixed layer depth were calculated from the water temperature profiles. Schmidt stability was calculated using the “rLakeAnalyzer” R package (Winslow et al. 2019). The mixed layer depth was defined as the depth where water density had increased by 0.15 kg/m³ relative to the uppermost measurement (similar method as Wilson et al. 2020).

Water samples to determine nutrient concentrations (phosphate, total phosphorus, nitrate, and ammonium) were collected every two weeks during the ice-free season. During stratification, separate integrated samples of the epilimnion and hypolimnion were taken. In winter, if the ice was accessible, a single integrated nutrient sample was taken through a hole in the ice approximately every month. Nutrients were analysed using standard laboratory techniques, described in Ahlgren and Ahlgren (1976) and Goedkoop and Sonesten (1995). Chlorophyll-a data were collected at the same time and depth resolution as the nutrient data. Material concentrated by filtration on glass fibre filters were analysed using spectrophotometry as described in Ahlgren and Ahlgren (1976).

MODEL DESCRIPTION AND SETUP

The General Ocean Turbulence Model (GOTM) is a one-dimensional (1D) k-epsilon model that simulates vertical thermal and turbulence dynamics in freshwater and marine water bodies (Umlauf et al. 2005). GOTM is interfaced to the Framework for Aquatic Biogeochemical Models (FABM), which allows coupling of a physical model with a biogeochemical model (Table 1, Bruggeman and Bolding 2014). At every simulation time step in this coupled setup, the biogeochemical equations are applied to each layer in GOTM, including surface and sediment exchange, and GOTM regulates the transport of biogeochemical substances between the layers. Using FABM, GOTM was coupled to a modified version of the SELMA model, which itself is a modular version of the ERGOM model (Table 1, Neumann et al. 2002). This new version was named “Selmaprotbas”, because apart from several code improvements, we implemented several features from the PROTBAS model described by Markensten and Pierson (2007).

The Selmaprotbas model describes oxygen, detritus, nitrogen, phosphorus, phytoplankton and zooplankton dynamics. Processes described in the model include (de-)nitrification, sediment resuspension, sediment solute release, mineralisation of detritus, phytoplankton growth regulated by nutrients and light, and grazing by zooplankton (Neumann et al. 2002). Chlorophyll-a content and biomass are linked through a fixed chlorophyll-to-carbon ratio. We modified the SELMA model code by 1) expressing biomass in carbon instead of nitrogen; 2) adding a silica cycle; 3) adding an option to use the phytoplankton light limitation and temperature growth dependence function described in Reynolds et al. (2001), 4) relating chlorophyll-a concentration directly to the carbon biomass of phytoplankton; 5) adding the possibility for buoyancy regulation of phytoplankton; and 6) allowing varying nutrient ratios over time in detritus and sediment. Advantages of these changes include a more comparable set-up to other biogeochemical models and a more complete description of potentially relevant processes. A more detailed common-language description of the model has been supplied in Supplement A and the model code is publicly available (see Software Availability).

Table 1. Software used or referred to in this study. Supplement A contains more information on how GOTM and Selmaprotbas are coupled to each other, and how the Selmaprotbas model was derived from the SELMA and PROTBAS models.

Abbreviation	Full name	Description	Reference
GOTM	General Ocean Turbulence Model	One-dimensional hydrodynamic model. Used in this study to simulate the vertical thermal structure	Umlauf et al., 2005
FABM	Framework for Aquatic Biogeochemical Models	Framework to couple a hydrodynamic to a biogeochemical model. Used in this study to couple GOTM and Selmaprotbas.	Bruggeman & Bolding, 2014
Selmaprotbas	Selmaprotbas (combination of the	Biogeochemical model. Used in this study to simulate oxygen, nutrient, and	<i>This study</i>

	<i>SELMA and PROTBAS models)</i>	phytoplankton dynamics. Based on SELMA and PROTBAS.	
SELMA	Simple EcoLogical Model for the Aquatic	Biogeochemical model. A modular (i.e. compartmentalised) version of ERGOM that can be coupled to FABM.	-
ERGOM	Ecological ReGional Ocean Model	Biogeochemical model.	Neumann et al., 2002
PROTBAS	PROTech-Based Algal Simulations	One-dimensional physical and biogeochemical model. Based on PROTECH.	Markensten & Pierson, 2007
PROTECH	Phytoplankton RespOnses To Environmental CHange	One-dimensional biogeochemical model.	Reynolds et al., 2001
ParSAC	Parallel Sensitivity Analysis and Calibration	Software for sensitivity analysis and calibration. Used in this study to perform a sensitivity analysis and calibrate the GOTM-Selmaprotbas coupled model.	Bruggeman & Bolding, 2020

The meteorological conditions and inflow data collected at Lake Erken were used as inputs for the model, and the GOTM model was run with an integration time step of 1 hour and 0.5 m thick layers. A fourth order Runge-Kutta time integration scheme was chosen for the Selmaprotbas model. The Selmaprotbas model was run with two phytoplankton groups: diatoms and cyanobacteria, both of which had growth regulated by light, temperature, and the concentrations of phosphorus and nitrogen. The diatom group was calibrated specifically for the spring period, had high sinking rates, and was also regulated by silica; cyanobacteria could fix nitrogen and regulated buoyancy based on light availability, with the same settings as *Anabaena* (now *Dolichospermum*) described by Reynolds et al. (2001). For the files used to run the model, see Software Availability.

CALIBRATION

After 5 years of spin-up, 13 years (2004-2016) were used for calibration, which was done using the ParSAC software (Table 1, Bruggeman and Bolding 2020), employing a differential evolution method to optimise the maximum likelihood objective function of RMSE between observations and simulations. A single set of parameter values was retrieved from the calibration. The calibration was split into two steps. First, the water temperature data was optimised using 10,000 iterations, by calibrating five parameters based on a previous study (Ayala et al. 2020): minimum turbulent kinetic energy, the extinction coefficient of visible light, and scaling factors for heat fluxes, wind speed, and incoming shortwave radiation. In the second step, 400,000 model iterations were done, varying 50 parameters that were determined in a sensitivity analysis (see next section). The objective function compared simulated in-lake concentrations of ammonium, nitrate, phosphate, total phosphorus, chlorophyll-a, water temperature, and oxygen with measured lake data. Physical parameters from the first step were also included in the second step of the calibration, but their ranges were constrained to +/- 10% of the value obtained in the first calibration step. Since the nutrient and chlorophyll-a samples were based on integrated samples for the epilimnion and hypolimnion, for the calibration we assumed these samples to be representative of 3 m and 15 m depth, respectively.

The ParSAC calibration attaches equal weight to each observation, so to avoid attaching too much value to the water temperature and oxygen measurements (which were collected at higher frequency) in the second step, we excluded temperature and oxygen measurements that were not collected on the same day as the nutrients, and we reduced the vertical resolution from 0.5 to 1.0 m. The full time series were used to assess goodness-of-fit.

The results of the calibration can be found in Supplement B.

SENSITIVITY ANALYSIS

To determine what parameters to include in the calibration of the Selmaprotbas model (biogeochemistry), we performed a sensitivity analysis using the ParSAC software (Bruggeman and Bolding 2020; Andersen et al. 2021), which applies the Sensitivity Analysis Library (SALib, Herman and Usher 2017) in Python. All parameters in the Selmaprotbas model, scaling factors for inflow discharge and concentrations, and the five calibrated parameters in GOTM were included in the sensitivity analysis (totalling 55 parameters), and responses in simulated mean values of ammonium, nitrate, phosphate, total phosphorus, chlorophyll-a, and oxygen were assessed.

We followed a density-based delta-sensitivity method (Borgonovo 2007), which has been described by Andersen et al. (2021) for the GOTM-FABM-PCLake model. First, a Latin hypercube sampling (McKay et al. 2000) was done to generate a number of parameter sets equal to 200 times the number of parameters. This number was based on a convergence test, where we found that values for sensitivity started to converge at this number (results of convergence test not shown). We then ran the model for all parameter sets in the Latin hypercube and used the delta-sensitivity analysis as described by Borgonovo (2007) on the results to do the sensitivity analysis. In this method, the global importance of a parameter is calculated based on its effect on the entire output distribution, which can be calculated even when parameters are correlated (Borgonovo 2007). A 95-percent confidence interval around the sensitivity values was obtained by 100 resamples using a bootstrapping approach (Plischke et al. 2013). To distinguish sensitive from insensitive parameters, we introduced a dummy parameter in the sensitivity analysis (Andersen et al. 2021). If a parameter's sensitivity value fell within the 95-percent confidence interval of the dummy for all variables (ammonium, nitrate, phosphate, chlorophyll-a, oxygen), that parameter was excluded from the calibration. For parameters that were repeated for the two phytoplankton groups, the parameter was excluded only if it fell in the dummy confidence interval for both groups. If not, the parameter was retained for both phytoplankton groups. The parameters that were excluded during the sensitivity analysis can be found in Supplement B.

VALIDATION

We calculated Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Error (ME), and Nash-Sutcliffe Efficiency (NSE, Nash and Sutcliffe 1970) from the simulated and measured values of water temperature, nutrients, oxygen, and chlorophyll-a as measures for the goodness-of-fit. All measured values at each depth were compared to the corresponding simulated values, by linear interpolation of simulated values if necessary. The last 4 years of the time series (2017-2020) were used for validation, and thus not used to train the model. The measures for the goodness-of-fit were compared between the calibration and validation period to assess the quality of the simulation. The simulation from 1999-2020 using the observed weather conditions and the calibrated parameter values is termed the "long-term simulation".

All calculations and data handling were done in the R software, version 4.0.1 (R Core Team 2020).

NUMERICAL EXPERIMENT 1: VARYING INITIAL CONDITIONS BEFORE A STORM

The aim of our first numerical experiment was to investigate which variables control the response of phytoplankton concentrations to storms. In order to achieve this aim, we induced a one-day storm event for different values of several meteorological and pre-event lake variables. Five variables were chosen that were expected to impact phytoplankton response to storms:

- Storm intensity (i.e. wind speed during the event); this represents the magnitude of the disturbance induced by the storm
- Mixed layer depth (MLD); MLD prior to the storm is a measure of the vulnerability of the thermal structure to mixing and controls the volume of the epilimnion
- Shortwave radiation; incoming solar radiation regulates the availability of light
- Surface water temperature; increases the strength of stratification, and therefore the resistance to mixing

- Hypolimnetic nutrients; these regulate the potential for nutrient upwelling

Ten levels of each variable were taken into consideration in a full factorial design, therefore totalling $10^5 = 100,000$ simulations. The storm perturbation had a duration of 24 hours and was initiated 24 hours after initialisation of the model run (Figure 1a).

We focused on the month of July to generate the weather conditions for this numerical experiment. This is because Lake Erken was always stratified in this month and stratification would have existed for a long enough time to allow for the build-up of hypolimnetic nutrients. In order to have a representative period with natural weather variations, we have selected the year in our dataset with the most generic weather conditions during this month. To that purpose, we calculated the mean and standard deviation for the meteorological driving variables measured in July (wind, pressure, temperature, relative humidity, shortwave radiation, and cloud cover) for each year separately and for the full period (1999-2020). For each year, we then calculated the root mean squared relative error (e.g. Despotovic et al. 2016) between the year and the full period values for both mean and standard deviation. July 2006 had the lowest error value and therefore most closely matched the long-term mean and variance, so these weather conditions were used as baseline in the first experiment (Figure 1, panels a-d).

This numerical experiment required calculation of generic in-lake conditions to be used as initial conditions, for all model variables. We used the long-term simulation during July to determine these, because we decided that this was more representative of average summer conditions in Lake Erken rather than using the initial profiles for July 2006. Due to the scenarios with different MLD and the importance of MLD for vertical profiles of temperature and solutes, we calculated average profiles for the epilimnion and hypolimnion separately. Both profiles were defined as ten equidistant values, interpolated from surface to the MLD for the epilimnion, and from the MLD to the maximum depth for the hypolimnion. As an example, when the MLD was 8 m, the epilimnetic profile would consist of ten values, a linear interpolation of the simulated values over 0 – 8 m, and when the MLD was 4 m, the epilimnetic profile would still have ten values, but interpolated over 0 – 4 m depth. Dates with a density difference between top and bottom of less than 0.15 kg/m^3 were excluded, as well as dates with an MLD shallower than 2 m or deeper than 15 m. The average of all calculated epilimnetic and hypolimnetic profiles during July were taken as initial conditions for our simulations, for each model variable. Because these initial conditions were defined relative to MLD, profiles for any value of MLD could be generated (see dashed lines in Figure 1, panels e-g).

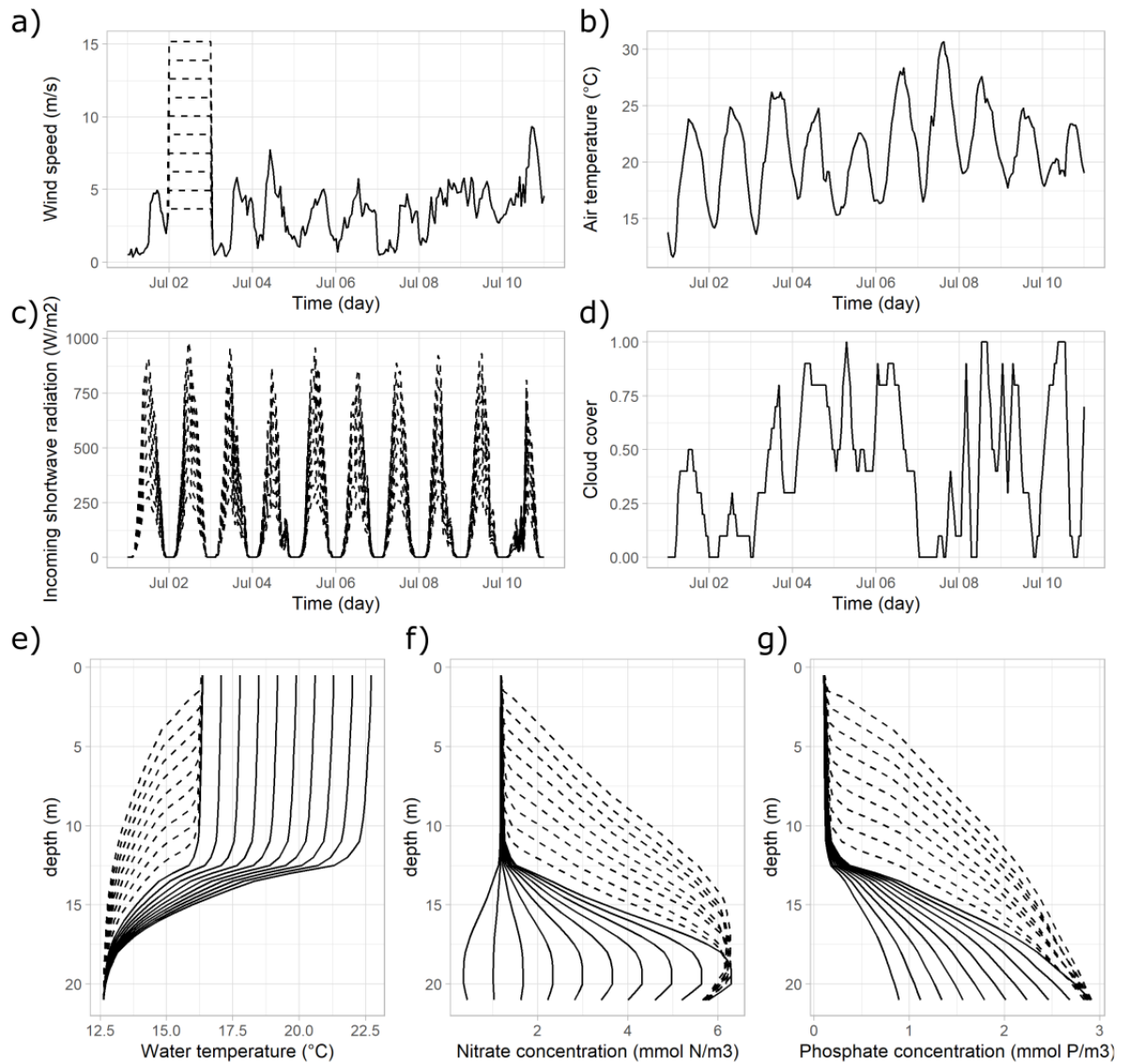


Figure 1. Set-up of the first numerical experiment. Panels a-d show the weather conditions used in the experiment – a) wind speed, b) air temperature, c) incoming shortwave radiation, and d) cloud cover. The solid lines were used in all simulations and the dashed lines indicate the different scenarios used in the numerical experiment, which were varied independently of one another. In panels e-g, the initial vertical profiles of e) water temperature, f) nitrate, and g) phosphate are shown. The initial profiles varied in both mixed layer depth (MLD, dashed lines) as well as the epilimnetic value for water temperature and the hypolimnetic value for nitrate and phosphorus (solid lines). Since it was a full factorial design, each of the panels e-g could contain hundred lines (varying both MLD and absolute value), but instead variation in either MLD (keeping the absolute value constant) or absolute value (keeping MLD constant) is shown. Nitrate and phosphate were part of the same scenario (i.e. “nutrients”) and therefore did not vary independently. These initial profiles were based on the average conditions during July in the long-term simulations. The values of the levels used in the scenarios can be found in Supplement C.

The ten different levels of wind speed, MLD, incoming solar radiation, surface temperature, and hypolimnetic nutrient concentration used in the simulations were also determined from the long-term simulation (1999-2020) using data from July. The 5th and 95th percentile of the daily averages were computed, and a linear sequence of ten values between these percentiles was used for the experiment (Figure 1). The only exception was wind speed. Since the main interest of the present study was high wind speed, the lowest wind speed considered was the median, and the highest wind speed was set to 3 m/s above the maximum recorded daily average wind speed, to anticipate the possibility of increased storm intensity in the future due to climate change (Mölter et al. 2016). Each combination of the independently-changed variables was a separate simulation.

As output of each model run, concentrations of chlorophyll-a, nitrate, and phosphate were volume-averaged over the euphotic zone for the first week after the end of the storm. The depth of the euphotic zone (i.e. the depth where 1% of the light remains) was kept constant and was calculated as $-\ln(0.01)$ times the calibrated value of the e-folding depth of visible light (“g2” parameter) in the GOTM model, which gave a euphotic zone depth of 8.0 m. We decided to average over the euphotic zone, because phytoplankton below this zone are unlikely to contribute to primary production and will likely degrade over time, yet they are still present as biomass in the model. Averaging over the full water column would therefore lead to underestimation of the effects of storms on production and chlorophyll-a due to mixed layer deepening. In addition to the average concentrations, average Schmidt stability was also calculated for the first week after the storm.

As the last step of this experiment, we fitted the volume-averaged chlorophyll-a concentrations in the experiment with a random forest model to discern what variables affected the result most, using permutation variable importance. The random forest model contained 1000 trees, and all data from the experiment were used - so no holdout -, as the aim was to find out what variables were most important, not prediction. The fitting of the random forest model and the calculation of the permutation importance were done using the “ranger” R package (Wright and Ziegler 2017).

NUMERICAL EXPERIMENT 2: INDUCING STORMS IN LONG-TERM SCENARIOS

Where the first numerical experiment investigated the effect of individual variables, the second experiment aimed at discerning the net effect of a warming climate on phytoplankton response to storms. The long-term simulation, from 1999 to 2020, under observed weather conditions, was taken as the baseline. To this baseline, every year ($N = 22$) a 24-hour wind perturbation was added. To avoid cumulative effects, only one perturbation was applied to each 22-year simulation. For the rest of the period, observed weather data were used. Based on average seasonal patterns of stratification, this perturbation occurred early (9th of June, corresponding to the first day-of-the-year when the averaged Schmidt stability over all the years exceeded 50% of the maximum) or later (4th of July, 80% of maximum stratification) in the year, and with moderate (7.2 m/s, i.e. 95th percentile of daily average wind speed) or high (9.0 m/s, 99th percentile) intensity (Table 2; for the determination of these thresholds, see Supplement D).

Table 2. Design for the second numerical experiment. Starting from the long-term simulation (1999-2020), 24-hour wind perturbations were added either early or late in the year, and with moderate or high intensity. These wind perturbations were added to every year in separate simulations, to avoid accretion of effects. This setup was repeated for a future-climate scenario, in which air temperatures were scaled to the level of 2040-2070 according to an RCP (Representative Concentration Pathway) 8.5 climate scenario.

	Present-climate (observed meteorological data)	RCP8.5 (scaled air temperatures)
Control (no perturbations)	1 simulation	1 simulation
Early, moderate intensity	22 simulations (1 perturbation for each year 1999-2020)	22 simulations
Early, high intensity	22 simulations	22 simulations
Late, moderate intensity	22 simulations	22 simulations
Late, high intensity	22 simulations	22 simulations

This design was repeated for a climate scenario in which the air temperature was scaled to the period 2041-2070 of an RCP8.5 emission scenario of the regional-downscaled output of the HadGEM2-ES global climate model (Collins et al. 2008) that was created as part of the EURO-CORDEX experiment (Table 2, Jacob et al. 2013). The measured Lake Erken air temperature was scaled according to the delta-decile method described in Perroud and Goyette (2010); for every month and every decile of daily-averaged air temperature (0-10th percentile, 10th to 20th percentile, etc.) the increase in temperature was calculated and applied to the historical time series. The other meteorological conditions, including relative humidity and wind speed, were kept the same. This approach

was chosen to isolate the effects of warming alone and to draw conclusions for a wider range of lakes, as local trends in other variables that may be specific to Lake Erken were not included. Atmospheric warming not only influences surface temperature and strength of stratification, but can also change the mixed layer depth and lead to an earlier onset of stratification and thus to different vertical profiles of nutrients and oxygen. As such, increased air temperature influences multiple potentially important lake variables that affect the relationship between storms and phytoplankton, which were investigated in isolation in the first numerical experiment.

In each simulation, the volume-averaged chlorophyll-a concentration between 0 and 8.0 m depth (the euphotic zone) was calculated. The maximum difference in concentration between the control and storm scenario, within one week after the storm, was compared between present-day and future climate.

RESULTS

CALIBRATION AND VALIDATION

During the calibration period, the model simulated water temperature with an RMSE of 0.9 °C. Seasonal cycles in oxygen, nitrate, and phosphate, were also reproduced, as indicated by NSE values above 0 (Table 3). The main cause for the low fit statistics of chlorophyll-a was the substantial underestimation of the spring chlorophyll-a peak (Supplement E). In the validation period, the model fit worsened slightly for phosphate, nitrate and chlorophyll-a, as indicated by the NSE values. Inspection of the time series (Supplement E) confirmed that seasonal cycles in water temperature were well simulated. Deep-water oxygen concentrations were also simulated accurately, except that under ice, oxygen depletion was underestimated by the model, and in 2014-2016 deep-water anoxia events were missed. Chlorophyll-a concentrations showed distinct spring and summer peaks, but in almost all years, the spring peak concentrations were underestimated, and sometimes simulated too late. Summer chlorophyll-a levels tended to be close to observed levels, with the exception of some summer blooms. Epilimnetic concentrations of both nitrate and phosphate were simulated to be low in summer, typical of values measured in the lake. However, the increase in nitrate concentrations in autumn was reproduced too early, and winter concentrations of phosphate tended to be underestimated.

Table 3. Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Error (ME), and Nash-Sutcliffe Efficiency (NSE) for the calibration ("Cal.", 2004-2016) and validation ("Val.", 2017-2020) periods. For RMSE, MAE, and ME, values close to 0 indicate an optimal fit, whereas for NSE a value close to 1 indicates an optimal fit. These metrics are calculated for the epilimnion in case of nitrate, phosphate, and chlorophyll-a, and for the full water column for oxygen and temperature.

Variable	RMSE		MAE		ME		NSE	
	Cal.	Val.	Cal.	Val.	Cal.	Val.	Cal.	Val.
Phosphate (mg P/l)	0.011	0.012	0.007	0.008	-0.003	-0.001	0.406	0.234
Nitrate (mg N/l)	0.050	0.051	0.037	0.038	0.017	0.024	0.375	0.346
Oxygen (mg O ₂ /l)	2.106	2.115	1.152	1.321	0.659	0.775	0.511	0.720
Chlorophyll-a (µg/l)	6.163	6.820	3.544	4.437	-1.797	-2.741	-0.054	-0.156
Water temperature (°C)	0.880	0.818	0.580	0.511	-0.065	-0.018	0.957	0.976

NUMERICAL EXPERIMENT 1: VARIABLES CONTROLLING PHYTOPLANKTON RESPONSE TO STORMS

Storm intensity, MLD, surface water temperature, hypolimnetic nutrient concentration, and incoming shortwave radiation all affected the phytoplankton response to storms. Wind speed had a nonlinear effect on the average phytoplankton biomass in the first week following the storm: moderate wind speeds increased chlorophyll-a concentrations, but strong winds (in the order of 10 m/s or higher) had a less positive, or even a reducing effect on chlorophyll-a concentration (Figure 2, panel b, inset). With an initial mixed layer deeper than about 8 m, even strong winds had substantially less effect on chlorophyll-a concentrations (Figure 2b).

Of the other variables included in the experiment, incoming shortwave radiation had the strongest influence (Table 4). At low incoming radiation (< 150 W/m² averaged), the effect of storms on phytoplankton was largely

negative, although at moderate wind speeds some increases could still be seen (Figure 2b). When incoming radiation increased above 200 W/m^2 , storms had an overall positive effect on phytoplankton concentration, moderate wind speeds more so than high wind speeds. Hypolimnetic nutrients were less influential than light or surface water temperature (Table 4), but higher concentrations resulted in increased phytoplankton biomass following storms at mixed layers deeper than about 4 m when incoming radiation was high (Figure 2b). At the shallowest mixed layer (2 m), wind speed had a negative effect on chlorophyll-a when hypolimnetic nutrients were high. This was caused by the setup of the experiment (Figure 1), as even under the lowest wind speed a large amount of the hypolimnetic nutrients entered the epilimnion, and high wind speed therefore mostly reduced growth due to mixed layer deepening. Surface water temperature before the storm (and therefore Schmidt stability) also influenced phytoplankton response to storms; a higher initial surface temperature caused a decrease of phytoplankton after storms (Supplement F-2).

Apart from changes in chlorophyll-a, we also looked at changes in Schmidt stability, and nutrient concentrations. The strongest decrease in Schmidt stability was diagnosed at strong wind speeds and shallow MLD (Supplement F), an indication of intense mixing. Although mixing events always entrained nutrients into the epilimnion, noticeable as a peak directly after the storm (not shown), the nutrient concentration averaged over the euphotic zone in the first week after the storm could be lower compared to no-storm conditions, especially for moderate wind speeds (5 – 10 m/s, Supplement F-1), due to enhanced phytoplankton uptake. If the initial mixed layer was deeper, the effect of the storms on thermal structure and nutrients was less strong (Supplement F-1).

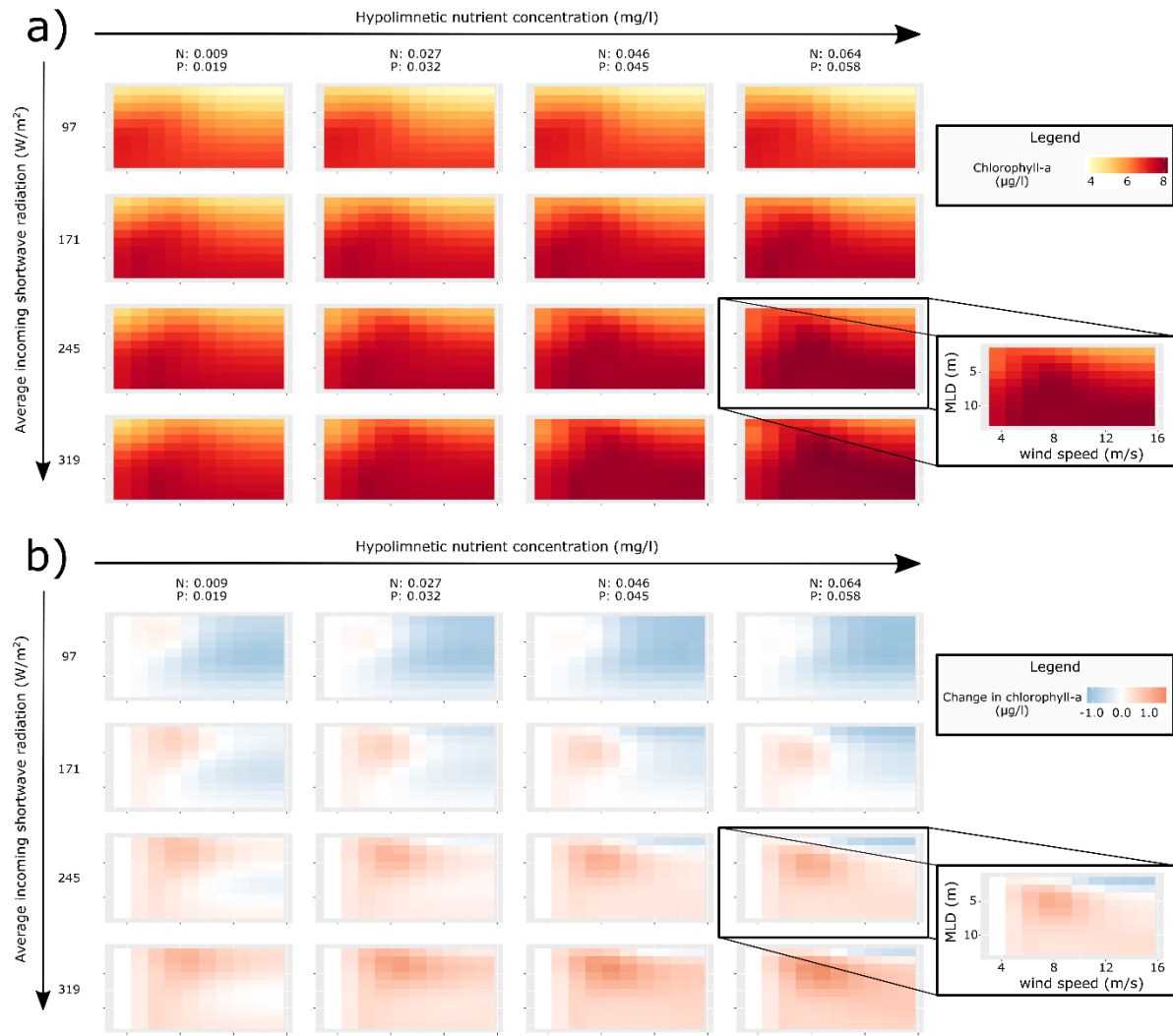


Figure 2. The figure shows two main panels, a and b, which are each composed of 16 sub-panels. Panel a shows the volume-averaged chlorophyll-a concentration in the euphotic zone (upper 8.0 m of the water column), averaged over the first week after an induced storm event in numerical experiment 1. In panel b the same data as in panel a are shown, but relative to no-storm conditions, while keeping MLD, nutrients, and light the same. The sub-panels each represent a scenario with a different hypolimnetic nutrient concentration (low on the left, high on the right; N and P concentrations are indicated on top) and a different average incoming shortwave radiation (low on top, high on bottom, values indicated on the left). Each sub-panel has the wind speed of the storm event on the horizontal axis and the mixed layer depth (MLD) on the vertical axis (see labels in the inserts), and each small rectangle inside each sub-panel corresponds to one simulation. The change in main panel b is calculated relative to the simulation with a wind speed of 3.7 m/s (which is why the left column of each sub-panel always has a value of 0). The numerical experiment was performed using ten levels of shortwave radiation and nutrient levels. Only four by four sub-panels are shown for visualisation purposes, as it turned out that the results for intermediate input values can be interpolated from the ones that are displayed in the figure.

Table 4. Permutation-based variable importance of wind speed, mixed layer depth, hypolimnetic nutrients, incoming shortwave radiation, and surface water temperature for predicting change in volume-averaged chlorophyll-a over the euphotic zone (i.e. the colours shown in Figure 2, panel b) in the first numerical experiment, based on a fitted random forest model. The out-of-the-bag R2 was 0.992. The importance values represent the degree to which the mean squared error of the fitted random forest model increases if the input column for that variable is randomly permuted. The greater the error after permutation, the more the model relies on the variable for making predictions, and therefore the more important the variable is to the model.

	Permutation-based importance
Incoming shortwave radiation	0.21
Wind speed	0.15

Surface water temperature	0.09
Mixed layer depth	0.07
Hypolimnetic nutrients	0.02

NUMERICAL EXPERIMENT 2: EFFECT OF A WARMER CLIMATE ON PHYTOPLANKTON RESPONSE TO STORMS

Figure 3 compares the simulated lake conditions under the present climate with those in the RCP8.5 scenario. Under the warming scenario, surface temperatures in summer increased by roughly 1.6 °C while deep-water temperatures remained around the same level, and therefore the Schmidt stability increased (increase in median by 43%, Figure 3). The mixed layer shoaled by 1.2 m (14%), and stratification tended to both form earlier and vanish later in the year (medians are 3.5 days earlier and 6.5 days later in the RCP8.5 scenario, respectively). Median deep-water oxygen concentrations decreased by 20% (1.17 mg/l), while deep-water nitrate and phosphate concentrations increased (nitrate increase in median of 50%, 14.4 µg/l; phosphate increase in median of 28%, 8.8 µg/l). Average summer chlorophyll-a concentration tended to be higher in the warming scenario as compared to the present-day conditions (0.56 µg/l higher, 10% increase, Figure 3).

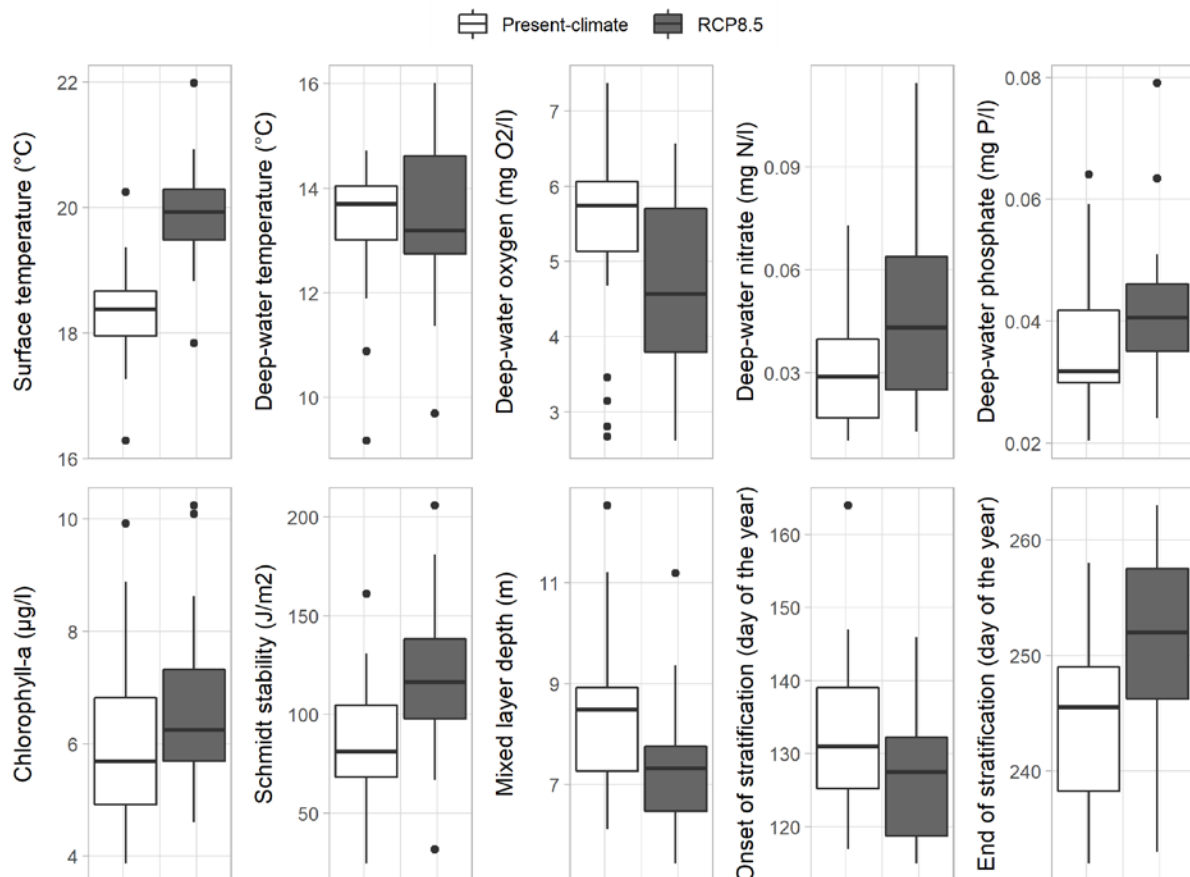


Figure 3. Comparison of summer long-term averages (June-August) between the unperturbed present-day and RCP8.5 climate scenarios of the Lake Erken simulations. Surface temperature and chlorophyll-a are taken from a depth of 3 m, and the variables marked “deep-water” are taken from 15 m depth. Onset and end of stratification were calculated as the first and last day-of-the-year that Schmidt stability continuously exceeded 10 J/m² for the duration of at least one week. The boxplots show the median and quartiles (N = 22). Whiskers extend to the smallest and largest value within 1.5 times the inter-quartile range from the nearest quartile, and values outside this range are marked as outliers (•) (made using the `geom_boxplot` function of the `ggplot2` R package, Wickham 2016).

Overall, impacts of identical storms under the RCP8.5 climate scenario did not have a drastically different effect compared to the present-day situation in our simulations (Figure 4). Both increasing and decreasing effects of storms on chlorophyll-a were found early and later in the stratified season and also with either moderate or high storm intensity (Figure 4). Storms with a higher intensity tended to have more effect than moderate-intensity

storms, but without shifting towards either more positive or more negative effects on chlorophyll-a. Moreover, the difference in effect between high- and moderate-intensity storms was small (Figure 4).

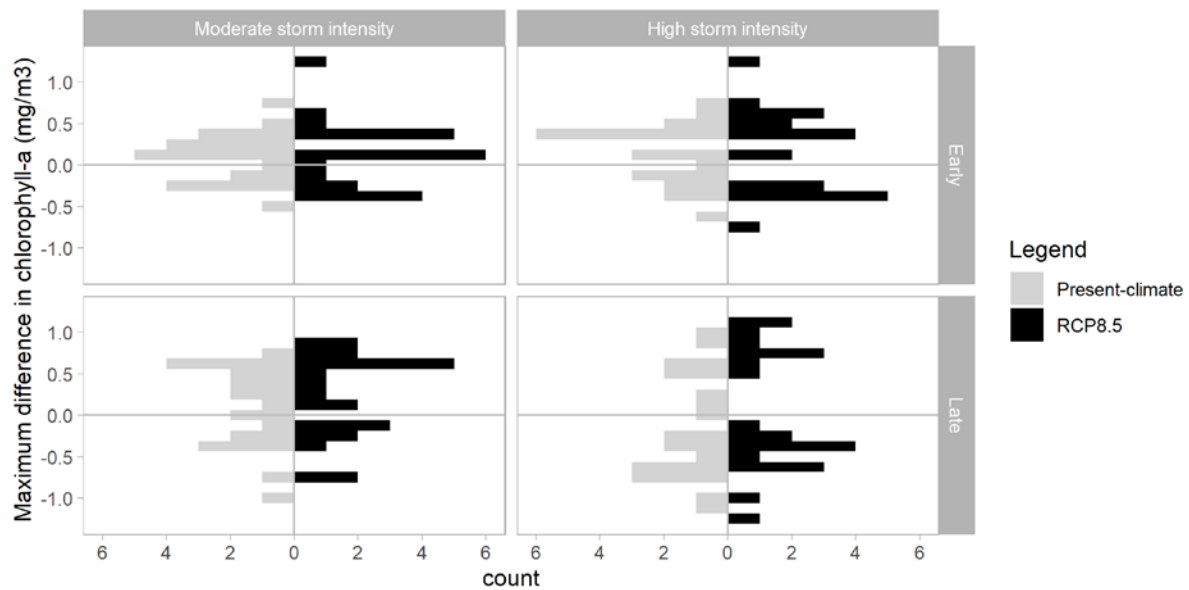


Figure 4. Comparison of the effect of storms on phytoplankton between present-day and RCP8.5 climate forcing in numerical experiment 2. Each histogram represents the maximum difference in volume-averaged chlorophyll-a concentration in the euphotic zone between storm and no-storm conditions in the simulations on the y-axis. The back-to-back histograms compare the present-climate (bars to the left, in light grey) against the RCP8.5-scaled climate scenario (bars to the right, in black). The four panels compare these outcomes in simulations when storms are moderate or severe (left, respectively right hand panels), and when they occur early in the season (9th of June) vs. later in the season (4th of July; top vs bottom panels). Each panel represents the outcome of multiple simulated storms, one for each year in the long-term simulation (N = 22).

DISCUSSION

MODEL VALIDATION

In this study, we applied a coupled physical-biogeochemical model, GOTM-Selmaprotbas, to investigate the effect of wind events on lake phytoplankton under present and future conditions. The model successfully reproduced the seasonal cycles of all variables. Water temperature was simulated well, and with an RMSE of 0.9 °C the fit was similar to those in previous studies in Lake Erken (Moras et al. 2019; Ayala et al. 2020). Periods of summer hypolimnetic hypoxia were captured well by the model in most years, although the clear underestimation of under-ice oxygen consumption did point towards an incomplete description of winter oxygen dynamics by the model. Also, the dynamics of dissolved nutrients (nitrate and phosphate) were reproduced rather well, with concentrations close to observed values in summer, the period under study. However, winter concentrations of phosphate and nitrate tended to be underestimated and the increase in nitrate in autumn was simulated too early, potentially due to a missing recalcitrant organic matter component, such as macrophytes near the shore. Additionally, expanding the model description of sediment dynamics may lead to improvements in oxygen and nutrient simulations. Compared to recent applications of the GLM-AED2 model in Lake Mendota, USA, (Ladwig et al. 2021) and of the CE-QUAL-W2 model in Rappbode Reservoir, Germany, (Mi et al. 2020), the nutrient fit statistics of the present study are similar.

The goodness-of-fit statistics were worst for the chlorophyll-a dynamics. This was largely due to the significant underestimation of the magnitude of the spring peak, and this peak was also simulated too late in some years. In Lake Erken, under-ice growth and resting stages can play an important role in phytoplankton dynamics (Weyhenmeyer et al. 1999; Yang et al. 2016b), and since these processes were not included in the model, this could be an explanation for why the model did not replicate the magnitude of the spring peak. However, in summer, during stratification, the long-term simulations matched the observed conditions well in most years,

except that short-term summer blooms were not well captured by the model. This may have been due to temporary surface accumulations of buoyant cyanobacteria, which were not reproduced by the model.

CAUSAL FACTORS REGULATING PHYTOPLANKTON RESPONSE TO STORMS

Storm intensity, mixed layer depth, surface water temperature, incoming shortwave radiation, and hypolimnetic nutrient concentrations all regulated phytoplankton response to wind perturbations in the first experiment. The variables also interacted with each other. The random forest permutation importance suggested that light had the strongest effect and hypolimnetic nutrients the least. However, this also depended on the numerical ranges of the variables used in the experiment, which were based on the summer conditions in Lake Erken. In lakes where the summer conditions are substantially different, the order of variable importance may therefore look differently.

The effect of storm intensity was non-monotonic, in the sense that the wind effect had a maximum around 5-10 m/s. It is possible that such moderate wind speeds caused nutrient upwelling without strongly deepening the mixed layer, and as such promoted growth. Stronger wind speeds, however, may have caused stronger nutrient upwelling, but also more mixed layer deepening, which led to stringent light limitation. This explanation is supported by the volume-averaged nutrient concentrations over the depth of the euphotic zone after storms (Supplement F); strong wind speeds increased nutrient concentrations in the mixed layer, but this was not accompanied by increased phytoplankton concentrations. Negative influence of wind on phytoplankton concentrations has been shown in various systems (e.g. Fitch and Moore 2007; Kuha et al. 2016; Jalil et al. 2020). However, a positive effect (relative to low wind speed) of moderate wind speed but a negative effect of high wind speeds has, to our knowledge, not often been shown in the literature. Due to the effect of storms on light and nutrient limitation, this non-monotonic relation of wind and phytoplankton could occur more frequently in stratifying lakes. It should be noted that we do not make a definite distinction between what is a storm and what is not, but rather explore the full range between median wind speeds and wind speeds that are higher than experienced in the past 22 years at Lake Erken. The non-monotonic effect of wind speed suggests that this entire wind speed distribution is relevant for lake ecosystem functioning, not just the extreme storms.

Storms had most effect on the investigated lake variables when the mixed layer was around 8 m deep or shallower prior to the storm. In case of a deeper antecedent mixed layer, the mechanical mixing generated at the water surface is largely dissipated at the depth of the maximum density gradient (Imboden and Wüest 1995), so that storms have less effect on thermal, nutrient, and phytoplankton vertical profiles. This threshold of 8 m did not change substantially when we averaged the response variables over a different depth than the euphotic zone depth (results not shown). A modelling study by Mi et al. (2018) also showed that storm-induced mixing has only a small effect on mixed layer depth and entrainment when stratification is deep and strong. While increases in surface temperature and Schmidt stability by climate warming have been reported in multiple studies (e.g. Fang and Stefan 2009; Kraemer et al. 2015; Pilla et al. 2020), trends in depth of stratification are more uncertain and might change only slightly (Pilla et al. 2020). Our simulations indicated that surface temperature and Schmidt stability in Lake Erken will increase under a warmer climate, but that the mixed layer depth will become shallower, similar to what was found by Ayala et al. (2020). A shoaling of the mixed layer would suggest a larger role of storms in the dynamics of stratified lakes.

Whether the net effect of a storm on phytoplankton concentration was positive or negative also depended on the other variables that were varied as part of the first numerical experiment. The effects of nutrients, light, and temperature could be understood from the perspective of nutrient and light limitation. If light conditions are optimal, nutrients are more likely to be limiting, and therefore nutrient upwelling during a storm is likely to promote an increase phytoplankton biomass. On the contrary, if light is the main limiting factor for growth, further deepening of the mixed layer due to mixing is likely to decrease phytoplankton concentrations. The results of the experiment were largely consistent with this. Higher nutrient concentrations in the hypolimnion slightly promoted higher chlorophyll-a concentrations after a storm, but only under high light conditions. The

potential of phytoplankton growth being boosted by storm-induced nutrient upwelling in lakes has been reported by observational studies (e.g. Soranno et al. 1997; MacIntyre and Jellison 2001; Crockford et al. 2015; Gilling et al. 2017a). Increases in phytoplankton after storms in the first numerical experiment were also seen when incoming shortwave radiation was high. Observed decreases in phytoplankton concentration after a storm have been explained by a combination of dilution due to mixed layer deepening and exposure to more stringent and dynamic light conditions (Ibelings et al. 1994; De Eyto et al. 2016; Kuha et al. 2016). Lastly, a higher pre-storm surface temperature resulted in more negative effects of wind on phytoplankton concentration in the first experiment. As water temperature only has a slight positive effect on cyanobacterial growth rates in the model, this result was mostly caused by the effect of surface water temperature on the thermal structure. Since we kept the hypolimnetic temperature constant, a higher surface temperature caused a higher Schmidt stability and therefore stronger stratification. Stronger stratification resisted mixing, as found by Mi et al. (2018), and as such less nutrients ended up in the epilimnion.

EFFECTS OF STORMS ON PHYTOPLANKTON UNDER A WARMER CLIMATE

Summer-averaged chlorophyll-a concentrations increased in simulations with warmer air temperatures in the second numerical experiment. This is in line with some previous studies, which report increases in phytoplankton with warming (Markensten et al. 2010; Trolle et al. 2014; Gray et al. 2019). However, trends in chlorophyll-a under atmospheric warming also depend on nutrient availability. The present study and the aforementioned studies were done in meso-/eutrophic systems. Under oligotrophic conditions, however, no change or decreasing trends are more likely because of the more stringent nutrient limitation due to earlier onset of stratification and higher nutrient requirements at increased temperatures (Tadonlélé 2010; Kraemer et al. 2017).

The projected increases in deep-water nutrient concentrations are also in line with previous studies. Climate warming mediates an increase in hypolimnetic nutrient levels in deep lakes through an increase in hypolimnetic anoxia (Sahoo et al. 2013; North et al. 2014) and incomplete winter mixing (Salmaso 2005; Yankova et al. 2017). Additionally, an earlier onset of stratification separates the epilimnion and hypolimnion earlier in the year, therefore both increasing nutrient concentrations in the hypolimnion and exacerbating nutrient limitation in the epilimnion. Earlier onset of stratification, lower oxygen concentrations, and increases in hypolimnetic nitrate and phosphate in a warmer climate were indeed reproduced by our simulations.

In the second experiment, model predictions suggested that the response of phytoplankton to summer storms would not deviate strongly from the present-day situation when air temperatures were increased to a level consistent with a RCP8.5 climate scenario. Based on the results of the first numerical experiment and projections for summer-average lake conditions in a warmer climate, either stimulating or reducing effects of storms were expected in the second experiment. The reason for this was that of the variables included in the first experiment, the mixed layer tended to become shallower, and hypolimnetic nutrient concentrations and surface water temperature (and therefore strength of stratification) increased as a consequence of atmospheric warming. The opposing effects of these trends in surface temperature and nutrient conditions may have compensated each other. Another potential reason for the lack of difference in the response to wind events between present climate and RCP8.5 could be that even under this high-emission scenario, the changes in the variables were rather small compared to the ranges that were included in the first numerical experiment (i.e. the variation experienced in July at Lake Erken over the past 22 years). Additionally, no strong response would be expected in years when the mixed layer stayed deeper than about 8 m, the depth below which the first numerical experiment showed a marked reduction of storm effects. It follows from the result of numerical experiment 2 that changes in atmospheric warming alone are not likely to strongly change the response of phytoplankton biomass to storms of similar intensity in Lake Erken.

IMPLICATIONS BEYOND LAKE ERKEN

The present study was set up for Lake Erken, and thus the range of the scenarios (surface temperature, nutrients, solar radiation, mixed layer depth, and wind speed) and morphometry were specific to this lake. The simulated phytoplankton groups (diatoms and cyanobacteria) were intentionally generic and not unique to Lake Erken, but during calibration the phytoplankton parameters were optimised to match the seasonal patterns of the phytoplankton community in Lake Erken. Different phytoplankton communities respond differently to storms (Stockwell et al. 2020). However, the effects of storms on light and nutrient availability occur widely (Stockwell et al. 2020), and the scenarios tested in the first numerical experiment covered a wide range of lake and atmospheric conditions. Therefore, the processes observed in Lake Erken are expected to be similar in other stratifying, mesotrophic lakes. Although the absolute thresholds found in the study may differ from lake to lake and are prone to model uncertainty, the findings in the present study are applicable to more lakes than Lake Erken alone and may facilitate general understanding of lake responses to storms.

Trends in extreme wind speeds (both frequency and intensity) strongly vary with geographic location (Sainsbury et al. 2018). In the area of Lake Erken, future trends in storm intensity and frequency are uncertain (Möller et al. 2016). However, in regions where storm intensity and frequency are predicted to increase, such as western Europe, an increased importance of storms for phytoplankton dynamics can be expected. Our first experiment showed that the effect of wind on phytoplankton can be non-monotonic, and that moderate wind speeds have different effects than high wind speeds. Therefore, any shift in the probability-distribution of wind speeds is relevant, not just trends in extreme wind speeds.

Air temperatures are increasing globally and this causes a rise in strength of stratification, but trends in mixed layer depth remain uncertain (Pilla et al. 2020). In the present study, mixed layer depth was identified as a key variable in responses to storms, so local trends in this variable may partially control storm impacts. Next to air temperature, mean wind speed (Stetler et al. 2021) and water transparency (Read and Rose 2013) determine mixed layer depth, and may change on local or regional scales. In regions that experience atmospheric stilling (Woolway et al. 2019) or lake brownification (Jennings et al. 2010), mixed layers might shoal and these lakes may be more strongly impacted by storm events. We only scaled air temperature in our climate warming scenario, by applying a change factor correction to a historical time series of air temperature. This allowed the comparison of identical storms under identical pre-event weather conditions, and the differences could be attributed to air temperature alone. However, a different experimental design using the full output from a climate scenario could give an indication of how the full effect of climate change will influence storm-effects on lakes, including trends in, for example, average wind speed.

Nutrient concentrations and their vertical profiles modulate the effect of storms on phytoplankton. Trends in nutrient loading are mostly controlled by human activities, and developing countries especially may experience increasing trends (Fink et al. 2018). Earlier onset of stratification with climate warming (Woolway et al. 2021) causes more nutrient build-up in the hypolimnion, so if nutrients are limiting in the epilimnion, phytoplankton increase after storms may become more prominent, although this was not observed in our second numerical experiment. In lakes where nutrients are high in the epilimnion throughout the year, a wind episode that deepens the mixed layer is likely to decrease phytoplankton concentration due to dilution and reduced light availability.

This study revealed new insights on the effects of storms on phytoplankton, but only certain aspects of this topic were tested. For example, we focused on summer only. In Europe, winter storms tend to be the most severe, but summer storms may have the most impact on a lake by mixing stratified waters (Andersen et al. 2020) and it is in summer that phytoplankton blooms occur most frequently. Additionally, we focused solely on wind. Passing storms tend to affect not only wind speed, but also air temperature and incoming solar radiation. Moreover, precipitation during storms will affect both the quantity and quality of catchment runoff. The retention time of Lake Erken is around 7 years, indicating that catchment runoff during storms is likely to have a minor influence, but in lakes with short residence times (e.g. < 1 year) this change in inflow can be at least as

impactful as wind (Klug et al. 2012; Reichwaldt and Ghadouani 2012; De Eyto et al. 2016). In addition, in the first experiment, only a limited number of variables that could affect the lake state prior to and after an event were assessed. Like for the effect of precipitation, the results in the present study do not discard the possibility that such other variables are important too.

The effect of phytoplankton community composition on the response to storms was not systematically explored in the present study. We only calibrated and validated total chlorophyll-a concentration, despite using two separate phytoplankton groups in the model. The diatoms dominated the spring peak and the summer peak contained more cyanobacteria, which was in line with the seasonal dynamics at Lake Erken. The chlorophyll-a data was more readily available and at higher frequency than taxonomic data. In order to assess the effect of storms on individual groups, the model would have to be calibrated and validated on group-specific data, and parameter values would have to be informed by a trait-based approach. Traits such as buoyancy regulation, nutrient storage, nutrient acquisition, growth rates, and photoadaptation are likely to be highly relevant for how a phytoplankton community responds to a storm (e.g. Visser et al. 1996; Kasprzak et al. 2017; Stockwell et al. 2020). As such, different communities may show distinct responses to storms under physically and chemically comparable situations. If storms already occur frequently in a system, the phytoplankton community may be adapted to such conditions (Stockwell et al. 2020), and therefore shifts in frequency of storms may be especially relevant when considering community composition. Acquisition of data of sufficient frequency and quality to investigate these topics is a key problem, but a combination of experiments, use of novel monitoring techniques, and modelling may elucidate some of this uncertainty in the near future. Also, our model results pointed at average concentrations and responses, not at phytoplankton bloom or scum formation. Prediction of blooms with data-driven or process-based models still remains a challenge (Rousso et al. 2020), and may require inclusion of processes that are not parameterised in our model, such as life cycles (Hense and Beckmann 2010) or selective grazing by zooplankton (Sommer et al. 2012). This may be part of the reason for why the spring peak and occasional summer spikes in chlorophyll-a were missed by the model used in this study.

CONCLUSION

High wind speeds ($\gtrsim 10$ m/s) always had more negative effects than moderate wind speeds ($\approx 5 - 10$ m/s), but the direction of the effect depended mostly on the level of incoming radiation, surface water temperature, and hypolimnetic nutrients. The effect of storms decreased markedly when the mixed layer depth was about 8 m or deeper. Higher incoming radiation and hypolimnetic nutrient concentrations promoted increases in chlorophyll-a concentrations after storms, whereas increases in surface temperature had a decreasing effect. These outcomes confirmed the conflicting effects of storms on phytoplankton light and nutrient limitation, and provide a mechanistic framework to better understand under what conditions storms tend to either increase or decrease phytoplankton biomass. A simulation forced by a future climate scenario showed earlier onset of stratification and a higher summer chlorophyll-a concentration, averaged over the euphotic zone. However, the response of phytoplankton to storms did not strongly change with warming air temperatures.

Increased understanding of the drivers of storm impacts on lakes can help short-term forecasting, and in some cases may be used to inform lake or reservoir management. Additionally, it facilitates assessment of how atmospheric trends will affect lakes, specifically those caused by climate change. Different regions are expected to experience different trends in air temperature, (extreme) wind speed, and nutrient loading. Studies evaluating the combined effects of these trends to assess the impacts of storms on lake phytoplankton could further our understanding of the global impact of extreme weather events on lake ecosystems.

ACKNOWLEDGEMENTS

This study was made possible thanks to data collected by the Erken Laboratory of Uppsala University and the Swedish Infrastructure for Ecosystem Science (SITES).

We would like to thank Karsten Bolding and Jorn Bruggeman for their advice during the development of the Selmaprotbas model, and Tobias Andersen for his help in setting up the sensitivity analysis.

J.P.M., A.I.A., M.W.T., R.M., and J.A.A.S. were funded by the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie grant agreement no. 722518 (MANTEL ITN).

The authors declare that they have no conflict of interest.

SOFTWARE AVAILABILITY

The GOTM code for the lake-branch is publicly available at <https://github.com/gotm-model/code/tree/lake> (Last accessed: 2021-07-29). The code for the Selmaprotbas model can be found at <https://github.com/jorritmesman/selmaprotbas> (doi: 10.5281/zenodo.5094298), including instructions on how to couple it to GOTM. The model set-up, including the configuration and input files, can be found at [https://github.com/jorritmesman/Erken GOTM SP setup](https://github.com/jorritmesman/Erken_GOTM_SP_setup).

Gap-filled hourly meteorological data for Lake Erken until 2018 have been published by Moras et al. (2019). Lake data until 2016 have been made available on <https://www.ieg.uu.se/erken-laboratory/lake-monitoring-programme/> (Last accessed: 2021-07-29). For the most recent data, contact Don Pierson (don.pierson@ebc.uu.se).

The HadGEM2-ES model output for the EURO-CORDEX experiment was downloaded from the ESGF node of the German Climate Computing Centre (DKRZ).

SYNTHESIS

The central topics of this thesis are the effects of extreme weather events on lakes, the interactions between physical and biogeochemical lake variables, and process-based lake modelling. Perhaps more than usual in a doctoral thesis, the methods and scopes of the chapters diverged rather strongly, with some chapters only looking at lake physics, others also at biogeochemistry, with some chapters being strongly focussed on the methodology, and others at the effects in the lake ecosystem, and Chapter 1 not using a modelling approach. However, the chapters did inform each other and build towards a novel understanding of the processes involved in extreme weather events, lake ecosystem dynamics, and climate change. In the final part of this doctoral thesis, I reflect upon the new knowledge generated by the thesis and discuss potential next steps for research into these topics.

LESSONS LEARNED

A FURTHER PROCESS-BASED UNDERSTANDING OF THE INTERACTIONS BETWEEN LAKE PHYSICS AND BIOGEOCHEMISTRY DURING EXTREME EVENTS

Understanding the interactions between biology and physics has been studied since the start of limnology as a research field, and there is a growing body of literature on extreme weather events as well. However, due to a lack of data during extreme events we often cannot link observations to processes, and we cannot be sure to what extent observed responses translate to other systems. Single-lake studies that discuss processes involved in a lake's response to an extreme event (e.g. De Eyto et al. 2016; Kasprzak et al. 2017; Tilahun and Kifle 2019) are immensely valuable, but it is often unclear if these processes are common in other lakes as well. The review by Stockwell et al. (2020) indeed confirmed that the response of lake variables to storms may diverge markedly between lakes. Process-based understanding is essential to work towards predicting future lake responses to extreme weather events.

This thesis contributed to a further process-based understanding on the interaction of lake thermal structure and biogeochemistry, and on lake responses to extreme weather events. In Chapter 1, we showed multiple feedback mechanisms that exist between thermal structure and lake biogeochemistry, and how they may influence mixing regimes. In Chapter 4, we investigated the influence of multiple drivers (in isolation and in interaction) of phytoplankton response to storms, for example showing novel patterns of how wind speed and mixed layer depth affect phytoplankton concentration shortly after a storm. Moreover, an important part of these chapters was the discussion about which lakes these patterns occur in, and to what extent. Chapter 1's transparency-reduction feedback is likely restricted to a small subset of lakes, and a shift to meromixis due to climate warming is most likely in lakes with a potential for strong solute release from the sediment and weak deep-water renewal. The results of the first numerical experiment in Chapter 4 are somewhat specific to Lake Erken, but the processes involved in the models occur in a wide range of stratifying lakes. By exploring large ranges of nutrient, light, and stratification conditions, the chapter also reveals important information for other stratifying lakes.

While these are small steps towards full process understanding, they provide starting points for further studies. They will be especially valuable for further scenario assessments using process-based models, as captured in the term "process-based". The future is looking bright for this research topic, as the necessary long-term high-frequency data needed to drive and evaluate these models is becoming increasingly common, due to advances in sensor development and continued long-term monitoring sites.

COMPLEX INTERACTIONS BETWEEN LONG-TERM CLIMATE WARMING AND SHORT-TERM EXTREME EVENTS

Long-term changes in lake variables due to climate warming interact with the consequences of extreme short-term events. This was shown in Chapter 1, where climate warming pushes lake mixing regimes in a certain direction, but a short-term event may tip the balance. This is the case for holomictic lakes, for example; climate warming makes incomplete mixing more likely, but it is a series of warm winters in a row that could potentially

cause a shift to a meromictic regime. Events in Lake Lugano in 2005 and 2006 show that the opposite is also possible, with a series of cold winters interfering with long-term trends (Lehmann et al. 2015).

The interaction between climate warming and lake responses to extreme weather is not often considered, but in Chapter 4 we compared the effect of storms on phytoplankton between present-day and future (RCP8.5-scaled air temperatures, 2040-2070 conditions) weather conditions. This revealed that differences do not need to be large; phytoplankton in Lake Erken did not react markedly different to storms in the warmer scenario compared to present-day conditions, according to the simulations. Inter-annual variation in lake variables had substantially larger effects than a shift in mean temperature due to warming. However, the relations between lake variables and phytoplankton dynamics found in the first numerical experiment in Chapter 4 did place this finding in perspective; would we expect such little changes also in other lakes? This is difficult to say without further study, but we found that several variables (e.g. mixed layer depth and strength of stratification) could affect phytoplankton biomass after storms. In Lake Erken, the projected changes in these variables were not so impactful, or compensated each other. But in other lakes, this may be different, and if trends in mixed layer depth, hypolimnetic nutrients, and surface temperature can be estimated, we can make a more educated guess of how phytoplankton response to storms will change. Other trends that are experienced in many lakes, such as browning and eutrophication, can factor in as well. Studies on multiple lakes are needed to see how transferable these relations are between lakes.

MODELLING AS A VIABLE APPROACH TO STUDY SHORT-TERM EFFECTS OF EXTREME EVENTS

This thesis showed that process-based modelling is a suitable method to study short-term effects of extreme weather events on lakes. Chapter 2 provided new data on model performance of one-dimensional hydrodynamic lake models during storms and heatwaves, adding credibility to studies that use such models. The results were overall favourable regarding the capacity of these models to replicate lake physics during extreme events, with the caveat that model uncertainty did increase compared to non-extreme conditions. Chapter 4 did not include validation of short-term effects on real data due to a lack of sufficient data for this purpose. However, the model responses were consistent with theory and revealed credible patterns. This evidence that models can be used to study extreme weather events is supported by other recent studies on this topic (e.g. Mi et al. 2018; Soares et al. 2019; Chen et al. 2020).

Chapter 3 discusses the ensemble technique. Although extreme events were not explicitly included in the chapter, ensemble modelling may be especially relevant for extreme events. Using an ensemble can be seen as a way of translating the limitations of process understanding into an uncertainty band around a model prediction. Uncertainty in meteorological forcing and process description are both higher in times of extreme weather, and therefore ensemble modelling can add to credibility in forecasting efforts involving extreme weather conditions.

NEXT STEPS

INCORPORATION OF THREE-DIMENSIONAL PROCESSES

This thesis involved the use of one-dimensional models, which have as advantages faster runtimes, less data requirements, and easier coupling of physics and ecology, compared to multi-dimensional models (Hamilton et al. 1997). However, the omission of horizontal processes may lead to an incomplete description of lake dynamics, particularly during extreme weather events. One such process is the excitation of internal waves by storm events, which can cause mixing over a prolonged period after a storm (Imboden and Wüest 1995), although some one-dimensional models take internal waves into account (Goudsmit et al. 2002; Stepanenko et al. 2020). Internal waves can be important for nutrient upwelling; thermocline tilting as a consequence of internal waves may lead to nutrient upwelling near-shore (MacIntyre and Jellison 2001), and breaking internal waves can entrain nutrients into the epilimnion (Kelly et al. 2019). As such, especially for looking at storm effects, using a multi-dimensional lake model could be a promising pathway for further investigation.

PRECIPITATION EVENTS AND CATCHMENT INFLOWS

One important type of extreme weather event, that is also projected to shift under influence of climate change (IPCC 2014), was not considered in this thesis: extreme precipitation events. Floods caused by such events have the potential to strongly influence lake ecosystems, by temporarily decreasing water residence time (i.e. flushing) and by importing large quantities of nutrients and organic material (Weyhenmeyer et al. 2004; Reichwaldt and Ghadouani 2012). One of the reasons for omitting flood events from this thesis was that catchment modelling of extreme weather events becomes a consideration as well, with its own data requirements, assumptions, and uncertainties. However, this topic is at least as relevant as storms or heatwaves and coupling catchment modelling scenarios involving extreme precipitation events (e.g. Ye et al. 2020) to lake (or coastal) models would be a promising path for further study.

BIOGEOCHEMICAL MODELLING TO STUDY SHIFTS IN MIXING REGIMES

Chapter 1 could have been the introduction for another thesis as well: one focused on modelling shifts in mixing regimes. Of the shifts discussed in this chapter, the change of holomictic to meromictic lakes would have the largest ecological implications, as meromictic lakes behave strikingly different from other lake mixing regimes (Gulati et al. 2017). Woolway and Merchant (2019) showed that changes to meromixis may become common under a warming climate, although it needs to be said that they followed a different definition of meromixis and did not consider biogeochemistry. Modelling the chance of formation of meromixis under climate warming with effects of biogeochemistry would involve simulation sediment solute release rates and redox conditions. In order to combine this with thermal stratification, the FABM software (Bruggeman and Bolding 2014), which was also used in Chapter 4, may be a promising pathway for this type of studies.

REPEATED PERTURBATIONS AND DIFFERENT DURATIONS OF PERTURBATIONS

Recent evidence suggests that repeated perturbations and different durations of perturbations also have important effects on phytoplankton communities (Thayne et al. 2021; Stelzer et al. in preparation). These effects are likely mediated through changes in community composition and the model used in Chapter 4 might not be complex enough to capture such changes. However, the changing frequencies of extreme events as part of climate change bring forward questions such as what happens when a second extreme event occurs before recovery from the first.

EFFECT OF SHORT-TERM EVENTS ON LONG-TERM DYNAMICS

One of the foundations of this PhD project was to stress the effect of long-term change (climate warming) on short-term effects of extreme weather events. In Chapter 4 we studied amongst others what the effect of climate warming was on phytoplankton response to storms. That is, we looked at effects of long-term change on short-term dynamics. However, short-term effects may also influence long-term dynamics. Prime examples in limnology are lakes Okeechobee and Apopka in Florida, USA, that were affected for multiple years by a series of hurricanes (Bachmann et al. 2000; Ji et al. 2018), but also local extinctions of for example fish caused by extreme events (Till et al. 2019). In Chapter 1 we looked at some effects of short-term events (e.g. a series of winters without complete mixing) on long-term dynamics, but we did not apply a modelling approach. For the topics included in this thesis, it would be interesting to study the effect of extreme weather events on long-term phytoplankton community composition.

CONCLUDING REMARKS

Altogether, this thesis increased process-based understanding of thermal structure and phytoplankton dynamics during extreme weather events, and helped to pioneer a mechanistic lake modelling approach to study extreme events. As we better understand how lake physics are affected by climate warming and extreme weather events and how this impacts biology, we can make informed projections of future conditions, assisted by mechanistic models. In this thesis, we reviewed existing literature involving feedbacks in lakes, assessed model performance during extreme events, developed new modelling tools, and lastly we used models to investigate drivers of

phytoplankton responses to storms and assess future effects of extreme events on lake ecosystem stability. This work is placed in a suite of other research articles produced in the MANTEL project, and contributes to further insight in the effects of extreme events and climate warming on lakes, which is of growing importance in these times of increasing human impacts on ecosystems and global climate change.

SUPPLEMENTARY MATERIAL

Chapters 2, 3, and 4 refer to supplementary material. These can be found online at:

- Chapter 2: <https://doi.org/10.1016/j.envsoft.2020.104852>
- Chapter 3: <https://doi.org/10.1016/j.envsoft.2021.105101>
- Chapter 4: <https://docs.google.com/document/d/17acOn7r95tn7OWGM8Z1RGb9knFPxx2l0/edit?usp=sharing&oid=117780408238442231298&rtpof=true&sd=true>

ACKNOWLEDGEMENTS

My first and sincere thanks go to my supervisors. Bas, thank you for your support and advice during my PhD, from start to finish. Your ideas always managed to steer me in the right direction and your support for the many collaborative projects in my PhD has proven its value over and over. Considering your many other responsibilities, I can nothing but admire the time and effort you took for supervision of me and the other PhDs; thank you so much. Don, thank you for your friendly advice and our stimulating discussions about modelling. Whether it was during my stays in Uppsala or when we were in different places, you were always there to help when I had a problem or question. Stéphane, your door was always open for questions and your critical thinking about modelling and heat fluxes helped me enormously: merci! Jérôme, I know you are not listed in this thesis as an “official” supervisor, but I always considered you one nonetheless. Your involvement from the start and incredibly valuable comments have improved the contents of this thesis immensely. I consider myself lucky with such a diverse group of great supervisors; depending on the nature of my problem, I could always find someone to go to. I cannot mention all the great things you’ve done, but know that it is appreciated!

Another important acknowledgement is to the members of the MANTEL project. Julio, thank you for your company; having someone to discuss, laugh, hike, and complain with was truly important. The fact that we didn’t get sick of each other after sharing apartment, office, supervisor, and research topic for so long, is a sign that we didn’t do so badly together, right? Ana, thank you as well for sticking with me. Your advice and conversations made my PhD better and more fun; I think we made a great team. Mike, Elias, and Maggie; hanging out with you during the MANTEL secondments was a lot of fun. But really I would like to thank all MANTEL supervisors and especially the students: Alexa, Ana, Cleo, Elias, Ewan, Hares, Harriet, Julio, Maggie, Mike, Nasim, Qing, and Truls. Being together during the MANTEL workshops and conferences was great, and I think we managed to do really cool research together. Being part of MANTEL enriched my PhD experience: the benefits in terms research opportunities, training, and camaraderie far exceeded the costs in terms of extra paperwork and bureaucracy. That being said, I need to thank the administrative staff at both the University of Geneva and Uppsala University - and extra kudos to Bas and Don - for arranging the agreement between the two universities.

I want to thank the members of the Microbial Ecology and Nonlinearity & Climate groups at the University of Geneva and the Limnology group at Uppsala University. I had the good fortune to be involved in all these groups, and I want to thank you for the work-related and non-work-related conversations, your enthusiasm, the after-work meet-ups, and for creating a great work environment. For those in Geneva, thank you Alonso, Bas, Ena, Evi, Fabio, Joren, Julio, Mridul, Patrick, Roxanne, Savina, Xu, and Ziyu in the MeCo group, and Alexis, Andrea, Ariadna, Debbie, Jérôme, Liliane, Marjorie, Maura, and Stéphane in the NLC group. I always was in close and good contact with the Aquatic Physics group as well; thanks César, Dan, Daphné, Timon, and Tonya. And of course Alexandra and Katia for keeping the department running. To the Uppsala team, thank you Ana, Anastasija, Anna B., Anna N., Anna S., Annika, Berenike, Bianka, Christoffer, Dolly, Don, Eva, Fabian, Fernando, Gesa, Gosia, Holger, Ingrid, Javier, Johan, JP, Karla, Karolina, Konstantinos, Kristin, Lars, Liam, Malineh, Maria, Marloes, Maté, Matilda, Moritz, Pablo, Peter, Rhiannon, Sarahi, Sebastian, Silke, Simone, Shuqi, Sofia, Stefan, Theresa, William, and Xavi. Also thank you to all the MSc students and guest researchers that I got to meet in both places. During my PhD I also stayed at ICRA in Girona and Sorbonne Université in Paris; thank you for hosting me there, Rafa and Vasilis – I had a great time working with you and exploring new places.

I was lucky enough to be involved in several organisations and committees during the past 4 years. Foremost, I need to thank the GLEON organisation. Bas made the good decision to introduce me and Julio to GLEON from the beginning, and one month after the start of our PhDs we attended our first GLEON meeting in New Paltz, USA. This was the first of a total of five GLEON meetings (three in-person, two virtual), up to now. Within GLEON, I met many amazing researchers and could join multiple research efforts. One of these culminated in the LakeEnsemblR R package. For this I want to especially thank my co-leaders in this project, Tadhg, Robert, and Johannes; it was a joy to work with you and I’m proud on what we achieved together. For the co-organisation

of two AEMON-J workshops and the membership of the GLEON GSA poster and workshop subcommittees, I additionally thank Abdou, Carolina, César, Cleo, Freya, Gregorio, Kaelin, Marieke, Mary, Michael, Muhammed, Patricia, Rosie, Ryan, Sofia, and Tobias. Also I need to give a shout-out to Julio and the GIMUN organisation for your involvement in the organisation of our event at the UN, which had to be cancelled due to a pandemic.

I'd like to express my gratitude to the members of my PhD defence committee, Thorsten Blenckner, Jean-Luc Loizeau, Karsten Rinke, Erik Sahlée, and Nele Schuwirth, for taking the time to read and review my thesis. Also, thanks to my co-authors on the papers that I got to be part of, and to the people that collected the data that were used in the creation of this thesis. Ena, Karla, and Peter, thank you for taking the time to correct the French and Swedish translations of the summary!

Lastly, I want to thank my friends and family in the Netherlands, for staying in touch despite my rare visits, and for being supportive and enthusiastic about my PhD. But most of all, I need to thank my parents. Your encouragement, support, and curiosity sparked my interest for limnology, brought me to the place where I am now, and enabled me to start and complete my PhD. These things are probably not said enough, but none of this would have been possible without you.

REFERENCES

- Adrian, R., C. M. O'Reilly, H. Zagarese, S. B. Baines, D. O. Hessen, W. Keller, D. M. Livingstone, R. Sommaruga, D. Straile, E. Van Donk, G. A. Weyhenmeyer, and M. Winder. 2009. Lakes as sentinels of climate change. *Limnology and Oceanography* 54: 2283-2297, doi:10.4319/lo.2009.54.6_part_2.2283
- Ahlgren, I., and G. Ahlgren. 1976. Vattenkemiska analysmetoder: sammanställda för undervisningen i limnologi. Institute of Limnology, Uppsala University.
- Allott, N., P. McGinnity, and B. O'Hea. 2005. Factors influencing the downstream transport of sediment in the Lough Feeagh catchment, Burrishoole, Co. Mayo, Ireland, p. 126-138. *Freshwater Forum*.
- Altwegg, R., V. Visser, L. D. Bailey, and B. Erni. 2017. Learning from single extreme events. *Phil. Trans. R. Soc. B* 372: 20160141, doi:10.1098/rstb.2016.0141
- Ambrosetti, W., L. Barbanti, and E. A. Carrara. 2010. Mechanisms of hypolimnion erosion in a deep lake (Lago Maggiore, N. Italy). *Journal of Limnology* 69: 3-14, doi:10.4081/jlimnol.2010.3
- Andersen, M. R., E. de Eyto, M. Dillane, R. Poole, and E. Jennings. 2020. 13 Years of Storms: An Analysis of the Effects of Storms on Lake Physics on the Atlantic Fringe of Europe. *Water* 12: 318, doi:10.3390/w12020318
- Andersen, T. K., K. Bolding, A. Nielsen, J. Bruggeman, E. Jeppesen, and D. Trolle. 2021. How morphology shapes the parameter sensitivity of lake ecosystem models. *Environmental Modelling & Software* 136: 104945, doi:10.1016/j.envsoft.2020.104945
- Anderson, G. B., M. L. Bell, and R. D. Peng. 2013. Methods to calculate the heat index as an exposure metric in environmental health research. *Environ Health Perspect* 121: 1111-1119, doi:10.1289/ehp.1206273
- Arhonditsis, G. B., B. A. Adams-VanHarn, L. Nielsen, C. A. Stow, and K. H. Reckhow. 2006. Evaluation of the current state of mechanistic aquatic biogeochemical modeling: citation analysis and future perspectives. *Environmental Science & Technology* 40: 6547-6554, doi:10.1021/es061030q
- Arhonditsis, G. B., and M. T. Brett. 2004. Evaluation of the current state of mechanistic aquatic biogeochemical modeling. *Marine Ecology Progress Series* 271: 13-26, doi:10.3354/meps271013
- Arhonditsis, G. B., C. A. Stow, Y. R. Rao, and G. Perhar. 2014. What has been accomplished twenty years after the Oreskes et al.(1994) critique? Current state and future perspectives of environmental modeling in the Great Lakes. *Journal of Great Lakes Research* 40: 1-7, doi:10.1016/j.jglr.2014.11.002
- Austin, J. A., and S. M. Colman. 2007. Lake Superior summer water temperatures are increasing more rapidly than regional air temperatures: A positive ice-albedo feedback. *Geophysical Research Letters* 34: L06604, doi:10.1029/2006gl029021
- Ayala, A. I., S. Moras, and D. C. Pierson. 2020. Simulations of future changes in thermal structure of Lake Erken: proof of concept for ISIMIP2b lake sector local simulation strategy. *Hydrology and Earth System Sciences* 24: 3311-3330, doi:10.5194/hess-24-3311-2020
- Bachmann, R. W., M. V. Hoyer, and D. E. Canfield. 2000. Internal heterotrophy following the switch from macrophytes to algae in Lake Apopka, Florida. *Hydrobiologia* 418: 217-227, doi:10.1023/A:1003997832707
- Bailey, L. D., and M. Pol. 2016. Tackling extremes: challenges for ecological and evolutionary research on extreme climatic events. *Journal of Animal Ecology* 85: 85-96, doi:10.1111/1365-2656.12451
- Baker, L., and D. Ellison. 2008. The wisdom of crowds — ensembles and modules in environmental modelling. *Geoderma* 147: 1-7, doi:10.1016/j.geoderma.2008.07.003
- Berberan-Santos, M. N., E. N. Bodunov, and L. Pogliani. 1997. On the barometric formula. *American Journal of Physics* 65: 404-412, doi:10.1119/1.18555
- Bertani, I., R. Primicerio, and G. Rossetti. 2016. Extreme climatic event triggers a lake regime shift that propagates across multiple trophic levels. *Ecosystems* 19: 16-31, doi:10.1007/s10021-015-9914-5
- Beven, K. 2006. A manifesto for the equifinality thesis. *Journal of Hydrology* 320: 18-36, doi:10.1016/j.jhydrol.2005.07.007
- Blenckner, T., A. Omstedt, and M. Rummukainen. 2002. A Swedish case study of contemporary and possible future consequences of climate change on lake function. *Aquatic Sciences* 64: 171-184, doi:10.1007/s00027-002-8065-x
- Bohrer, B., and M. Schultze. 2008. Stratification of lakes. *Reviews of Geophysics* 46: RG2005, doi:10.1029/2006rg000210
- Borgonovo, E. 2007. A new uncertainty importance measure. *Reliability Engineering & System Safety* 92: 771-784, doi:10.1016/j.res.2006.04.015

- Bormans, M., B. S. Sherman, and I. T. Webster. 1999. Is buoyancy regulation in cyanobacteria an adaptation to exploit separation of light and nutrients? *Marine and Freshwater Research* 50: 897-906, doi:10.1071/mf99105
- Brothers, S., J. Köhler, K. Attermeyer, H.-P. Grossart, T. Mehner, N. Meyer, K. Scharnweber, and S. Hilt. 2014. A feedback loop links brownification and anoxia in a temperate, shallow lake. *Limnology and Oceanography* 59: 1388-1398, doi:10.4319/lo.2014.59.4.1388
- Bruce, L. C., M. A. Frassl, G. B. Arhonditsis, G. Gal, D. P. Hamilton, P. C. Hanson, A. L. Hetherington, J. M. Melack, J. S. Read, K. Rinke, A. Rigosi, D. Trolle, L. Winslow, R. Adrian, A. I. Ayala, S. A. Bocaniov, B. Boehrer, C. Boon, J. D. Brookes, T. Bueche, B. D. Busch, D. Copetti, A. Cortés, E. de Eyto, J. A. Elliott, N. Gallina, Y. Gilboa, N. Guyennon, L. Huang, O. Kerimoglu, J. D. Lenters, S. MacIntyre, V. Makler-Pick, C. G. McBride, S. Moreira, D. Özkundakci, M. Pilotti, F. J. Rueda, J. A. Rusak, N. R. Samal, M. Schmid, T. Shatwell, C. Snorheim, F. Soulignac, G. Valerio, L. van der Linden, M. Vetter, B. Vinçon-Leite, J. Wang, M. Weber, C. Wickramaratne, R. I. Woolway, H. Yao, and M. R. Hipsey. 2018. A multi-lake comparative analysis of the General Lake Model (GLM): Stress-testing across a global observatory network. *Environmental Modelling & Software* 102: 274-291, doi:10.1016/j.envsoft.2017.11.016
- Bruggeman, J., and K. Bolding. 2014. A general framework for aquatic biogeochemical models. *Environmental Modelling & Software* 61: 249-265, doi:10.1016/j.envsoft.2014.04.002
- Bruggeman, J., and K. Bolding. 2020. parsac (Version 0.5.7). doi:10.5281/zenodo.4280520
- Bueche, T., D. P. Hamilton, and M. Vetter. 2017. Using the General Lake Model (GLM) to simulate water temperatures and ice cover of a medium-sized lake: a case study of Lake Ammersee, Germany. *Environmental Earth Sciences* 76, doi:10.1007/s12665-017-6790-7
- Burchard, H., K. Bolding, W. Kühn, A. Meister, T. Neumann, and L. Umlauf. 2006. Description of a flexible and extendable physical-biogeochemical model system for the water column. *Journal of Marine Systems* 61: 180-211, doi:10.1016/j.jmarsys.2005.04.011
- Burchard, H., K. Bolding, and M. R. Villarreal. 1999. GOTM, a general ocean turbulence model: theory, implementation and test cases. Space Applications Institute.
- Calderó-Pascual, M., E. de Eyto, E. Jennings, M. Dillane, M. R. Andersen, S. Kelly, H. L. Wilson, and V. McCarthy. 2020. Effects of Consecutive Extreme Weather Events on a Temperate Dystrophic Lake: A Detailed Insight into Physical, Chemical and Biological Responses. *Water* 12, doi:10.3390/w12051411
- Camacho, A., M. R. Miracle, L. Romero-Viana, A. Picazo, and E. Vicente. 2017. Lake La Cruz, an iron-rich karstic meromictic lake in Central Spain, p. 187-233. *In* R. D. Gulati, E. S. Zadereev and A. G. Degermendzhi [eds.], *Ecology of Meromictic Lakes*. Springer.
- Cann, K. F., D. R. Thomas, R. L. Salmon, A. P. Wyn-Jones, and D. Kay. 2013. Extreme water-related weather events and waterborne disease. *Epidemiology & Infection* 141: 671-686, doi:10.1017/S0950268812001653
- Carey, C. C., W. M. Woelmer, M. E. Lofton, R. J. Figueiredo, B. J. Bookout, R. S. Corrigan, V. Daneshmand, A. G. Hounshell, D. W. Howard, A. S. L. Lewis, R. P. McClure, H. L. Wander, N. K. Ward, and R. Q. Thomas. 2021. Advancing lake and reservoir water quality management with near-term, iterative ecological forecasting. *Inland Waters* 1: 1-14, doi:10.1080/20442041.2020.1816421
- Carpenter, S. R., E. G. Booth, and C. J. Kucharik. 2017. Extreme precipitation and phosphorus loads from two agricultural watersheds. *Limnology and Oceanography* 63: 1221-1233, doi:10.1002/lno.10767
- Chen, W., A. Nielsen, T. K. Andersen, F. Hu, Q. Chou, M. Søndergaard, E. Jeppesen, and D. Trolle. 2020. Modeling the Ecological Response of a Temporarily Summer-Stratified Lake to Extreme Heatwaves. *Water* 12: 94, doi:10.3390/w12010094
- Ciglenečki, I., I. Janeković, M. Marguš, E. Bura-Nakić, M. Carić, Z. Ljubešić, M. Batistić, E. Hrustić, I. Dupčić, and R. Garić. 2015. Impacts of extreme weather events on highly eutrophic marine ecosystem (Rogoznica Lake, Adriatic coast). *Continental Shelf Research* 108: 144-155, doi:10.1016/j.csr.2015.05.007
- Coats, R., J. Perez-Losada, G. Schladow, R. Richards, and C. Goldman. 2006. The warming of lake Tahoe. *Climatic Change* 76: 121-148, doi:10.1007/s10584-005-9006-1
- Collins, W., N. Bellouin, M. Doutriaux-Boucher, N. Gedney, T. Hinton, C. Jones, S. Liddicoat, G. Martin, F. O'Connor, and J. Rae. 2008. Evaluation of the HadGEM2 model. Met Office Exeter, UK.
- Couture, R. M., S. J. Moe, Y. Lin, O. Kaste, S. Haande, and A. Lyche Solheim. 2018. Simulating water quality and ecological status of Lake Vansjø, Norway, under land-use and climate change by linking process-oriented models with a Bayesian network. *Science of the Total Environment* 621: 713-724, doi:10.1016/j.scitotenv.2017.11.303
- Couture, R. M., H. A. Wit, K. Tominaga, P. Kiuru, and I. Markelov. 2015. Oxygen dynamics in a boreal lake responds to long-term changes in climate, ice phenology, and DOC inputs. *Journal of Geophysical Research: Biogeosciences* 120: 2441-2456, doi:10.1002/2015jg003065

- Crockford, L., P. Jordan, A. Melland, and D. Taylor. 2015. Storm-triggered, increased supply of sediment-derived phosphorus to the epilimnion in a small freshwater lake. *Inland Waters* 5: 15-26, doi:10.5268/iw-5.1.738
- Csanady, G. 1975. Hydrodynamics of large lakes. *Annual Review of Fluid Mechanics* 7: 357-386, doi:10.1146/annurev.fl.07.010175.002041
- Danis, P.-A., U. von Grafenstein, V. Masson-Delmotte, S. Planton, D. Gerdeaux, and J. M. Moisselin. 2004. Vulnerability of two European lakes in response to future climatic changes. *Geophysical Research Letters* 31: L21507, doi:10.1029/2004gl020833
- De Boyer Montégut, C., G. Madec, A. S. Fisher, A. Lazar, and D. Iudicone. 2004. Mixed layer depth over the global ocean: An examination of profile data and a profile-based climatology. *Journal of Geophysical Research* 109: C12003, doi:10.1029/2004jc002378
- De Brabandere, L., S. Bonaglia, M. Y. Kononets, L. Viktorsson, A. Stigebrandt, B. Thamdrup, and P. O. J. Hall. 2015. Oxygenation of an anoxic fjord basin strongly stimulates benthic denitrification and DNRA. *Biogeochemistry* 126: 131-152, doi:10.1007/s10533-015-0148-6
- De Eyto, E., M. Dillane, T. Moore, H. Wilson, J. Cooney, P. Hughes, M. Murphy, P. Nixon, D. Sweeney, and R. Poole. 2020. Lough Feeagh water temperature profiles Marine Institute, Ireland.
- De Eyto, E., E. Jennings, E. Ryder, K. Sparber, M. Dillane, C. Dalton, and R. Poole. 2016. Response of a humic lake ecosystem to an extreme precipitation event: physical, chemical, and biological implications. *Inland Waters* 6: 483-498, doi:10.1080/IW-6.4.875
- Del Don, C., K. W. Hanselmann, R. Peduzzi, and R. Bachofen. 2001. The meromictic alpine Lake Cadagno: orographical and biogeochemical description. *Aquatic Sciences* 63: 70-90, doi:10.1007/PL00001345
- Despotovic, M., V. Nedic, D. Despotovic, and S. Cvetanovic. 2016. Evaluation of empirical models for predicting monthly mean horizontal diffuse solar radiation. *Renewable and Sustainable Energy Reviews* 56: 246-260, doi:10.1016/j.rser.2015.11.058
- Diehl, S., S. Berger, R. Ptacnik, and A. Wild. 2002. Phytoplankton, light, and nutrients in a gradient of mixing depths: field experiments. *Ecology* 83: 399-411, doi:10.1890/0012-9658(2002)083[0399:PLANIA]2.0.CO;2
- Dinno, A. 2017. dunn.test: Dunn's Test of Multiple Comparisons Using Rank Sums.
- Dodds, W. K., C. T. Robinson, E. E. Gaiser, G. J. A. Hansen, H. Powell, J. M. Smith, N. B. Morse, S. L. Johnson, S. V. Gregory, T. Bell, T. K. Kratz, and W. H. McDowell. 2012. Surprises and Insights from Long-Term Aquatic Data Sets and Experiments. *BioScience* 62: 709-721, doi:10.1525/bio.2012.62.8.4
- Doherty, J. 2015. Calibration and uncertainty analysis for complex environmental models. *Watermark Numerical Computing*.
- Donohue, I., H. Hillebrand, J. M. Montoya, O. L. Petchey, S. L. Pimm, M. S. Fowler, K. Healy, A. L. Jackson, M. Lurgi, and D. McClean. 2016. Navigating the complexity of ecological stability. *Ecology Letters* 19: 1172-1185, doi:10.1111/ele.12648
- Driescher, E., H. Behrendt, G. Schellenberger, and R. Stellmacher. 1993. Lake Müggelsee and its environment—natural conditions and anthropogenic impacts. *Internationale Revue der gesamten Hydrobiologie und Hydrographie* 78: 327-343.
- Elliott, J., A. Irish, C. Reynolds, and P. Tett. 2000. Modelling freshwater phytoplankton communities: an exercise in validation. *Ecological Modelling* 128: 19-26, doi:10.1016/S0304-3800(99)00221-5
- Enstad, L. I., K. Rygg, P. M. Haugan, and G. Alendal. 2008. Dissolution of a CO₂ lake, modeled by using an advanced vertical turbulence mixing scheme. *International Journal of Greenhouse Gas Control* 2: 511-519, doi:10.1016/j.ijggc.2008.04.001
- Fang, X., S. R. Alam, H. G. Stefan, L. Jiang, P. C. Jacobson, and D. L. Pereira. 2012. Simulations of water quality and oxythermal cisco habitat in Minnesota lakes under past and future climate scenarios. *Water Quality Research Journal of Canada* 47: 375-388, doi:10.2166/wqrjc.2012.031
- Fang, X., and H. G. Stefan. 1999. Projections of climate change effects on water temperature characteristics of small lakes in the contiguous US. *Climatic Change* 42: 377-412, doi:10.1023/A:1005431523281
- Fang, X., and H. G. Stefan. 2009. Simulations of climate effects on water temperature, dissolved oxygen, and ice and snow covers in lakes of the contiguous US under past and future climate scenarios. *Limnology and Oceanography* 54: 2359-2370, doi:10.4319/lo.2009.54.6_part_2.2359
- Fee, E. J. 1976. The vertical and seasonal distribution of chlorophyll in lakes of the Experimental Lakes Area, northwestern Ontario: Implications for primary production estimates. *Limnology and Oceanography* 21: 767-783, doi:10.4319/lo.1976.21.6.0767

- Fee, E. J., R. E. Hecky, S. E. M. Kasian, and D. R. Cruikshank. 1996. Effects of lake size, water clarity, and climatic variability on mixing depths in Canadian Shield lakes. *Limnology and Oceanography* 41: 912-920, doi:10.4319/lo.1996.41.5.0912
- Feldbauer, J., D. Kneis, T. Hegewald, T. U. Berendonk, and T. Petzoldt. 2020. Managing climate change in drinking water reservoirs: potentials and limitations of dynamic withdrawal strategies. *Environmental Sciences Europe* 32: 48, doi:10.1186/s12302-020-00324-7
- Fenocchi, A., M. Rogora, S. Sibilla, M. Ciampittello, and C. Dresti. 2018. Forecasting the evolution in the mixing regime of a deep subalpine lake under climate change scenarios through numerical modelling (Lake Maggiore, Northern Italy/Southern Switzerland). *Climate Dynamics* 51: 3521-3536, doi:10.1007/s00382-018-4094-6
- Ficke, A. D., C. A. Myrick, and L. J. Hansen. 2007. Potential impacts of global climate change on freshwater fisheries. *Reviews in Fish Biology and Fisheries* 17: 581-613, doi:10.1007/s11160-007-9059-5
- Ficker, H., M. Luger, and H. Gassner. 2017. From dimictic to monomictic: Empirical evidence of thermal regime transitions in three deep alpine lakes in Austria induced by climate change. *Freshwater Biology* 62: 1335-1345, doi:10.1111/fwb.12946
- Fink, G., J. Alcamo, M. Flörke, and K. Reder. 2018. Phosphorus Loadings to the World's Largest Lakes: Sources and Trends. *Global Biogeochemical Cycles* 32: 617-634, doi:10.1002/2017gb005858
- Fink, G., M. Wessels, and A. Wüest. 2016. Flood frequency matters: Why climate change degrades deep-water quality of peri-alpine lakes. *Journal of Hydrology* 540: 457-468, doi:10.1016/j.jhydrol.2016.06.023
- Fitch, D. T., and J. K. Moore. 2007. Wind speed influence on phytoplankton bloom dynamics in the Southern Ocean Marginal Ice Zone. *Journal of Geophysical Research* 112: C08006, doi:10.1029/2006jc004061
- Foley, B., I. D. Jones, S. C. Maberly, and B. Rippey. 2012. Long-term changes in oxygen depletion in a small temperate lake: effects of climate change and eutrophication. *Freshwater Biology* 57: 278-289, doi:10.1111/j.1365-2427.2011.02662.x
- Forbes, S. A. 1887. The lake as a microcosm. *Illinois Natural History Survey Bulletin*; v. 015, no. 09.
- Forel, F. A. 1880. Températures lacustres. *Recherches sur la température du lac Léman et d'autres lacs d'eau douce. Archives des Sciences physiques et naturelles de Genève* 3: 501-515.
- Frassl, M. A., J. M. Abell, D. A. Botelho, K. Cinque, B. R. Gibbes, K. D. Jöhnk, K. Muraoka, B. J. Robson, M. Wolski, M. Xiao, and D. P. Hamilton. 2019. A short review of contemporary developments in aquatic ecosystem modelling of lakes and reservoirs. *Environmental Modelling & Software* 117: 181-187, doi:10.1016/j.envsoft.2019.03.024
- French, R. H., and J. Imberger. 1984. Lake modeling: State of the art. *Critical Reviews in Environmental Science and Technology* 13: 311-357, doi:10.1080/10643388409381710
- Friedrich, J., F. Janssen, D. Aleynik, H. W. Bange, N. Boltacheva, M. N. Çagatay, A. W. Dale, G. Etiope, Z. Erdem, M. Geraga, A. Gilli, M. T. Gomoiu, P. O. J. Hall, D. Hansson, Y. He, M. Holtappels, M. K. Kirf, M. Kononets, S. Konovalov, A. Lichtschlag, D. M. Livingstone, G. Marinaro, S. Mazlumyan, S. Naeher, R. P. North, G. Papatheodorou, O. Pfannkuche, R. Prien, G. Rehder, C. J. Schubert, T. Soltwedel, S. Sommer, H. Stahl, E. V. Stanev, A. Teaca, A. Tengberg, C. Waldmann, B. Wehrli, and F. Wenzhöfer. 2014. Investigating hypoxia in aquatic environments: diverse approaches to addressing a complex phenomenon. *Biogeosciences* 11: 1215-1259, doi:10.5194/bg-11-1215-2014
- Frieler, K., R. Betts, J. Burke, E. Burke, P. Ciais, S. Denvil, D. Deryng, K. Ebi, T. Eddy, K. Emanuel, J. Elliott, E. Galbraith, S. N. Gosling, K. Halladay, F. Hattermann, T. Hickler, J. Hinkel, V. Huber, C. Jones, V. Krysanova, S. Lange, H. K. Lotze, H. Lotze-Campen, M. Mengel, I. Mouratiadou, H. Müller Schmied, S. Ostberg, F. Piontek, A. Popp, C. P. Reyer, J. Schewe, M. Stevanovic, T. Suzuki, K. Thonicke, H. Tian, D. P. Tittensor, R. Vautard, M. van Vliet, L. Warszawski, and F. Zhao. 2017. Assessing the impacts of 1.5 C global warming—simulation protocol of the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP2b). *Geoscientific Model Development* 10: 4321-4345, doi:10.5194/gmd-10-4321-2017
- Fukushima, T., B. Matsushita, L. Subehi, F. Setiawan, and H. Wibowo. 2017. Will hypolimnetic waters become anoxic in all deep tropical lakes? *Scientific Reports* 7: 45320, doi:10.1038/srep45320
- Gal, G., V. Makler-Pick, and N. Shachar. 2014. Dealing with uncertainty in ecosystem model scenarios: Application of the single-model ensemble approach. *Environmental Modelling & Software* 61: 360-370, doi:10.1016/j.envsoft.2014.05.015
- Gal, G., G. Yael, S. Noam, E. Moshe, and D. Schlabing. 2020. Ensemble Modeling of the Impact of Climate Warming and Increased Frequency of Extreme Climatic Events on the Thermal Characteristics of a Sub-Tropical Lake. *Water* 12: 1982, doi:10.3390/w12071982

- Gaudard, A., L. Råman Vinnå, F. Bärenbold, M. Schmid, and D. Bouffard. 2019. Toward an open access to high-frequency lake modeling and statistics data for scientists and practitioners—the case of Swiss lakes using Simstrat v2. 1. *Geoscientific Model Development* 12: 3955-3974, doi:10.5194/gmd-12-3955-2019
- Gertman, I., and A. Hecht. 2002. The Dead Sea hydrography from 1992 to 2000. *Journal of Marine Systems* 35: 169-181, doi:10.1016/S0924-7963(02)00079-9
- Giling, D. P., J. C. Nejstgaard, S. A. Berger, H. P. Grossart, G. Kirillin, A. Penske, M. Lentz, P. Casper, J. Sareyka, and M. O. Gessner. 2017a. Thermocline deepening boosts ecosystem metabolism: evidence from a large-scale lake enclosure experiment simulating a summer storm. *Global Change Biology* 23: 1448-1462, doi:10.1111/gcb.13512
- Giling, D. P., P. A. Staehr, H. P. Grossart, M. R. Andersen, B. Boehrer, C. Escot, F. Evrendilek, L. Gómez-Gener, M. Honti, I. D. Jones, N. Karakaya, A. Laas, E. Moreno-Ostos, K. Rinke, U. Scharfenberger, S. R. Schmidt, M. Weber, R. I. Woolway, J. A. Zwart, and B. Obrador. 2017b. Delving deeper: Metabolic processes in the metalimnion of stratified lakes. *Limnology and Oceanography* 62: 1288-1306, doi:10.1002/lno.10504
- Gneiting, T., and A. E. Raftery. 2005. Weather forecasting with ensemble methods. *Science* 310: 248-249, doi:10.1126/science.1115255
- Goedkoop, W., and L. Sonesten. 1995. Laborationsmanual för kemiska och fysikaliska analyser av inlandsvatten och sediment. Institute of Limnology, Uppsala University.
- Goudsmit, G. H., H. Burchard, F. Peeters, and A. Wüest. 2002. Application of k- ϵ turbulence models to enclosed basins: The role of internal seiches. *Journal of Geophysical Research: Oceans* 107, doi:10.1029/2001JC000954
- Grasset, C., R. Mendonça, G. Villamor Saucedo, D. Bastviken, F. Roland, and S. Sobek. 2018. Large but variable methane production in anoxic freshwater sediment upon addition of allochthonous and autochthonous organic matter. *Limnology and Oceanography* 63: 1488-1501, doi:10.1002/lno.10786
- Gray, E., J. A. Elliott, E. B. Mackay, A. M. Folkard, P. O. Keenan, and I. D. Jones. 2019. Modelling lake cyanobacterial blooms: Disentangling the climate-driven impacts of changing mixed depth and water temperature. *Freshwater Biology* 64: 2141-2155, doi:10.1111/fwb.13402
- Gudas, C., D. Bastviken, K. Steger, K. Premke, S. Sobek, and L. J. Tranvik. 2010. Temperature-controlled organic carbon mineralization in lake sediments. *Nature* 466: 478-481, doi:10.1038/nature09186
- Gulati, R. D., E. S. Zadereev, and A. G. Degermendzhi. 2017. *Ecology of Meromictic Lakes*. Springer.
- Gurkan, Z., J. Zhang, and S. E. Jørgensen. 2006. Development of a structurally dynamic model for forecasting the effects of restoration of Lake Fure, Denmark. *Ecological Modelling* 197: 89-102, doi:10.1016/j.ecolmodel.2006.03.006
- Hamilton-Taylor, J., W. Davison, and K. Morfett. 1996. The biogeochemical cycling of Zn, Cu, Fe, Mn, and dissolved organic C in a seasonally anoxic lake. *Limnology and Oceanography* 41: 408-418, doi:10.4319/lno.1996.41.3.0408
- Hamilton, D. P., G. C. Hocking, and J. C. Patterson. 1997. Criteria for selection of spatial dimension in the application of one-and two-dimensional water quality models. *Mathematics and computers in simulation* 43: 387-393, doi:10.1016/S0378-4754(97)00023-2
- Hansson, L. A., M. K. Ekvall, L. He, Z. Li, M. Svensson, P. Urrutia-Cordero, and H. Zhang. 2020. Different climate scenarios alter dominance patterns among aquatic primary producers in temperate systems. *Limnology and Oceanography* 65: 2328-2336, doi:10.1002/lno.11455
- Havens, K. E., K. R. Jin, A. J. Rodusky, B. Sharfstein, M. A. Brady, T. L. East, N. Iricanin, R. T. James, M. C. Harwell, and A. D. Steinman. 2001. Hurricane effects on a shallow lake ecosystem and its response to a controlled manipulation of water level. *The Scientific World Journal* 1: 44-70, doi:10.1100/tsw.2001.14
- Hellweger, F. L. 2017. 75 years since Monod: It is time to increase the complexity of our predictive ecosystem models (opinion). *Ecological Modelling* 346: 77-87, doi:10.1016/j.ecolmodel.2016.12.001
- Heming, J. T., F. Prates, M. A. Bender, R. Bowyer, J. Cangialosi, P. Caroff, T. Coleman, J. D. Doyle, A. Dube, G. Faure, J. Fraser, B. C. Howell, Y. Igarashi, R. McTaggart-Cowan, M. Mohapatra, J. R. Moskaitis, J. Murtha, R. Rivett, M. Sharma, C. J. Short, A. A. Singh, V. Tallapragada, H. A. Titley, and Y. Xiao. 2019. Review of Recent Progress in Tropical Cyclone Track Forecasting and Expression of Uncertainties. *Tropical Cyclone Research and Review* 8: 181-218, doi:10.1016/j.tcrr.2020.01.001
- Henriksen, A., and R. F. Wright. 1977. Effects of Acid Precipitation on a Small Acid Lake in Southern Norway: Paper presented at the Nordic Hydrological Conference (Reykjavik, Iceland, Aug-Sep, 1976). *Hydrology Research* 8: 1-10, doi:10.2166/nh.1977.0001
- Hense, I., and A. Beckmann. 2010. The representation of cyanobacteria life cycle processes in aquatic ecosystem models. *Ecological Modelling* 221: 2330-2338, doi:10.1016/j.ecolmodel.2010.06.014

- Herman, J., and W. Usher. 2017. SALib: an open-source Python library for sensitivity analysis. *Journal of Open Source Software* 2: 97, doi:10.21105/joss.00097
- Hilt, S., I. Henschke, J. Rucker, and B. Nixdorf. 2010. Can submerged macrophytes influence turbidity and trophic state in deep lakes? Suggestions from a case study. *Journal of Environmental Quality* 39: 725-733, doi:10.2134/jeq2009.0122
- Hipsey, M. R., L. C. Bruce, C. Boon, B. Busch, C. C. Carey, D. P. Hamilton, P. C. Hanson, J. S. Read, E. de Sousa, M. Weber, and L. A. Winslow. 2019. A General Lake Model (GLM 3.0) for linking with high-frequency sensor data from the Global Lake Ecological Observatory Network (GLEON). *Geoscientific Model Development* 12: 473-523, doi:10.5194/gmd-12-473-2019
- Hipsey, M. R., G. Gal, G. B. Arhonditsis, C. C. Carey, J. A. Elliott, M. A. Frassl, J. H. Janse, L. de Mora, and B. J. Robson. 2020. A system of metrics for the assessment and improvement of aquatic ecosystem models. *Environmental Modelling & Software* 128, doi:10.1016/j.envsoft.2020.104697
- Hoke, A., J. Woodhouse, L. Zoccarato, V. McCarthy, E. de Eyto, M. Calderó-Pascual, E. Geffroy, M. Dillane, H.-P. Grossart, and E. Jennings. 2020. Impacts of Extreme Weather Events on Bacterial Community Composition of a Temperate Humic Lake. *Water* 12, doi:10.3390/w12102757
- Huber, V., R. Adrian, and D. Gerten. 2010. A matter of timing: heat wave impact on crustacean zooplankton. *Freshwater Biology* 55: 1769-1779, doi:10.1111/j.1365-2427.2010.02411.x
- Huber, V., C. Wagner, D. Gerten, and R. Adrian. 2012. To bloom or not to bloom: contrasting responses of cyanobacteria to recent heat waves explained by critical thresholds of abiotic drivers. *Oecologia* 169: 245-256, doi:10.1007/s00442-011-2186-7
- Huisman, J., J. Sharples, J. M. Stroom, P. M. Visser, W. E. A. Kardinaal, J. M. Verspagen, and B. Sommeijer. 2004. Changes in turbulent mixing shift competition for light between phytoplankton species. *Ecology* 85: 2960-2970, doi:10.1890/03-0763
- Huisman, J., P. van Oostveen, and F. J. Weissing. 1999. Critical depth and critical turbulence: two different mechanisms for the development of phytoplankton blooms. *Limnology and Oceanography* 44: 1781-1787, doi:10.4319/lo.1999.44.7.1781
- Hupfer, M., and J. Lewandowski. 2008. Oxygen Controls the Phosphorus Release from Lake Sediments - a Long-Lasting Paradigm in Limnology. *International Review of Hydrobiology* 93: 415-432, doi:10.1002/iroh.200711054
- Hutchinson, G. E. 1957. *A Treatise on Limnology*. Wiley.
- Hutchinson, G. E., and H. Löffler. 1956. The thermal classification of lakes. *Proceedings of the National Academy of Sciences* 42: 84-86, doi:10.1073/pnas.42.2.84
- Hutter, K., and K. Jöhnk. 2004. *Continuum methods of physical modeling: continuum mechanics, dimensional analysis, turbulence*. Springer Science & Business Media.
- Ibelings, B. W., B. M. Kroon, and L. R. Mur. 1994. Acclimation of photosystem II in a cyanobacterium and a eukaryotic green alga to high and fluctuating photosynthetic photon flux densities, simulating light regimes induced by mixing in lakes. *New Phytologist* 128: 407-424, doi:10.1111/j.1469-8137.1994.tb02987.x
- Ibelings, B. W., R. Portielje, E. H. R. R. Lammens, R. Noordhuis, M. S. van den Berg, W. Joosse, and M. L. Meijer. 2007. Resilience of Alternative Stable States during the Recovery of Shallow Lakes from Eutrophication: Lake Veluwe as a Case Study. *Ecosystems* 10: 4-16, doi:10.1007/s10021-006-9009-4
- Idso, S. B. 1973. On the concept of lake stability. *Limnology and Oceanography* 18: 681-683, doi:10.4319/lo.1973.18.4.0681
- Imberger, J. 1985. The diurnal mixed layer 1. *Limnology and Oceanography* 30: 737-770, doi:10.4319/lo.1985.30.4.0737
- Imberger, J., and P. F. Hamblin. 1982. Dynamics of lakes, reservoirs, and cooling ponds. *Annual Review of Fluid Mechanics* 14: 153-187.
- Imboden, D. M. 1973. Limnologische Transport- und Nährstoffmodelle. *Schweiz. Z. Hydrol.* 35: 29-68, doi:10.1007/BF02502063
- Imboden, D. M., and A. Wüest. 1995. Mixing mechanisms in lakes, p. 83-138. *In* A. Lerman, D. M. Imboden and J. R. Gat [eds.], *Physics and chemistry of lakes*. Springer.
- IPCC. 2014. *Climate Change 2014: Synthesis Report. Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change*, p. 151. *In* Core Writing Team, Pachauri, R.K. and Meyer, L.A. [ed.].
- Ito, Y., and K. Momii. 2015. Impacts of regional warming on long-term hypolimnetic anoxia and dissolved oxygen concentration in a deep lake. *Hydrological Processes* 29: 2232-2242, doi:10.1002/hyp.10362

- Jachner, S., G. Van den Boogaart, and T. Petzoldt. 2007. Statistical methods for the qualitative assessment of dynamic models with time delay (R Package qualV). *Journal of Statistical Software* 22: 1-30, doi:10.18637/jss.v022.i08
- Jacob, D., J. Petersen, B. Eggert, A. Alias, O. B. Christensen, L. M. Bouwer, A. Braun, A. Colette, M. Déqué, G. Georgievski, E. Georgopoulou, A. Gobiet, L. Menut, G. Nikulin, A. Haensler, N. Hempelmann, C. Jones, K. Keuler, S. Kovats, N. Kröner, S. Kotlarski, A. Kriegsmann, E. Martin, E. van Meijgaard, C. Moseley, S. Pfeifer, S. Preuschmann, C. Radermacher, K. Radtke, D. Rechid, M. Rounsevell, P. Samuelsson, S. Somot, J.-F. Soussana, C. Teichmann, R. Valentini, R. Vautard, B. Weber, and P. Yiou. 2013. EURO-CORDEX: new high-resolution climate change projections for European impact research. *Regional Environmental Change* 14: 563-578, doi:10.1007/s10113-013-0499-2
- Jalil, A., K. Zhang, L. Qi, Y. Li, and M. Aleem. 2020. Phytoplankton response to long-term wind dynamics at large shallow Lake Taihu (shallow lake phytoplankton response to long-term wind dynamics). *International Journal of Environmental Science and Technology* 18: 341-352, doi:10.1007/s13762-020-02827-5
- Jankowski, T., D. M. Livingstone, H. Bührer, R. Forster, and P. Niederhauser. 2006. Consequences of the 2003 European heat wave for lake temperature profiles, thermal stability, and hypolimnetic oxygen depletion: Implications for a warmer world. *Limnology and Oceanography* 51: 815-819, doi:10.4319/lo.2006.51.2.0815
- Janssen, A. B. G., G. B. Arhonditsis, A. Beusen, K. Bolding, L. Bruce, J. Bruggeman, R.-M. Couture, A. S. Downing, J. A. Elliott, M. A. Frassl, G. Gal, D. J. Gerla, M. R. Hipsey, F. Hu, S. C. Ives, J. H. Janse, E. Jeppesen, K. D. Jöhnk, D. Kneis, X. Kong, J. J. Kuiper, M. K. Lehmann, C. Lemmen, D. Ozkundakci, T. Petzoldt, K. Rinke, B. J. Robson, R. Sachse, S. A. Schep, M. Schmid, H. Scholten, S. Teurlincx, D. Trolle, T. A. Troost, A. A. Van Dam, L. Van Gerven, M. Weijerman, S. A. Wells, and W. M. Mooij. 2015. Exploring, exploiting and evolving diversity of aquatic ecosystem models: a community perspective. *Aquatic Ecology* 49: 513-548, doi:10.1007/s10452-015-9544-1
- Jansson, M., P. Blomqvist, A. Jonsson, and A. K. Bergström. 1996. Nutrient limitation of bacterioplankton, autotrophic and mixotrophic phytoplankton, and heterotrophic nanoflagellates in Lake Östräsket. *Limnology and Oceanography* 41: 1552-1559, doi:10.4319/lo.1996.41.7.1552
- Jennings, E., M. Järvinen, N. Allott, L. Arvola, K. Moore, P. Naden, C. N. Aonghusa, T. Nöges, and G. A. Weyhenmeyer. 2010. Impacts of climate on the flux of dissolved organic carbon from catchments, p. 199-220. *In* G. George [ed.], *The Impact of Climate Change on European Lakes*. Springer.
- Jennings, E., S. Jones, L. Arvola, P. A. Staehr, E. Gaiser, I. D. Jones, K. C. Weathers, G. A. Weyhenmeyer, C. Y. CHIU, and E. De Eyto. 2012. Effects of weather-related episodic events in lakes: an analysis based on high-frequency data. *Freshwater Biology* 57: 589-601, doi:10.1111/j.1365-2427.2011.02729.x
- Ji, G., K. E. Havens, J. R. Beaver, and T. L. East. 2018. Recovery of plankton from hurricane impacts in a large shallow lake. *Freshwater Biology* 63: 366-379, doi:10.1111/fwb.13075
- Jöhnk, K. D., J. Huisman, J. Sharples, B. Sommeijer, P. M. Visser, and J. M. Stroom. 2008. Summer heatwaves promote blooms of harmful cyanobacteria. *Global Change Biology* 14: 495-512, doi:10.1111/j.1365-2486.2007.01510.x
- Johnson, S. G. 2014. The NLOpt nonlinear-optimization package.
- Jones, I., G. George, and C. Reynolds. 2005. Quantifying effects of phytoplankton on the heat budgets of two large limnetic enclosures. *Freshwater Biology* 50: 1239-1247, doi:10.1111/j.1365-2427.2005.01397.x
- Jørgensen, S. E. 1995. State of the art of ecological modelling in limnology. *Ecological Modelling* 78: 101-115, doi:10.1016/0304-3800(94)00120-7
- Julià, R., F. Burjachs, M. J. Dasí, F. Mezquita, M. R. Miracle, J. R. Roca, G. Seret, and E. Vicente. 1998. Meromixis origin and recent trophic evolution in the Spanish mountain lake La Cruz. *Aquatic Sciences* 60: 279-299, doi:10.1007/s000270050042
- Kaden, H., F. Peeters, A. Lorke, R. Kipfer, Y. Tomonaga, and M. Karabiyikoglu. 2010. Impact of lake level change on deep-water renewal and oxic conditions in deep saline Lake Van, Turkey. *Water Resources Research* 46: W11508, doi:10.1029/2009wr008555
- Kangur, K., P. Kangur, K. Ginter, K. Orru, M. Haldna, T. Möls, and A. Kangur. 2013. Long-term effects of extreme weather events and eutrophication on the fish community of shallow Lake Peipsi (Estonia/Russia). *Journal of Limnology* 72: 376-387, doi:10.4081/jlimnol.2013.e30
- Karlsson-Elfgren, I., E. Rydin, P. Hyenstrand, and K. Pettersson. 2003. Recruitment and Pelagic Growth of *Gloeotrichia Echinulata* (Cyanophyceae) in Lake Erken 1. *Journal of Phycology* 39: 1050-1056, doi:10.1111/j.0022-3646.2003.03-030.x

- Kasprzak, P., T. Shatwell, M. O. Gessner, T. Gonsiorczyk, G. Kirillin, G. Selmecky, J. Padisák, and C. Engelhardt. 2017. Extreme Weather Event Triggers Cascade Towards Extreme Turbidity in a Clear-water Lake. *Ecosystems* 20: 1407-1420, doi:10.1007/s10021-017-0121-4
- Kelly, M. R., V. W. Moriarty, G. Auger, C. Watson, H. R. Kolar, and K. C. Rose. 2019. Understanding the factors contributing to harmful algal bloom formation in a large oligotrophic lake: the important role of physics (Poster). GLEON21.
- Kelly, S., B. Doyle, E. de Eyto, M. Dillane, P. McGinnity, R. Poole, M. White, and E. Jennings. 2020. Impacts of a record-breaking storm on physical and biogeochemical regimes along a catchment-to-coast continuum. *PLoS one* 15: e0235963, doi:10.1371/journal.pone.0235963
- Khan, S. J., D. Deere, F. D. Leusch, A. Humpage, M. Jenkins, and D. Cunliffe. 2015. Extreme weather events: Should drinking water quality management systems adapt to changing risk profiles? *Water Research* 85: 124-136, doi:10.1016/j.watres.2015.08.018
- Kirillin, G. 2010. Modeling the impact of global warming on water temperature and seasonal mixing regimes in small temperate lakes. *Boreal Environment Research* 15: 279-293.
- Kirillin, G., and T. Shatwell. 2016. Generalized scaling of seasonal thermal stratification in lakes. *Earth-Science Reviews* 161: 179-190, doi:10.1016/j.earscirev.2016.08.008
- Kitaigorodskii, S., and Y. Z. Miropolsky. 1970. On theory of open ocean active layer. *Izvestiya Akademii Nauk SSSR Fizika Atmosfery i Okeana* 6: 178-+.
- Klug, J. L., D. C. Richardson, H. A. Ewing, B. R. Hargreaves, N. R. Samal, D. Vachon, D. C. Pierson, A. M. Lindsey, D. M. O'Donnell, S. W. Effler, and K. C. Weathers. 2012. Ecosystem effects of a tropical cyclone on a network of lakes in northeastern North America. *Environmental Science & Technology* 46: 11693-11701, doi:10.1021/es302063v
- Kobler, U. G., and M. Schmid. 2019. Ensemble modelling of ice cover for a reservoir affected by pumped-storage operation and climate change. *Hydrological Processes* 33: 2676-2690, doi:10.1002/hyp.13519
- Koenings, J. P., and J. A. Edmundson. 1991. Secchi disk and photometer estimates of light regimes in Alaskan lakes: effects of yellow color and turbidity. *Limnology and Oceanography* 36: 91-105, doi:10.4319/lo.1991.36.1.0091
- Konzelmann, T., R. S. van de Wal, W. Greuell, R. Bintanja, E. A. Henneken, and A. Abe-Ouchi. 1994. Parameterization of global and longwave incoming radiation for the Greenland Ice Sheet. *Global and Planetary change* 9: 143-164, doi:10.1016/0921-8181(94)90013-2
- Kraemer, B. M., O. Anneville, S. Chandra, M. Dix, E. Kuusisto, D. M. Livingstone, A. Rimmer, S. G. Schladow, E. Silow, L. M. Sitoki, R. Tamatamah, Y. Vadeboncoeur, and P. B. McIntyre. 2015. Morphometry and average temperature affect lake stratification responses to climate change. *Geophysical Research Letters* 42: 4981-4988, doi:10.1002/2015GL064097
- Kraemer, B. M., T. Mehner, and R. Adrian. 2017. Reconciling the opposing effects of warming on phytoplankton biomass in 188 large lakes. *Scientific Reports* 7: 10762, doi:10.1038/s41598-017-11167-3
- Krishnamurti, T. N., C. Kishtawal, Z. Zhang, T. LaRow, D. Bachiochi, E. Williford, S. Gadgil, and S. Surendran. 2000. Multimodel ensemble forecasts for weather and seasonal climate. *Journal of Climate* 13: 4196-4216, doi:10.1175/1520-0442(2000)013<4196:MEFFWA>2.0.CO;2
- Kuha, J., L. Arvola, P. C. Hanson, J. Huotari, T. Huttula, J. Juntunen, M. Järvinen, K. Kallio, M. Ketola, K. Kuoppamäki, A. Lepistö, A. Lohila, R. Paavola, J. Vuorenmaa, L. Winslow, and J. Karjalainen. 2016. Response of boreal lakes to episodic weather-induced events. *Inland Waters* 6: 523-534, doi:10.1080/IW-6.4.886
- Ladwig, R., E. Furusato, G. Kirillin, R. Hinkelmann, and M. Hupfer. 2018. Climate Change Demands Adaptive Management of Urban Lakes: Model-Based Assessment of Management Scenarios for Lake Tegel (Berlin, Germany). *Water* 10, doi:10.3390/w10020186
- Ladwig, R., P. C. Hanson, H. A. Dugan, C. C. Carey, Y. Zhang, L. Shu, C. J. Duffy, and K. M. Cobourn. 2021. Lake thermal structure drives interannual variability in summer anoxia dynamics in a eutrophic lake over 37 years. *Hydrology and Earth System Sciences* 25: 1009-1032, doi:10.5194/hess-25-1009-2021
- Lehmann, M. F., M. Simona, S. Wyss, J. Blees, C. H. Frame, H. Niemann, M. Veronesi, and J. Zopfi. 2015. Powering up the "biogeochemical engine": the impact of exceptional ventilation of a deep meromictic lake on the lacustrine redox, nutrient, and methane balances. *Frontiers in Earth Science* 3: 45, doi:10.3389/feart.2015.00045
- Lepori, F., M. Bartosiewicz, M. Simona, and M. Veronesi. 2018. Effects of winter weather and mixing regime on the restoration of a deep perialpine lake (Lake Lugano, Switzerland and Italy). *Hydrobiologia* 824: 229-242, doi:10.1007/s10750-018-3575-2

- Lepori, F., and J. J. Roberts. 2015. Past and future warming of a deep European lake (Lake Lugano): What are the climatic drivers? *Journal of Great Lakes Research* 41: 973-981, doi:10.1016/j.jglr.2015.08.004
- Leppäranta, M. 2015. Freezing of lakes and the evolution of their ice cover. Springer Science & Business Media.
- Leutbecher, M., and T. N. Palmer. 2008. Ensemble forecasting. *Journal of Computational Physics* 227: 3515-3539, doi:10.1016/j.jcp.2007.02.014
- Lewis Jr, W. M. 1973. The Thermal Regime Of Lake Lanao (Philippines) And Its Theoretical Implications For Tropical Lakes 1. *Limnology and Oceanography* 18: 200-217, doi:10.4319/lo.1973.18.2.0200
- Lewis Jr, W. M. 1983. A revised classification of lakes based on mixing. *Canadian Journal of Fisheries and Aquatic Sciences* 40: 1779-1787, doi:10.1139/f83-207
- Lewis Jr, W. M. 1996. Tropical lakes: How latitude makes a difference. *In* S. Academic [ed.], *Perspectives Tropical Limnology*. SPB Academic.
- Li, C., D. Notz, S. Tietsche, and J. Marotzke. 2013. The Transient versus the Equilibrium Response of Sea Ice to Global Warming. *Journal of Climate* 26: 5624-5636, doi:10.1175/jcli-d-12-00492.1
- Lin, L. 1989. A concordance correlation coefficient to evaluate reproducibility. *Biometrics* 45: 255-268, doi:10.2307/2532051
- Lindenmayer, D. B., G. E. Likens, A. Andersen, D. Bowman, C. M. Bull, E. Burns, C. R. Dickman, A. A. Hoffmann, D. A. Keith, M. J. Liddell, A. J. Lowe, D. J. Metcalfe, S. R. Phinn, J. Russell-Smith, N. Thurgate, and G. M. Wardle. 2012. Value of long-term ecological studies. *Austral Ecology* 37: 745-757, doi:10.1111/j.1442-9993.2011.02351.x
- Lindström, G., C. Pers, J. Rosberg, J. Strömqvist, and B. Arheimer. 2010. Development and testing of the HYPE (Hydrological Predictions for the Environment) water quality model for different spatial scales. *Hydrology Research* 41: 295-319, doi:10.2166/nh.2010.007
- Livingstone, D. M. 1993. Temporal structure in the deep-water temperature of four Swiss lakes: A short-term climatic change indicator? *Internationale Vereinigung für theoretische und angewandte Limnologie: Verhandlungen* 25: 75-81, doi:10.1080/03680770.1992.11900062
- Livingstone, D. M. 1997. An example of the simultaneous occurrence of climate-driven "sawtooth" deep-water warming/cooling episodes in several Swiss lakes. *Internationale Vereinigung für theoretische und angewandte Limnologie: Verhandlungen* 26: 822-828, doi:10.1080/03680770.1995.11900832
- Livingstone, D. M. 2008. A change of climate provokes a change of paradigm: taking leave of two tacit assumptions about physical lake forcing. *International Review of Hydrobiology* 93: 404-414, doi:10.1002/iroh.200811061
- Loizeau, J.-L., and J. Dominik. 2000. Evolution of the Upper Rhone River discharge and suspended sediment load during the last 80 years and some implications for Lake Geneva. *Aquatic Sciences* 62: 54-67, doi:10.1007/s000270050075
- MacIntyre, S., and R. Jellison. 2001. Nutrient fluxes from upwelling and enhanced turbulence at the top of the pycnocline in Mono Lake, California, p. 13-29. *Saline Lakes*. Springer.
- Mackay, E. B., A. M. Folkard, and I. D. Jones. 2014. Interannual variations in atmospheric forcing determine trajectories of hypolimnetic soluble reactive phosphorus supply in a eutrophic lake. *Freshwater Biology* 59: 1646-1658, doi:10.1111/fwb.12371
- Magee, M. R., and C. H. Wu. 2017. Response of water temperatures and stratification to changing climate in three lakes with different morphometry. *Hydrology and Earth System Sciences* 21: 6253-6274, doi:10.5194/hess-21-6253-2017
- Magnuson, J. J., D. M. Robertson, B. J. Benson, R. H. Wynne, D. M. Livingstone, T. Arai, R. A. Assel, R. G. Barry, V. Card, E. Kuusisto, N. G. Granin, T. D. Prowse, K. M. Stewart, and V. S. Vuglinski. 2000. Historical trends in lake and river ice cover in the Northern Hemisphere. *Science* 289: 1743-1746, doi:10.1126/science.289.5485.1743
- Markensten, H., K. Moore, and I. Persson. 2010. Simulated lake phytoplankton composition shifts toward cyanobacteria dominance in a future warmer climate. *Ecological Applications* 20: 752-767, doi:10.1890/08-2109.1
- Markensten, H., and D. C. Pierson. 2007. Weather driven influences on phytoplankton succession in a shallow lake during contrasting years: application of PROTBAS. *Ecological Modelling* 207: 128-136, doi:10.1016/j.ecolmodel.2007.04.023
- Martin, J. L., and S. C. McCutcheon. 1999. *Hydrodynamics and transport for water quality modeling*. CRC press.
- Matzinger, A., M. Schmid, E. Veljanoska-Sarafiloska, S. Patceva, D. Guseska, B. Wagner, B. Müller, M. Sturm, and A. Wüest. 2007. Eutrophication of ancient Lake Ohrid: Global warming amplifies detrimental effects of increased nutrient inputs. *Limnology and Oceanography* 52: 338-353, doi:10.4319/lo.2007.52.1.0338

- Matzinger, A., Z. Spirkovski, S. Patceva, and A. Wüest. 2006. Sensitivity of ancient Lake Ohrid to local anthropogenic impacts and global warming. *Journal of Great Lakes Research* 32: 158-179, doi:10.3394/0380-1330(2006)32[158:SOALOT]2.0.CO;2
- McKay, M. D., R. J. Beckman, and W. J. Conover. 2000. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics* 42: 55-61, doi:10.1080/00401706.2000.10485979
- Melack, J. M., and R. Jellison. 1998. Limnological conditions in Mono Lake: contrasting monomixis and meromixis in the 1990s. *Hydrobiologia* 384: 21-39, doi:10.1023/A:1003352511328
- Mesman, J. P., A. I. Ayala, R. Adrian, E. De Eyto, M. A. Frassl, S. Goyette, J. Kasparian, M. Perroud, J. A. A. Stelzer, D. C. Pierson, and B. W. Ibelings. 2020. Performance of one-dimensional hydrodynamic lake models during short-term extreme weather events. *Environmental Modelling & Software* 133: 104852, doi:10.1016/j.envsoft.2020.104852
- Mesman, J. P., J. A. A. Stelzer, V. Dakos, S. Goyette, I. D. Jones, J. Kasparian, D. F. McGinnis, and B. W. Ibelings. 2021. The role of internal feedbacks in shifting deep lake mixing regimes under a warming climate. *Freshwater Biology* 66: 1021-1035, doi:10.1111/fwb.13704
- Met Éireann. 2018. Met Éireann Data licensed under a Creative Commons Attribution-ShareAlike 4.0 International licence.
- Mi, C., M. A. Frassl, B. Boehrer, and K. Rinke. 2018. Episodic wind events induce persistent shifts in the thermal stratification of a reservoir (Rappbode Reservoir, Germany). *International Review of Hydrobiology* 103: 71-82, doi:10.1002/iroh.201701916
- Mi, C., T. Shatwell, J. Ma, V. C. Wentzky, B. Boehrer, Y. Xu, and K. Rinke. 2020. The formation of a metalimnetic oxygen minimum exemplifies how ecosystem dynamics shape biogeochemical processes: A modelling study. *Water Research* 175: 115701, doi:10.1016/j.watres.2020.115701
- Mironov, D., E. Heise, E. Kourzeneva, B. Ritter, N. Schneider, and A. Terzhevik. 2010. Implementation of the lake parameterisation scheme FLake into the numerical weather prediction model COSMO. *Boreal Environment Research* 15: 218-230.
- Mironov, D. V. 2005. Parameterization of lakes in numerical weather prediction. Part 1: Description of a lake model (technical report No. 11). Deutscher Wetterdienst.
- Mironov, D. V. 2008. Parameterization of lakes in numerical weather prediction. Part 1: Description of a lake model. German Weather Service, Offenbach am Main, Germany.
- Mischke, U. 2003. Cyanobacteria associations in shallow polytrophic lakes: influence of environmental factors. *Acta Oecologica* 24: S11-S23, doi:10.1016/S1146-609X(03)00003-1
- Möller, T., D. Schindler, A. Albrecht, and U. Kohnle. 2016. Review on the Projections of Future Storminess over the North Atlantic European Region. *Atmosphere* 7: 60, doi:10.3390/atmos7040060
- Mooij, W. M., D. Trolle, E. Jeppesen, G. Arhonditsis, P. V. Belolipetsky, D. B. R. Chitamwebwa, A. G. Degermendzhy, D. L. DeAngelis, L. N. De Senerpont Domis, A. S. Downing, J. A. Elliott, C. R. Fragoso, U. Gaedke, S. N. Genova, R. D. Gulati, L. Håkanson, D. P. Hamilton, M. R. Hipsey, J. 't Hoen, S. Hülsmann, F. H. Los, V. Makler-Pick, T. Petzoldt, I. G. Prokopkin, K. Rinke, S. A. Schep, K. Tominaga, A. A. Van Dam, E. H. Van Nes, S. A. Wells, and J. H. Janse. 2010. Challenges and opportunities for integrating lake ecosystem modelling approaches. *Aquatic Ecology* 44: 633-667, doi:10.1007/s10452-010-9339-3
- Moras, S., A. I. Ayala, and D. C. Pierson. 2019. Historical modelling of changes in Lake Erken thermal conditions. *Hydrology and Earth System Sciences* 23: 5001-5016, doi:10.5194/hess-23-5001-2019
- Mu, M., W. Duan, and Y. Tang. 2017. The predictability of atmospheric and oceanic motions: Retrospect and prospects. *Science China Earth Sciences* 60: 2001-2012, doi:10.1007/s11430-016-9101-x
- Müller, B., L. D. Bryant, A. Matzinger, and A. Wüest. 2012. Hypolimnetic oxygen depletion in eutrophic lakes. *Environmental Science & Technology* 46: 9964-9971, doi:10.1021/es301422r
- Nash, J. E., and J. V. Sutcliffe. 1970. River flow forecasting through conceptual models: Part 1 - A discussion of principles. *Journal of Hydrology* 10: 282-290, doi:10.1016/0022-1694(70)90255-6
- Nelder, J. A., and R. Mead. 1965. A simplex method for function minimization. *The computer journal* 7: 308-313, doi:10.1093/comjnl/7.4.308
- Neumann, T., W. Fennel, and C. Kremp. 2002. Experimental simulations with an ecosystem model of the Baltic Sea: A nutrient load reduction experiment. *Global Biogeochemical Cycles* 16: 1033, doi:10.1029/2001gb001450
- Nielsen, A., D. Trolle, R. Bjerring, M. Søndergaard, J. E. Olesen, J. H. Janse, W. M. Mooij, and E. Jeppesen. 2014. Effects of climate and nutrient load on the water quality of shallow lakes assessed through ensemble runs by PCLake. *Ecological Applications* 24: 1926-1944, doi:10.1890/13-0790.1

- Nöges, T., P. Nöges, A. Jolma, and J. Kaitaranta. 2009. Impacts of climate change on physical characteristics of lakes in Europe. JRC Scientific and Technical Reports, EUR 24064, doi:10.2788/41235
- North, R. P., R. L. North, D. M. Livingstone, O. Köster, and R. Kipfer. 2014. Long-term changes in hypoxia and soluble reactive phosphorus in the hypolimnion of a large temperate lake: consequences of a climate regime shift. *Global Change Biology* 20: 811-823, doi:10.1111/gcb.12371
- Nowlin, W. H., J. L. Evarts, and M. J. Vanni. 2005. Release rates and potential fates of nitrogen and phosphorus from sediments in a eutrophic reservoir. *Freshwater Biology* 50: 301-322, doi:10.1111/j.1365-2427.2004.01316.x
- O'Reilly, C. M., S. R. Alin, P.-D. Plisnier, A. S. Cohen, and B. A. McKee. 2003. Climate change decreases aquatic ecosystem productivity of Lake Tanganyika, Africa. *Nature* 424: 766, doi:10.1038/nature01833
- O'Reilly, C. M., S. Sharma, D. K. Gray, S. E. Hampton, J. S. Read, R. J. Rowley, P. Schneider, J. D. Lenters, P. B. McIntyre, B. M. Kraemer, G. A. Weyhenmeyer, D. Straile, B. Dong, R. Adrian, M. G. Allan, O. Anneville, L. Arvola, J. Austin, J. L. Bailey, J. S. Baron, J. D. Brookes, E. de Eyto, M. T. Dokulil, D. P. Hamilton, K. Havens, A. L. Hetherington, S. N. Higgins, S. Hook, L. R. Izmet'seva, K. D. Jöhnk, K. Kangur, P. Kasprzak, M. Kumagai, E. Kuusisto, G. Leshkevich, D. M. Livingstone, S. MacIntyre, L. May, J. M. Melack, D. C. Mueller-Navarra, M. Naumenko, P. Nöges, T. Nöges, R. P. North, P.-D. Plisnier, A. Rigosi, A. Rimmer, M. Rogora, L. G. Rudstam, J. A. Rusak, N. Salmaso, N. R. Samal, D. E. Schindler, S. G. Schladow, M. Schmid, S. R. Schmidt, E. Silow, M. E. Soylu, K. Teubner, P. Verburg, A. Voutilainen, A. Watkinson, C. E. Williamson, and G. Zhang. 2015. Rapid and highly variable warming of lake surface waters around the globe. *Geophysical Research Letters* 42: 10,773-710,781, doi:10.1002/2015gl066235
- Obrador, B., P. A. Staehr, and J. P. C. Christensen. 2014. Vertical patterns of metabolism in three contrasting stratified lakes. *Limnology and Oceanography* 59: 1228-1240, doi:10.4319/lo.2014.59.4.1228
- Padisák, J., and C. S. Reynolds. 2003. Shallow lakes: the absolute, the relative, the functional and the pragmatic. *Hydrobiologia* 506: 1-11, doi:10.1023/B:HYDR.0000008630.49527.29
- Paerl, H. W., and J. Huisman. 2009. Climate change: a catalyst for global expansion of harmful cyanobacterial blooms. *Environmental Microbiology Reports* 1: 27-37, doi:10.1111/j.1758-2229.2008.00004.x
- Page, T., P. J. Smith, K. J. Beven, I. D. Jones, J. A. Elliott, S. C. Maberly, E. B. Mackay, M. De Ville, and H. Feuchtmayr. 2018. Adaptive forecasting of phytoplankton communities. *Water Research* 134: 74-85, doi:10.1016/j.watres.2018.01.046
- Parker, W. S. 2010. Predicting weather and climate: Uncertainty, ensembles and probability. *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics* 41: 263-272, doi:10.1016/j.shpsb.2010.07.006
- Parker, W. S. 2013. Ensemble modeling, uncertainty and robust predictions. *WIREs Climate Change* 4: 213-223, doi:10.1002/wcc.220
- Patterson, J., P. Hamblin, and J. Imberger. 1984. Classification and dynamic simulation of the vertical density structure of lakes 1. *Limnology and Oceanography* 29: 845-861, doi:10.4319/lo.1984.29.4.0845
- Peeters, F., D. Finger, M. Hofer, M. Brennwald, D. M. Livingstone, and R. Kipfer. 2003. Deep-water renewal in Lake Issyk-Kul driven by differential cooling. *Limnology and Oceanography* 48: 1419-1431, doi:10.4319/lo.2003.48.4.1419
- Peeters, F., D. M. Livingstone, G.-H. Goudsmit, R. Kipfer, and R. Forster. 2002. Modeling 50 years of historical temperature profiles in a large central European lake. *Limnology and Oceanography* 47: 186-197, doi:10.4319/lo.2002.47.1.0186
- Perga, M. E., R. Bruel, L. Rodriguez, Y. Guénand, and D. Bouffard. 2018. Storm impacts on alpine lakes: antecedent weather conditions matter more than the event intensity. *Global Change Biology* 24: 5004-5016, doi:10.1111/gcb.14384
- Perroud, M., and S. Goyette. 2010. Impacts of warmer climate on Lake Geneva water-temperature profiles. *Boreal Environment Research* 15: 255-278.
- Persson, I., and I. D. Jones. 2008. The effect of water colour on lake hydrodynamics: a modelling study. *Freshwater Biology* 53: 2345-2355, doi:10.1111/j.1365-2427.2008.02049.x
- Pettersson, K., K. Grust, G. Weyhenmeyer, and T. Blenckner. 2003. Seasonality of chlorophyll and nutrients in Lake Erken—effects of weather conditions. *Hydrobiologia* 506: 75-81, doi:10.1023/B:HYDR.0000008582.61851.76
- Pilla, R. M., C. E. Williamson, B. V. Adamovich, R. Adrian, O. Anneville, S. Chandra, W. Colom-Montero, S. P. Devlin, M. A. Dix, M. T. Dokulil, E. E. Gaiser, S. F. Girdner, K. D. Hambright, D. P. Hamilton, K. Havens, D. O. Hessen, S. N. Higgins, T. H. Huttula, H. Huuskonen, P. D. F. Isles, K. D. Joehnk, I. D. Jones, W. B. Keller, L. B. Knoll, J. Korhonen, B. M. Kraemer, P. R. Leavitt, F. Lepori, M. S. Luger, S. C. Maberly, J. M. Melack, S. J. Melles, D. C. Muller-Navarra, D. C. Pierson, H. V. Pislegina, P. D. Plisnier, D. C. Richardson, A.

- Rimmer, M. Rogora, J. A. Rusak, S. Sadro, N. Salmaso, J. E. Saros, E. Saulnier-Talbot, D. E. Schindler, M. Schmid, S. V. Shimaraeva, E. A. Silow, L. M. Sitoki, R. Sommaruga, D. Straile, K. E. Strock, W. Thiery, M. A. Timofeyev, P. Verburg, R. D. Vinebrooke, G. A. Weyhenmeyer, and E. Zadereev. 2020. Deeper waters are changing less consistently than surface waters in a global analysis of 102 lakes. *Scientific Reports* 10: 20514, doi:10.1038/s41598-020-76873-x
- Pimm, S. L., I. Donohue, J. M. Montoya, and M. Loreau. 2019. Measuring resilience is essential to understand it. *Nature Sustainability* 2: 895-897, doi:10.1038/s41893-019-0399-7
- Plischke, E., E. Borgonovo, and C. L. Smith. 2013. Global sensitivity measures from given data. *European Journal of Operational Research* 226: 536-550, doi:10.1016/j.ejor.2012.11.047
- R Core Team. 2019. R: A language and environment for statistical computing. R Foundation for Statistical Computing.
- R Core Team. 2020. R: A language and environment for statistical computing. R Foundation for Statistical Computing.
- Ravens, T. M., O. Kocsis, A. Wüest, and N. Granin. 2000. Small-scale turbulence and vertical mixing in Lake Baikal. *Limnology and Oceanography* 45: 159-173, doi:10.4319/lo.2000.45.1.0159
- Read, J. S., C. Gries, E. K. Read, J. Klug, P. Hanson, M. R. Hipsey, E. Jennings, C. M. O'Reilly, L. A. Winslow, D. Pierson, C. McBride, and D. Hamilton. 2018. Generating community-built tools for data sharing and analysis in environmental networks. *Inland Waters* 6: 637-644, doi:10.1080/iw-6.4.889
- Read, J. S., D. P. Hamilton, I. D. Jones, K. Muraoka, L. A. Winslow, R. Kroiss, C. H. Wu, and E. Gaiser. 2011. Derivation of lake mixing and stratification indices from high-resolution lake buoy data. *Environmental Modelling & Software* 26: 1325-1336, doi:10.1016/j.envsoft.2011.05.006
- Read, J. S., and K. C. Rose. 2013. Physical responses of small temperate lakes to variation in dissolved organic carbon concentrations. *Limnology and Oceanography* 58: 921-931, doi:10.4319/lo.2013.58.3.0921
- Reichwaldt, E. S., and A. Ghadouani. 2012. Effects of rainfall patterns on toxic cyanobacterial blooms in a changing climate: between simplistic scenarios and complex dynamics. *Water Research* 46: 1372-1393, doi:10.1016/j.watres.2011.11.052
- Rey, J., G. Rohat, M. Perroud, S. Goyette, and J. Kasparian. 2020. Shifting velocity of temperature extremes under climate change. *Environmental Research Letters* 15, doi:10.1088/1748-9326/ab6c6f
- Reynolds, C., A. Irish, and J. Elliott. 2001. The ecological basis for simulating phytoplankton responses to environmental change (PROTECH). *Ecological Modelling* 140: 271-291, doi:10.1016/S0304-3800(01)00330-1
- Ridley, J. K., J. A. Lowe, and H. T. Hewitt. 2012. How reversible is sea ice loss? *The Cryosphere* 6: 193-198, doi:10.5194/tc-6-193-2012
- Riis, T., and K. Sand-Jensen. 1998. Development of vegetation and environmental conditions in an oligotrophic Danish lake over 40 years. *Freshwater Biology* 40: 123-134, doi:10.1046/j.1365-2427.1998.00338.x
- Rippey, B., and C. McSorley. 2009. Oxygen depletion in lake hypolimnia. *Limnology and Oceanography* 54: 905-916, doi:10.4319/lo.2009.54.3.0905
- Rodi, W. 1980. Turbulence models and their application in hydraulics - A state-of-the-art review. CRC Press.
- Rousoo, B. Z., E. Bertone, R. Stewart, and D. P. Hamilton. 2020. A systematic literature review of forecasting and predictive models for cyanobacteria blooms in freshwater lakes. *Water Research* 182: 115959, doi:10.1016/j.watres.2020.115959
- Sachse, R., T. Petzoldt, M. Blumstock, S. Moreira, M. Pätzig, J. Rücker, J. H. Janse, W. M. Mooij, and S. Hilt. 2014. Extending one-dimensional models for deep lakes to simulate the impact of submerged macrophytes on water quality. *Environmental Modelling & Software* 61: 410-423, doi:10.1016/j.envsoft.2014.05.023
- Sahoo, G. B., and S. G. Schladow. 2008. Impacts of climate change on lakes and reservoirs dynamics and restoration policies. *Sustainability Science* 3: 189-199, doi:10.1007/s11625-008-0056-y
- Sahoo, G. B., S. G. Schladow, J. E. Reuter, R. Coats, M. Dettinger, J. Riverson, B. Wolfe, and M. Costa-Cabral. 2013. The response of Lake Tahoe to climate change. *Climatic Change* 116: 71-95, doi:10.1007/s10584-012-0600-8
- Sainsbury, N. C., M. J. Genner, G. R. Saville, J. K. Pinnegar, C. K. O'Neill, S. D. Simpson, and R. A. Turner. 2018. Changing storminess and global capture fisheries. *Nature Climate Change* 8: 655-659, doi:10.1038/s41558-018-0206-x
- Salmaso, N. 2005. Effects of climatic fluctuations and vertical mixing on the interannual trophic variability of Lake Garda, Italy. *Limnology and Oceanography* 50: 553-565, doi:10.4319/lo.2005.50.2.0553
- Saloranta, T. M., and T. Andersen. 2007. MyLake—A multi-year lake simulation model code suitable for uncertainty and sensitivity analysis simulations. *Ecological Modelling* 207: 45-60, doi:10.1016/j.ecolmodel.2007.03.018

- Saloranta, T. M., M. Forsius, M. Järvinen, and L. Arvola. 2009. Impacts of projected climate change on the thermodynamics of a shallow and a deep lake in Finland: model simulations and Bayesian uncertainty analysis. *Hydrology Research* 40: 234-248, doi:10.2166/nh.2009.030
- Saulnier-Talbot, É., I. Gregory-Eaves, K. G. Simpson, J. Efitre, T. E. Nowlan, Z. E. Taranu, and L. J. Chapman. 2014. Small changes in climate can profoundly alter the dynamics and ecosystem services of tropical crater lakes. *PLoS one* 9: e86561, doi:10.1371/journal.pone.0086561
- Scheffer, M. 1998. *Ecology of Shallow Lakes*. Chapman & Hall.
- Scheffer, M., S. Carpenter, J. A. Foley, C. Folke, and B. Walker. 2001. Catastrophic shifts in ecosystems. *Nature* 413: 591-596, doi:10.1038/35098000
- Schmid, M., K. Tietze, M. Halbwachs, A. Lorke, D. F. McGinnis, and A. Wüest. 2002. The volcanic risk-How hazardous is the gas accumulation in Lake Kivu? Arguments for a risk assesment in light of the Nyiragongo Volcano eruption of 2002. *Acta Vulcanologica* 14: 115-122, doi:10.1400/19084
- Schmidt, W. 1928. Über die Temperatur- und Stabilitätsverhältnisse Von Seen. *Geografiska Annaler* 10: 145-177, doi:10.1080/20014422.1928.11880475
- Schultze, M., B. Boehrer, K. Wendt-Potthoff, S. Katsev, and E. T. Brown. 2017. Chemical Setting and Biogeochemical Reactions in Meromictic Lakes, p. 35-59. *In* R. D. Gulati, E. S. Zadereev and A. G. Degermendzhi [eds.], *Ecology of Meromictic Lakes*. Springer.
- Schwefel, R., A. Gaudard, A. Wüest, and D. Bouffard. 2016. Effects of climate change on deepwater oxygen and winter mixing in a deep lake (Lake Geneva): Comparing observational findings and modeling. *Water Resources Research* 52: 8811-8826, doi:10.1002/2016WR019194
- Schwefel, R., B. Müller, H. Boisgontier, and A. Wüest. 2019. Global warming affects nutrient upwelling in deep lakes. *Aquatic Sciences* 81: 50, doi:10.1007/s00027-019-0637-0
- Schwefel, R., T. Steinsberger, D. Bouffard, L. D. Bryant, B. Müller, and A. Wüest. 2018. Using small-scale measurements to estimate hypolimnetic oxygen depletion in a deep lake. *Limnology and Oceanography* 63: S54-S67, doi:10.1002/lno.10723
- Seneviratne, S., N. Nicholls, D. Easterling, C. Goodess, S. Kanae, J. Kossin, Y. Luo, J. Marengo, K. McInnes, M. Rahimi, M. Reichstein, A. Sorteberg, C. Vera, and X. Zhang. 2012. Changes in climate extremes and their impacts on the natural physical environment, p. 109-230. *In* C. B. Field et al. [eds.], *Managing the Risks of Extreme Events and Disasters to Advance Climate Change Adaptation*.
- Šeparović, L., A. Alexandru, R. Laprise, A. Martynov, L. Sushama, K. Winger, K. Tete, and M. Valin. 2013. Present climate and climate change over North America as simulated by the fifth-generation Canadian regional climate model. *Climate Dynamics* 41: 3167-3201, doi:10.1007/s00382-013-1737-5
- Sharma, S., K. Blagrove, J. J. Magnuson, C. M. O'Reilly, S. Oliver, R. D. Batt, M. R. Magee, D. Straile, G. A. Weyhenmeyer, L. Winslow, and R. I. Woolway. 2019. Widespread loss of lake ice around the Northern Hemisphere in a warming world. *Nature Climate Change* 9: 227-231, doi:10.1038/s41558-018-0393-5
- Shatwell, T., R. Adrian, and G. Kirillin. 2016. Planktonic events may cause polymictic-dimictic regime shifts in temperate lakes. *Scientific Reports* 6: 24361, doi:10.1038/srep24361
- Shatwell, T., W. Thiery, and G. Kirillin. 2019. Future projections of temperature and mixing regime of European temperate lakes. *Hydrology and Earth System Sciences* 23: 1533-1551, doi:10.5194/hess-23-1533-2019
- Shimoda, Y., and G. B. Arhonditsis. 2016. Phytoplankton functional type modelling: Running before we can walk? A critical evaluation of the current state of knowledge. *Ecological Modelling* 320: 29-43, doi:10.1016/j.ecolmodel.2015.08.029
- Shimoda, Y., M. E. Azim, G. Perhar, M. Ramin, M. A. Kenney, S. Sadraddini, A. Gudimov, and G. B. Arhonditsis. 2011. Our current understanding of lake ecosystem response to climate change: What have we really learned from the north temperate deep lakes? *Journal of Great Lakes Research* 37: 173-193, doi:10.1016/j.jglr.2010.10.004
- Shrestha, A., M. B. Green, J. N. Boyer, and L. A. Doner. 2020. Effects of Storm Events on Phosphorus Concentrations in a Forested New England Stream. *Water, Air, & Soil Pollution* 231: 376, doi:10.1007/s11270-020-04738-0
- Soares, L. M. V., T. F. d. G. Silva, B. Vinçon-Leite, J. C. Eleutério, L. C. d. Lima, and N. d. O. Nascimento. 2019. Modelling drought impacts on the hydrodynamics of a tropical water supply reservoir. *Inland Waters* 9: 422-437, doi:10.1080/20442041.2019.1596015
- Soetaert, K., and P. M. Herman. 2008. *A practical guide to ecological modelling: using R as a simulation platform*. Springer Science & Business Media.
- Soetaert, K., and T. Petzoldt. 2010. Inverse Modelling, Sensitivity and Monte Carlo Analysis in R Using Package FME. *Journal of Statistical Software* 33: 1-28, doi: 10.18637/jss.v033.i03

- Sommer, U., R. Adrian, L. De Senerpont Domis, J. J. Elser, U. Gaedke, B. Ibelings, E. Jeppesen, M. Lürling, J. C. Molinero, W. M. Mooij, E. van Donk, and M. Winder. 2012. Beyond the Plankton Ecology Group (PEG) Model: Mechanisms Driving Plankton Succession. *Annual Review of Ecology, Evolution, and Systematics* 43: 429-448, doi:10.1146/annurev-ecolsys-110411-160251
- Søndergaard, M., J. P. Jensen, and E. Jeppesen. 2003. Role of sediment and internal loading of phosphorus in shallow lakes. *Hydrobiologia* 506: 135-145, doi:10.1023/B:HYDR.0000008611.12704.dd
- Soranno, P. A., S. R. Carpenter, and R. C. Lathrop. 1997. Internal phosphorus loading in Lake Mendota: response to external loads and weather. *Canadian Journal of Fisheries and Aquatic Sciences* 54: 1883-1893, doi:10.1139/f97-095
- Soullignac, F., P.-A. Danis, D. Bouffard, V. Chanudet, E. Dambrine, Y. Guénand, T. Harmel, B. W. Ibelings, D. Trevisan, R. Uittenbogaard, and O. Anneville. 2018. Using 3D modeling and remote sensing capabilities for a better understanding of spatio-temporal heterogeneities of phytoplankton abundance in large lakes. *Journal of Great Lakes Research* 44: 756-764, doi:10.1016/j.jglr.2018.05.008
- Spigel, R. H., and J. Imberger. 1980. The classification of mixed-layer dynamics of lakes of small to medium size. *Journal of Physical Oceanography* 10: 1104-1121, doi:10.1175/1520-0485(1980)010<1104:TCOMLD>2.0.CO;2
- Spigel, R. H., J. Imberger, and K. N. Rayner. 1986. Modeling the diurnal mixed layer. *Limnology and Oceanography* 31: 533-556, doi:10.4319/lo.1986.31.3.0533.
- Stelzer, J. A. A., J. P. Mesman, R. Adrian, A. S. Gsell, L. N. De Senerpont Domis, P. M. Visser, and B. W. Ibelings. in preparation. The effects of eutrophication on the phytoplankton responses to repeated pulse perturbations.
- Stelzer, J. A. A., J. P. Mesman, R. Adrian, and B. W. Ibelings. 2021. Early warning signals of regime shifts for aquatic systems: Can experiments help to bridge the gap between theory and real-world application? *Ecological Complexity* 47: 100944, doi:10.1016/j.ecocom.2021.100944
- Stepanenko, V. M., S. Goyette, A. Martynov, M. Perroud, X. Fang, and D. Mironov. 2010. First steps of a Lake Model intercomparison project: LakeMIP. *Boreal Environment Research* 15: 191-202.
- Stepanenko, V. M., A. Martynov, K. D. Jöhnk, Z. M. Subin, M. Perroud, X. Fang, F. Beyrich, D. Mironov, and S. Goyette. 2013. A one-dimensional model intercomparison study of thermal regime of a shallow, turbid midlatitude lake. *Geoscientific Model Development* 6: 1337-1352, doi:10.5194/gmd-6-1337-2013
- Stepanenko, V. M., G. Valerio, and M. Pilotti. 2020. Horizontal Pressure Gradient Parameterization for One-Dimensional Lake Models. *Journal of Advances in Modeling Earth Systems* 12, doi:10.1029/2019ms001906
- Stetler, J. T., S. Girdner, J. Mack, L. A. Winslow, T. H. Leach, and K. C. Rose. 2021. Atmospheric stilling and warming air temperatures drive long-term changes in lake stratification in a large oligotrophic lake. *Limnology and Oceanography* 66: 954-964, doi:10.1002/lno.11654
- Stockwell, J. D., J. P. Doubek, R. Adrian, O. Anneville, C. C. Carey, L. Carvalho, L. N. De Senerpont Domis, G. Dur, M. A. Frassl, H. P. Grossart, B. W. Ibelings, M. J. Lajeunesse, A. M. Lewandowska, M. E. Llames, S. S. Matsuzaki, E. R. Nodine, P. Noges, V. P. Patil, F. Pomati, K. Rinke, L. G. Rudstam, J. A. Rusak, N. Salmaso, C. T. Seltmann, D. Straile, S. J. Thackeray, W. Thiery, P. Urrutia-Cordero, P. Venail, P. Verburg, R. I. Woolway, T. Zohary, M. R. Andersen, R. Bhattacharya, J. Hejzlar, N. Janatian, A. Kpodonu, T. J. Williamson, and H. L. Wilson. 2020. Storm impacts on phytoplankton community dynamics in lakes. *Global Change Biology* 26: 2756-2784, doi:10.1111/gcb.15033
- Straile, D., K. Jöhnk, and R. Henno. 2003. Complex effects of winter warming on the physicochemical characteristics of a deep lake. *Limnology and Oceanography* 48: 1432-1438, doi:10.4319/lo.2003.48.4.1432
- Sugiyama, N., S. Kravtsov, and P. Roebber. 2017. Multiple climate regimes in an idealized lake-ice-atmosphere model. *Climate Dynamics* 50: 655-676, doi:10.1007/s00382-017-3633-x
- Tadonlélé, R. D. 2010. Evidence of warming effects on phytoplankton productivity rates and their dependence on eutrophication status. *Limnology and Oceanography* 55: 973-982, doi:10.4319/lo.2010.55.3.0973
- Tanentzap, A. J., N. D. Yan, B. Keller, R. Girard, J. Heneberry, J. M. Gunn, D. P. Hamilton, and P. A. Taylor. 2008. Cooling lakes while the world warms: Effects of forest regrowth and increased dissolved organic matter on the thermal regime of a temperate, urban lake. *Limnology and Oceanography* 53: 404-410, doi:10.4319/lo.2008.53.1.0404
- Thayne, M. W., B. M. Kraemer, J. P. Mesman, B. W. Ibelings, and R. Adrian. 2021. Antecedent lake conditions shape resistance and resilience of a shallow lake ecosystem following extreme wind storms. *Limnology and Oceanography*, doi:10.1002/lno.11859

- Thiery, W. I. M., V. M. Stepanenko, X. Fang, K. D. Jöhnk, Z. Li, A. Martynov, M. Perroud, Z. M. Subin, F. Darchambeau, D. Mironov, and N. P. M. Van Lipzig. 2014. LakeMIP Kivu: evaluating the representation of a large, deep tropical lake by a set of one-dimensional lake models. *Tellus A: Dynamic Meteorology and Oceanography* 66, doi:10.3402/tellusa.v66.21390
- Thomas, R. Q., R. J. Figueiredo, V. Daneshmand, B. J. Bookout, L. K. Puckett, and C. C. Carey. 2020. A Near-Term Iterative Forecasting System Successfully Predicts Reservoir Hydrodynamics and Partitions Uncertainty in Real Time. *Water Resources Research* 56, doi:10.1029/2019wr026138
- Tilahun, S., and D. Kifle. 2019. The influence of El Niño-induced drought on cyanobacterial community structure in a shallow tropical reservoir (Koka Reservoir, Ethiopia). *Aquatic Ecology* 53: 61–77, doi:10.1007/s10452-019-09673-9
- Till, A., A. L. Rypel, A. Bray, and S. B. Fey. 2019. Fish die-offs are concurrent with thermal extremes in north temperate lakes. *Nature Climate Change* 9: 637–641, doi:10.1038/s41558-019-0520-y
- Todini, E. 2004. Role and treatment of uncertainty in real-time flood forecasting. *Hydrological Processes* 18: 2743–2746, doi:10.1002/hyp.5687
- Trolle, D., J. A. Elliott, W. M. Mooij, J. H. Janse, K. Bolding, D. P. Hamilton, and E. Jeppesen. 2014. Advancing projections of phytoplankton responses to climate change through ensemble modelling. *Environmental Modelling & Software* 61: 371–379, doi:10.1016/j.envsoft.2014.01.032
- Trombetta, T., F. Vidussi, S. Mas, D. Parin, M. Simier, and B. Mostajir. 2019. Water temperature drives phytoplankton blooms in coastal waters. *PLoS one* 14: e0214933, doi:10.1371/journal.pone.0214933
- Umlauf, L., H. Burchard, and K. Bolding. 2005. GOTM: Sourcecode and Test Case Documentation.
- Ummenhofer, C. C., and G. A. Meehl. 2017. Extreme weather and climate events with ecological relevance: a review. *Phil. Trans. R. Soc. B* 372: 20160135, doi:10.1098/rstb.2016.0135
- Urrutia-Cordero, P., H. Zhang, F. Chaguaceda, H. Geng, and L. A. Hansson. 2020. Climate warming and heat waves alter harmful cyanobacterial blooms along the benthic–pelagic interface. *Ecology* 101: e03025, doi:10.1002/ecy.3025
- Vachon, D., T. Langenegger, D. Donis, and D. F. McGinnis. 2019. Influence of water column stratification and mixing patterns on the fate of methane produced in deep sediments of a small eutrophic lake. *Limnology and Oceanography* 64: 2114–2128, doi:10.1002/lno.11172
- Van de Pol, M., S. Jenouvrier, J. H. C. Cornelissen, and M. E. Visser. 2017. Behavioural, ecological and evolutionary responses to extreme climatic events: challenges and directions. *Phil. Trans. R. Soc. B* 372, doi:10.1098/rstb.2016.0134
- Van Meerbeek, K., T. Jucker, J. C. Svenning, and I. Stott. 2021. Unifying the concepts of stability and resilience in ecology. *Journal of Ecology*, doi:10.1111/1365-2745.13651
- van Vliet, M. T. H., M. Flörke, J. A. Harrison, N. Hofstra, V. Keller, F. Ludwig, J. E. Spanier, M. Stokal, Y. Wada, Y. Wen, and R. J. Williams. 2019. Model inter-comparison design for large-scale water quality models. *Current Opinion in Environmental Sustainability* 36: 59–67, doi:10.1016/j.cosust.2018.10.013
- Vanderkelen, I., N. P. M. Lipzig, D. M. Lawrence, B. Droppers, M. Golub, S. N. Gosling, A. B. G. Janssen, R. Marcé, H. M. Schmied, M. Perroud, D. Pierson, Y. Pokhrel, Y. Satoh, J. Schewe, S. I. Seneviratne, V. M. Stepanenko, Z. Tan, R. I. Woolway, and W. Thiery. 2020. Global Heat Uptake by Inland Waters. *Geophysical Research Letters* 47: e2020GL087867, doi:10.1029/2020gl087867
- Vannitsem, S., J. B. Bremnes, J. Demayer, G. R. Evans, J. Flowerdew, S. Hemri, S. Lerch, N. Roberts, S. Theis, A. Atencia, Z. Ben Bouallègue, J. Bhend, M. Dabernig, L. De Cruz, L. Hieta, O. Mestre, L. Moret, I. O. Plenković, M. Schmeits, M. Taillardat, J. Van den Bergh, B. Van Schaeybroeck, K. Whan, and J. Ylhäisi. 2021. Statistical Postprocessing for Weather Forecasts: Review, Challenges, and Avenues in a Big Data World. *Bulletin of the American Meteorological Society* 102: E681–E699, doi:10.1175/bams-d-19-0308.1
- Veraart, A. J., E. J. Faassen, V. Dakos, E. H. van Nes, M. Lurling, and M. Scheffer. 2011. Recovery rates reflect distance to a tipping point in a living system. *Nature* 481: 357–359, doi:10.1038/nature10723
- Visser, P., B. Ibelings, B. Van Der Veer, J. Koedood, and L. Mur. 1996. Artificial mixing prevents nuisance blooms of the cyanobacterium *Microcystis* in Lake Nieuwe Meer, the Netherlands. *Freshwater Biology* 36: 435–450, doi:10.1046/j.1365-2427.1996.00093.x
- Vörös, M., V. Istvanovics, and T. Weidinger. 2010. Applicability of the FLake model to Lake Balaton. *Boreal Environment Research* 15: 245–254.
- Vrede, K., T. Vrede, A. Isaksson, and A. Karlsson. 1999. Effects of nutrients (phosphorous, nitrogen, and carbon) and zooplankton on bacterioplankton and phytoplankton—a seasonal study. *Limnology and Oceanography* 44: 1616–1624, doi:10.4319/lo.1999.44.7.1616

- Weber, M., K. Rinke, M. R. Hipsey, and B. Boehrer. 2017. Optimizing withdrawal from drinking water reservoirs to reduce downstream temperature pollution and reservoir hypoxia. *Journal of Environmental Management* 197: 96-105, doi:10.1016/j.jenvman.2017.03.020
- Wetzel, R. G. 2001. *Limnology: lake and river ecosystems*. gulf professional publishing.
- Weyhenmeyer, G. A., T. Blenckner, and K. Pettersson. 1999. Changes of the plankton spring outburst related to the North Atlantic Oscillation. *Limnology and Oceanography* 44: 1788-1792, doi:10.4319/lo.1999.44.7.1788
- Weyhenmeyer, G. A., E. Willén, and L. Sonesten. 2004. Effects of an extreme precipitation event on water chemistry and phytoplankton in the Swedish Lake Mälaren. *Boreal Environment Research* 9: 409-420.
- Whitt, D. B., M. Lévy, and J. R. Taylor. 2019. Submesoscales Enhance Storm-Driven Vertical Mixing of Nutrients: Insights From a Biogeochemical Large Eddy Simulation. *Journal of Geophysical Research: Oceans* 124: 8140-8165, doi:10.1029/2019jc015370
- Wickham, H. 2016. *ggplot2: Elegant Graphics for Data Analysis*. Springer-Verlag.
- Wickham, H., J. Hester, and W. Chang. 2020. *devtools: Tools to Make Developing R Packages Easier*. R package version 2.3.0.
- Wilhelm, S., and R. Adrian. 2008. Impact of summer warming on the thermal characteristics of a polymictic lake and consequences for oxygen, nutrients and phytoplankton. *Freshwater Biology* 53: 226-237, doi:10.1111/j.1365-2427.2007.01887.x
- Wilhelm, S., T. Hintze, D. M. Livingstone, and R. Adrian. 2006. Long-term response of daily epilimnetic temperature extrema to climate forcing. *Canadian Journal of Fisheries and Aquatic Sciences* 63: 2467-2477, doi:10.1139/F06-140
- Wilson, H. L., A. I. Ayala, I. D. Jones, A. Rolston, D. Pierson, E. de Eyto, H.-P. Grossart, M.-E. Perga, R. I. Woolway, and E. Jennings. 2020. Variability in epilimnion depth estimations in lakes. *Hydrology and Earth System Sciences* 24: 5559-5577, doi:10.5194/hess-24-5559-2020
- Winder, M., and D. A. Hunter. 2008. Temporal organization of phytoplankton communities linked to physical forcing. *Oecologia* 156: 179-192, doi:10.1007/s00442-008-0964-7
- Winder, M., and U. Sommer. 2012. Phytoplankton response to a changing climate. *Hydrobiologia* 698: 5-16, doi:10.1007/s10750-012-1149-2
- Winslow, L. A., J. S. Read, R. I. Woolway, J. A. Brentrup, T. Leach, J. Zwart, S. Albers, and D. Collinge. 2019. *rLakeAnalyzer: Lake Physics Tools*. R package version 1.11.4.1.
- Winslow, L. A., J. A. Zwart, R. D. Batt, H. A. Dugan, R. I. Woolway, J. R. Corman, P. C. Hanson, and J. S. Read. 2016. *LakeMetabolizer: an R package for estimating lake metabolism from free-water oxygen using diverse statistical models*. *Inland Waters* 6: 622-636, doi:10.1080/iw-6.4.883
- Woolway, R. I., E. Jennings, and L. Carrea. 2020. Impact of the 2018 European heatwave on lake surface water temperature. *Inland Waters* 10: 322-332, doi:10.1080/20442041.2020.1712180
- Woolway, R. I., and C. J. Merchant. 2018. Intralake Heterogeneity of Thermal Responses to Climate Change: A Study of Large Northern Hemisphere Lakes. *Journal of Geophysical Research: Atmospheres* 123: 3087-3098, doi:10.1002/2017jd027661
- Woolway, R. I., and C. J. Merchant. 2019. Worldwide alteration of lake mixing regimes in response to climate change. *Nature Geoscience* 12: 271-276, doi:10.1038/s41561-019-0322-x
- Woolway, R. I., C. J. Merchant, J. Van Den Hoek, C. Azorin-Molina, P. Nöges, A. Laas, E. B. Mackay, and I. D. Jones. 2019. Northern Hemisphere Atmospheric Stilling Accelerates Lake Thermal Responses to a Warming World. *Geophysical Research Letters* 46: 11983-11992, doi:10.1029/2019gl082752
- Woolway, R. I., S. Sharma, G. A. Weyhenmeyer, A. Debolskiy, M. Golub, D. Mercado-Bettín, M. Perroud, V. Stepanenko, Z. Tan, L. Grant, R. Ladwig, J. Mesman, T. N. Moore, T. Shatwell, I. Vanderkelen, J. A. Austin, C. L. DeGasperi, M. Dokulil, S. La Fuente, E. B. Mackay, S. G. Schladow, S. Watanabe, R. Marcé, D. C. Pierson, W. Thiery, and E. Jennings. 2021. Phenological shifts in lake stratification under climate change. *Nature Communications* 12: 2318, doi:10.1038/s41467-021-22657-4
- Wright, M. N., and A. Ziegler. 2017. *ranger: A Fast Implementation of Random Forests for High Dimensional Data in C++ and R*. 77: 17, doi:10.18637/jss.v077.i01
- Wright, R. F. 1983. Input-output budgets at Langtjern, a small acidified lake in southern Norway. *Hydrobiologia* 101: 1-12, doi:10.1007/BF00008651
- Wu, W., R. Emerton, Q. Duan, A. W. Wood, F. Wetterhall, and D. E. Robertson. 2020. Ensemble flood forecasting: Current status and future opportunities. *WIREs Water* 7: e1432, doi:10.1002/wat2.1432
- Wüest, A., D. Bouffard, J. Guillard, B. W. Ibelings, S. Lavanchy, M. E. Perga, and N. Pasche. 2021. LÉXPLORE: A floating laboratory on Lake Geneva offering unique lake research opportunities. *WIREs Water* 8: e1544, doi:10.1002/wat2.1544

- Wüest, A., G. Piepke, and D. C. Van Senden. 2000. Turbulent kinetic energy balance as a tool for estimating vertical diffusivity in wind-forced stratified waters. *Limnology and Oceanography* 45: 1388-1400, doi:10.4319/lo.2000.45.6.1388
- Yang, Y., W. Colom, D. Pierson, and K. Pettersson. 2016a. Water column stability and summer phytoplankton dynamics in a temperate lake (Lake Erken, Sweden). *Inland Waters* 6: 499-508, doi:10.1080/IW-6.4.874
- Yang, Y., K. Pettersson, and J. Padisák. 2016b. Repetitive baselines of phytoplankton succession in an unstably stratified temperate lake (Lake Erken, Sweden): a long-term analysis. *Hydrobiologia* 764: 211-227, doi:10.1007/s10750-015-2314-1
- Yankova, Y., S. Neuenschwander, O. Koster, and T. Posch. 2017. Abrupt stop of deep water turnover with lake warming: Drastic consequences for algal primary producers. *Scientific Reports* 7: 13770, doi:10.1038/s41598-017-13159-9
- Yao, H., N. R. Samal, K. D. Jöhnk, X. Fang, L. C. Bruce, D. C. Pierson, J. A. Rusak, and A. James. 2014. Comparing ice and temperature simulations by four dynamic lake models in Harp Lake: past performance and future predictions. *Hydrological Processes* 28: 4587-4601, doi:10.1002/hyp.10180
- Ye, S., M. Sivapalan, and Q. Ran. 2020. Synergistic Impacts of Rainfall Variability and Land Use Heterogeneity on Nitrate Retention in River Networks: Exacerbation or Compensation? *Water Resources Research* 56, doi:10.1029/2018wr024226
- Ye, X., E. J. Anderson, P. Y. Chu, C. Huang, and P. Xue. 2019. Impact of Water Mixing and Ice Formation on the Warming of Lake Superior: A Model-guided Mechanism Study. *Limnology and Oceanography* 64: 558-574, doi:10.1002/lno.11059
- Zhan, Q., C. N. Stratmann, H. G. Van der Geest, A. J. Veraart, K. Brenzinger, M. Lürling, and L. N. De Senerpont Domis. under review. Effectiveness of phosphorus control under extreme heatwaves: implications for sediment nutrient releases and greenhouse gas emissions. *Biogeochemistry*.
- Zhong, Y., M. Notaro, S. J. Vavrus, and M. J. Foster. 2016. Recent accelerated warming of the Laurentian Great Lakes: Physical drivers. *Limnology and Oceanography* 61: 1762-1786, doi:10.1002/lno.10331
- Zohary, T., and I. Ostrovsky. 2011. Ecological impacts of excessive water level fluctuations in stratified freshwater lakes. *Inland Waters* 1: 47-59, doi:10.5268/iw-1.1.406