

Improving algal bloom modelling for lake management using remote sensing and process-based modelling approaches

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Abstract

Freshwater ecosystems are increasingly threatened by eutrophication and harmful algal blooms, which negatively impact water quality and security. As freshwater availability declines globally, the need for effective monitoring and forecasting systems becomes more urgent. In the face of climate change, algal blooms are projected to increase in bloom frequency and severity through rising temperatures and altered hydrological cycles. Current monitoring approaches, based on in situ sampling and sensors, are accurate but resource-intensive and rarely provide forecasting capabilities. Forecast models, while potentially useful for proactive water management, are often limited by data availability due to low frequency or inconsistent datasets. Remote sensing offers a scalable, cost-effective alternative for chlorophyll-a monitoring, a proxy for algal biomass, but its integration into operational forecasting remains limited due to data quality concerns and methodological challenges. This thesis investigates how we can use and advance algal bloom modelling techniques for water management under present and future climate conditions. It aims to incorporate existing data sources, such as remote sensing, to enhance process-based model calibration and improve the forecasting of algal blooms. Through three data-driven chapters, we explore the roles of data availability, remote sensing data, and model transferability in forecasting chl-a concentrations and bloom events across UK waterbodies.

In Chapter 2, the relative importance of different input data for model calibration and bloom detection is assessed. Demonstrating high-frequency calibration data to improve predictions across the full chl-a spectrum, while high-frequency meteorological data are particularly critical for detecting bloom events.

Chapter 3 focuses on improving model calibration with remote sensing data as a supplement to in situ monitoring. Showing that remote sensing can significantly enhance chl-a forecasts and bloom detection when subjected to robust quality filtering. Highlighting the potential for remote sensing data to improve model output and make calibration available in water bodies with low data availability. A novel, easy-to-implement quality control approach is introduced using conformal prediction to improve the reliability of satellite-derived inputs.

Chapter 4 evaluates climate change impacts on three UK waterbodies using high-frequency calibrated models. By spatially relocating models across a latitudinal gradient, it is shown that northern reservoirs are likely to experience the greatest increases in chl-a under all climate scenarios. This novel approach provides a unique opportunity to explore how latitude,

local waterbody characteristics, and climate interact to influence bloom dynamics across the UK. These findings underscore the importance of tailoring mitigation strategies to both geographic location and waterbody type.

Together, the data chapters demonstrate that reliable forecasts of algal blooms can be achieved across different water body types and data frequencies, advancing our understanding of how data quantity and quality influence model performance. The results show that satellite Earth observation data can effectively support the calibration of lake ecosystem models, enabling their application in systems where in situ monitoring is currently limited or absent. By integrating remote sensing with process-based models, this approach offers a scalable and cost-effective way to fill data gaps while preserving site-specific characteristics. The modelling framework also proves valuable for exploring the effects of climate change on bloom dynamics across diverse lakes and regions, highlighting its broader utility for water management. Strengthening these tools will aid in building climate resilience across freshwater management systems.

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List of common abbreviations

- **ACOLITE:** Atmospheric Correction for OLI ‘lite’
- **Chl-a:** Chlorophyll-a
- **CP:** Conformal Prediction
- **CV:** coefficient of variation
- **C2RCC:** Case 2 Regional CoastColour (atmospheric correction)
- **EO:** Earth Observation
- **GCM:** Global Climate Models
- **GLM-AED:** General Lake Model - AquaticEcodynamics
- **LWBC:** Latitude Waterbody Combination
- **MAE:** Mean Absolute Error
- **MdSA:** Median Symmetric Accuracy
- **MSI:** Multi Spectral Imagery
- **NC:** Non-conformity
- **OWT:** Optical Water Type
- **Polymer:** POLYnomial-based approach of MERIS data (atmospheric correction)
- **RCP:** Representative Concentration Pathways
- **SSP:** Shared Socioeconomic Pathways
- **SSPB:** Symmetric Signed Percentage Bias
- **S2:** Sentinel 2 satellite constellation

Statement of original authorship

I certify that the work contained within this thesis, including text, figures and tables, is my own, except where specifically stated. The thesis has been composed by me and has not previously been accepted for a degree or professional qualification.

Date: 04-07-2025

Signature:

X 
Maud Siebers

Declarations

During the preparation of this work the author used Chat-GPT to improve language clarity and sentence structure. After using this tool/service, the author reviewed and edited the content as needed and takes full responsibility for the content of the publication.

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The version presented in this thesis reflects the manuscript published. To maintain consistency with the other chapters, an additional appendix B has been included, providing details on model validation and calibration, as referenced in the main text.

Chapter 1: General introduction

Only 2.5% of the world's water is freshwater, and of this only 0.3 % is readily available in surface waterbodies. The rest of it locked up in glaciers and permanent snow or found deep underground. Despite its scarcity, global water use amounts to about 28 km³ per day, most of which is freshwater, and demand is still growing (Mittermeier et al., 2010).

These scarce freshwater bodies provide essential ecosystem services (Paetzold et al., 2010; Rinke et al., 2019) like provision of food and water for fishing (McIntyre et al., 2016), drinking water, irrigation and energy (Van Vliet et al., 2017) and cultural purposes like recreation, aesthetic and educational (Millennium Ecosystem Assessment, 2005).

Furthermore, these systems support and regulate ecosystem services like habitat provision, primary production and nutrient cycling which are crucial for nature preservation and therefore critical for survival of all life forms (Millennium Ecosystem Assessment, 2005; Mittermeier et al., 2010). Moreover, lakes and rivers are among the freshwater systems that provide the most ecosystem services (17 out of 19 described ecosystem services) listed in Mittermeier et al., (2010). These are a few of the many reasons why freshwater bodies are invaluable to the world and why keeping their water quality high is important.

Despite their importance and scarcity, the value of these freshwater resources is increasingly undermined by deteriorating water quality and loss of biodiversity. Freshwater systems are experiencing the most significant loss of biodiversity worldwide, despite covering a small portion of the Earth's surface. These habitats are home to about one-third of all vertebrate species and around 10% of all known species (Dudgeon et al., 2006; Reid et al., 2019; Strayer & Dudgeon, 2010; Tickner et al., 2020). Furthermore, a variety of environmental pressures disrupts freshwater systems, preventing them from sustaining nutrient cycles and ecological balance, many of which are driven by human activities. These cumulative impacts pose even more serious threats to these ecosystems (Bănăduc et al., 2024).

In Europe, key threats include nutrient loading, chemical pollution, and habitat degradation caused by physical alterations to water bodies (European Environment Agency et al., 2018).

Among these, nutrient loading is of particular concern due to its direct role in triggering algal blooms, which are one of the most visible and disruptive manifestations of freshwater degradation (Wurtsbaugh et al., 2019). Harmful algal blooms can deplete oxygen, release toxins, and cause widespread ecological and economic harm (Merel et al., 2013). Satellite observations have shown that harmful algal blooms affected 11.7% of global lake area between 1982 and 2019 (Hou et al., 2022), underscoring their widespread impact. Compared to other stressors, algal blooms represent an acute, dynamic threat that directly impairs water use, biodiversity, and ecosystem stability. Moreover, algal blooms have already been growing in frequency and severity over the past decades, highlighting the urgency of addressing this issue (Fang et al., 2022; Ho et al., 2019; Hou et al., 2022; Kraemer et al., 2022).

1.1 Algal blooms

Algal blooms consist of phytoplankton, which are microscopic, photosynthetic organisms floating in the water column. Different groups of phytoplankton exist including diatoms, cyanobacteria, dinoflagellates, green algae and cryptophytes and can occur in both freshwater and marine environments. A rapid increase in the growth and accumulation of algae in a waterbody is called an algal bloom. These blooms are often visible as green, red, or brown discoloration of the water surface depending on the dominant taxa. Despite algal growth being a natural phenomenon in freshwater ecosystems, blooms more typically signify a substantial ecological imbalance as a result from excessive nutrient enrichment and disrupt the normal functioning of the ecosystem.

1.1.1 Formation of algal blooms

Human activities increase nutrient loading to water bodies, which is called cultural eutrophication (Wurtsbaugh et al., 2019). Nitrogen (N) and phosphorus (P) are essential components of algal biomass, while silica (Si) plays a key role in supporting diatom growth. Nutrient bioavailability is crucial, as the effects of eutrophication may be minimal if N or P cannot be taken up by the algae (Glibert, 2017). Several distinct stages of eutrophication exist which influence the abundance of algae in a waterbody. The oligotrophic state, characterised by low nutrient levels, clear water, and relatively low biological activity could be disrupted by a nutrient increase shifting the waterbody into a mesotrophic phase. The mesotrophic phase has algal growth, due to moderate nutrient levels supporting greater productivity resulting in a more diverse aquatic community. However, continued nutrient enrichment leads to a eutrophic state, marked by excessive algal growth and reduced water clarity. In severe

cases, the lake may reach a hypertrophic state, where excessive nutrient accumulation causes extreme ecological imbalances with bloom dominating the surface water layers.

Other environmental factors play a significant role in whether a bloom will form. Increased light, higher temperatures, and limited water movement all favour the growth of algal blooms (Klemas, 2012; Paerl et al., 2020). These conditions are typically more prominent in summer conditions, especially in the UK and Europe. The increased temperature and light accelerate the phytoplankton photosynthesis, increasing their growth rate and overall biomass within the water column. Additional contributing factors include the influence of site-specific characteristics, such as hydraulic retention time. Since algae are mainly transported by water currents, increased water movement can enhance flushing, making blooms less likely to occur in flowing rivers. These secondary triggers vary widely between waterbodies, contributing to the complexity of managing algal blooms (Rousso et al., 2020) and can have more indirect consequences.

1.1.2 Impacts of algal blooms

Excessive algal growth can have severe consequences on the water quality of a waterbody (Figure 1.1 **Error! Reference source not found.**) (Feng et al., 2024). The primary, and most easily identified effects are turbidity, algal scums, toxins and odours (Huisman et al., 2018; Klemas, 2012; Paerl et al., 2001), resulting directly from decomposition of excess biomass. Secondary effects include reduced light penetration, which inhibits photosynthesis in submerged vegetation, leading to habitat loss and decreased oxygen production (Scheffer et al., 1993; Scheffer & Van Nes, 2007). Decomposition of excess algae consumes oxygen, leading to hypoxic or anoxic conditions that cause fish kills and disrupt aquatic life (Rabalais et al., 2010). In deeper lakes and reservoirs, trophic state, depth, and mixing (stratification) play an important role in duration and dimensions of the blooms (Lepori & Roberts, 2017). Toxins produced by certain algal species, such as cyanobacteria, can further exacerbate fish and shellfish mortality. The blooms can also outcompete native species of algae and plants, reduce biodiversity and alter food web dynamics (Scheffer et al., 1993).

The phytoplankton group composition of algal blooms strongly influences their impacts. Cyanobacteria (also referred to as blue-green algae) can cause serious health problems due to

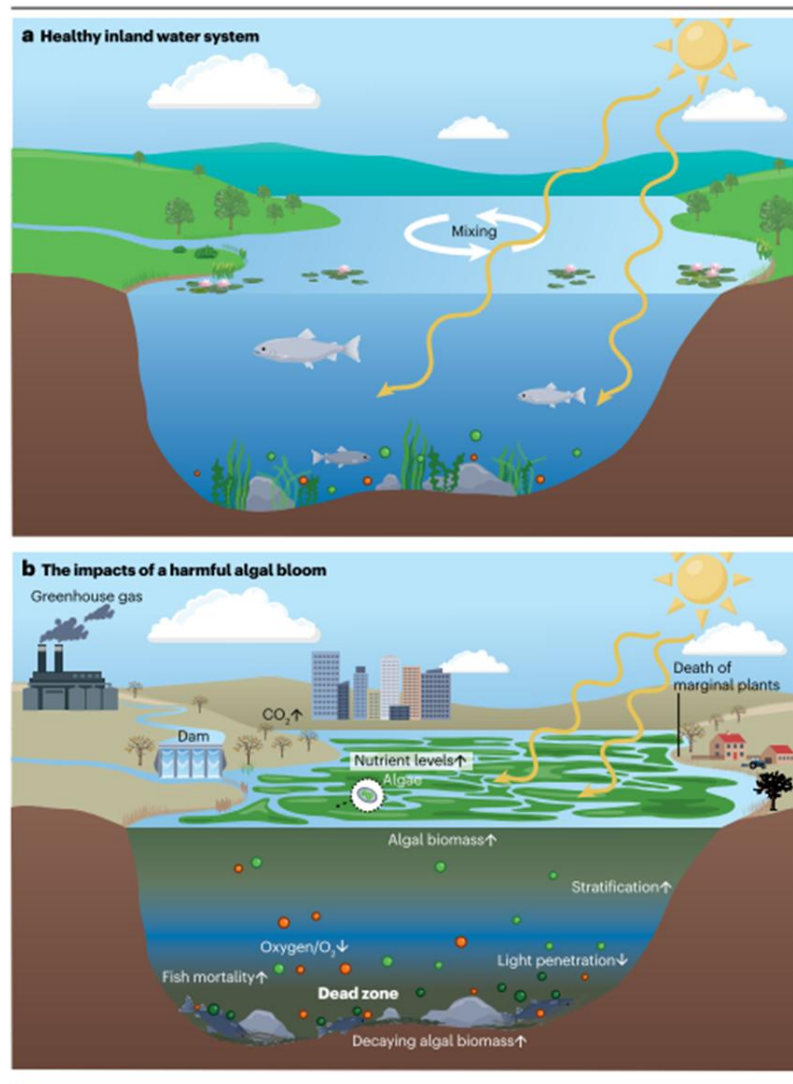


Figure 1.1 Summary of impacts resulting from harmful algal blooms by (Feng et al., 2024).

harmful toxins leaching into the water (Carmichael, 2012). These toxins, depending on the specific cyanobacteria species, can result in minor skin irritations, stomach upsets and, in very rare extreme cases, death (Kouakou & Poder, 2019). Therefore, when drinking water or recreational waters are contaminated, waterbodies are often (partially) closed to mitigate risks. Diatoms are more likely to bloom in spring or even winter, due to being better adapted to colder temperatures and less stable mixing patterns and the clear water phase letting lighter deeper in the water column (Townsend et al., 1992). Although diatoms are not generally known for their toxicity, some species can produce neurotoxins such as BMAA. However, this trait is relatively rare, with only around 30 known species globally reported to produce

such compounds (Catherine et al., 2013). Diatom blooms are often smaller and less invasive, however may still cause non-toxic effects from biomass accumulation like bad odours, deoxygenation and light inhibition.

Harmful algal blooms can create unsafe conditions for recreation, leading to reduced tourism revenue and declining property values. These impacts, along with increased costs for water treatment and disruptions to commercial fisheries and agriculture, result in substantial economic losses. Affected sectors include tourism, housing, wastewater treatment, industry, agriculture, and local communities, as well as broader water management systems (Hoagland & Scatasta, 2006). Water treatment costs rise due to the need for additional filtration of toxins and biomass. Excess biomass can also disrupt shipping and clog hydropower stations, impacting industries. Commercial fisheries suffer from fish kills due to oxygen depletion or toxic contamination in shellfish. In agriculture, contaminated water can harm crops and livestock or increase costs for alternative sources. In severe cases where monitoring and management is needed as result of a bloom, government intervention is required (Hoagland & Scatasta, 2006; Kouakou & Poder, 2019).

1.1.3 Monitoring of algal blooms

Given their wide-ranging impacts and potential for rapid onset, algal blooms are a priority for freshwater resource managers. Their sudden and often unpredictable appearance demands timely and effective monitoring and intervention. Traditionally, monitoring has relied on in situ sampling campaigns or fixed-point sensors, which provide valuable data on water quality parameters but are often costly, resource-intensive, spatially limited, and unable to provide early warnings of risks to utility or health.

A commonly used metric to monitor algal biomass is chlorophyll-a (chl-a) (Søndergaard et al., 2011), a green pigment present in all photosynthetic algae. Chl-a absorbs light most efficiently in the blue and red portions of the spectrum, making it detectable through both direct sampling and optical methods. Chl-a has become central in water quality assessments and regulatory thresholds, such as those used by the World Health Organization and the EU Water Framework Directive (WFD-UKTAG, 2014; World Health Organization, 2021).

However, while traditional monitoring techniques provide crucial ground truth data, their limitations have spurred interest in more scalable, cost-effective, and predictive approaches. Methods that integrate remote sensing technologies and ecological modelling offer the potential to complement existing monitoring systems by extending coverage, increasing

temporal resolution, and enabling early detection and forecasting of bloom events. These approaches are increasingly essential in water bodies where rapid response and proactive management are needed.

1.1.4 Algal blooms: three UK case studies

In this thesis, three contrasting freshwater systems in the UK: Esthwaite Water, Loch Leven, and Alton Water, which all experience algal blooms but differ in morphology (polymictic lake, monomictic lake, and reservoir) and in their management and monitoring strategies are examined. These three sites were selected to capture a range of morphological and geographical conditions across the UK, offering insights into how algal blooms develop and are managed under differing environmental and hydrological contexts (Table 1.1).

Table 1.1 Key characteristics of the three UK freshwater systems studied: Loch Leven, Esthwaite Water, and Alton Water. The lakes differ in geographic location, morphometry, trophic status, land use, and management practices (Hughes et al., 2004), offering contrasting contexts for understanding algal bloom dynamics.

	LOCH LEVEN	ESTHWAITE WATER	ALTON WATER
LATITUDE	North	Central	South
COORDINATES	56.19°N, 3.39°W	54.36°N, 2.98°W	51.99°N, 1.12°E
MORPHOMETRY	Shallow and large	Medium depth and small	Deeper and small
SURFACE AREA (KM²)	13.3	0.96	1.62
MEAN DEPTH (M)	3.9	6.9	5.76
MAXIMUM DEPTH (M)	25.5 (only one small area)	25	20
FUNCTIONALITY	Nature reserve	Nature reserve	Drinking Water reservoir, recreational
MEAN ANNUAL LAKE TEMPERATURE	~10-13°C	~7 – 10.5°C	~8-15 °C
MEAN ANNUAL CHL-A CONCENTRATION	High (14 - 40 µg/L)	Moderate–high (14-29 µg/L)	Moderate (12–23 µg/L)
EUTROPHIC STATUS	Eutrophic	Eutrophic	Mesotrophic/Eutrophic
CATCHMENT LAND USE	Agriculture, urban, nature conservation	Mixed agriculture, woodland	Agriculture, urban
MANAGEMENT	Extensive (nutrient input reduction, reed beds)	Eutrophication management	Water quality management for drinking water
LAKE TYPE	Polymictic	Monomictic	Monomictic
HUMAN IMPACTS	Nutrient loading	Agricultural runoff, wastewater overflow	Recreational use, water abstraction

Loch Leven is the most northerly lake, relatively shallow with a larger surface area located in lowland Scotland (Carvalho et al., 2012). Esthwaite Water is a small lake with a surface area with a deeper mean depth, located slightly further south in the UK in the English Lake District (Mackay et al., 2012, 2014; Mortimer, 1942). Alton Water is a manmade drinking water reservoir with actively managed in and outflows commissioned in 1987 in Suffolk, England.

Together, these case studies provide a basis for examining how lake morphology, latitude, and management strategies influence the occurrence and dynamics of algal blooms under current and future climate conditions.

1.2 Algal blooms in a changing climate

The risks posed by algal blooms is not stationary and has been increasing over the decades and are expected to increase further in both magnitude and frequency in the future (Gobler, 2020; Hou et al., 2022; Klemas, 2012). Global climate change and additional anthropomorphic stressors are expected to exacerbate eutrophication, leading to an increased dominance of algal blooms (Havens & Paerl, 2015; Huisman et al., 2018; Paerl et al., 2020; Paerl & Huisman, 2008; Wurtsbaugh et al., 2019). The higher frequency of extreme weather events and rising temperatures has been speculated to have an impact on the frequency of algal blooms (Havens et al., 2016; Huisman et al., 2018; Paerl et al., 2001; Paerl & Huisman, 2008).

To better understand how future environmental and socio-economic conditions may shape the trajectory of algal bloom development, it is essential to consider the broader climate projections and pathways that influence these stressors. The IPCC has presented different climate scenarios based on human behaviour called Shared Socioeconomic Pathways (SSPs). These SSPs describe different narratives (O'Neill et al., 2017), which range from 'Taking the Green Road' (SSP1) where the world shifts gradually toward a more sustainable path, to 'Taking the Highway' (SSP5) in which the push for economic and social developments is coupled with the exploitation of abundant fossil fuel resources and the adoption of resources and energy intensive lifestyles around the world. In between the two extreme scenarios, are the 'Middle of the road' scenario (SSP2) in which the world follows historical trends with slow progress on sustainability and persistent inequality. The 'A rocky Road' scenario (SSP3) which focusses on nationalism and regional policies and 'A Road Divided' (SSP4) which

expects degradation of social cohesion due to well developed areas to keep developing, but low developing countries staying undeveloped (Figure 1.2).

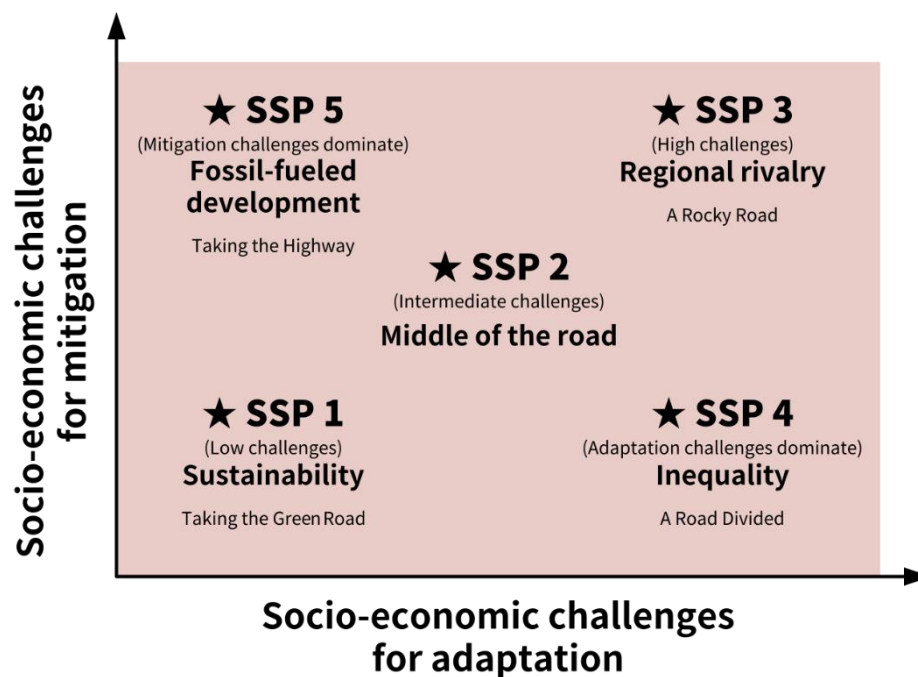


Figure 1.2 Description of the Representative Concentration Pathways (RCPs), their potential Shared Socioeconomic Pathway (SSP) pairings, and projected greenhouse gas (GHG) emissions and global mean temperature increases by 2100 relative to pre-industrial levels.

The SSP scenarios can be coupled to Representative Concentration Pathways (RCP), which are possible outcomes of greenhouse gas emissions in the atmosphere (Table 1.2). The SSP is the pathway humanity follows, and the RCP is the likely outcome in greenhouse gas emissions and temperature that result from that pathway.

Table 1.2 Description of the Representative Concentration Pathways (RCPs), their potential Shared Socioeconomic Pathway (SSP) pairings, and projected greenhouse gas (GHG) emissions and global mean temperature increases by 2100 relative to pre-industrial levels.

RCP	Description	Possible SSP Pairings	Expected Temp Increase (2100, relative to pre- industrial)	GHG Emissions (CO₂ equivalent in 2100)
RCP1.9	Very low emissions, net-zero CO ₂ by ~2050	SSP1	≤1.5°C	~0 GtCO ₂ /year (net negative)
RCP2.6	Low emissions, requires rapid mitigation	SSP1, SSP2	1.5–2°C	~10 GtCO ₂ /year
RCP4.5	Moderate emissions, peak mid-century then decline	SSP1, SSP2, SSP4	2.5–3°C	~25 GtCO ₂ /year
RCP6.0	Medium-high emissions, slow decline after 2100	SSP2, SSP3, SSP4	3–4°C	~50 GtCO ₂ /year
RCP7.0	High emissions, rising through the century	SSP3, SSP5	~4°C	~70 GtCO ₂ /year
RCP8.5	Worst-case, fossil-fuel-intensive, "business-as-usual"	SSP5, SSP3	4.5–5.5°C	~100+ GtCO ₂ /year

These SSP-RCP combinations represent potential climate futures and as previously mentioned, climate has been shown to influence algal dynamics and blooms in the past. Predicting the future of algal blooms is challenging due to their complex nature and the considerable heterogeneity across lakes (Neil et al., 2019; Spyrakos et al., 2018), which has made large-scale forecasting difficult (Richardson et al., 2018). Nevertheless, the increasing frequency and severity of algal bloom events highlight the pressing need for advanced management strategies. Given the complexity of these phenomena, an interdisciplinary approach is essential, even better, one that integrates the expertise of researchers,

policymakers, and water managers, while making full use of available tools, such as predictive modelling (Visser et al., 2016). Modelling offers a powerful means to anticipate future trends and inform mitigation efforts, making it a crucial focus for the next stage of research into algal bloom management.

1.3 Modelling of algal blooms

The current and future impacts of algal blooms call for increased monitoring and additional efforts in maintaining the health of aquatic ecosystems (Stumpf et al., 2016). An important step towards mitigation and prevention is being able to prioritise regions for attention, evaluate management strategies and adapt to future ecological changes (Richardson et al., 2018). Traditional monitoring methods provide valuable information on the current state of freshwater systems but are limited in their ability to anticipate future changes. In contrast, modelling approaches offer a means to generate predictions, supporting both operational and strategic decision-making in water management (Janssen et al., 2019). These methods can capture bloom dynamics and provide the added benefit of predicting algal blooms, offering valuable insights into both short- and long-term bloom evolution (Rousso et al., 2020) thereby supporting management efforts. Additionally, they have the potential to be scaled up to a broader range of lakes (Tigli et al., 2025), enhancing their applicability and effectiveness which has been supported and actively worked on by initiatives like ISMIP (<https://www.isimip.org/>) and GLEON (<http://gleon.org/>).

The development and implementation of models for simulating and forecasting algal blooms has been ongoing for several decades (Carey et al., 2022; Mi et al., 2020; Scheffer, 1989; Seppälä et al., 2007; Stumpf et al., 2016). With the added pressures of climate change, these efforts have gained renewed urgency and focus (Havens & Paerl, 2015; Kong et al., 2021; Moss et al., 2011). Despite ongoing progress, significant challenges remain in modelling algal blooms. These include adequately capturing system complexity, which is especially difficult for ecological systems, managing uncertainties, addressing limitations in validation data, and operating across appropriate spatial scales (Janssen et al., 2019). To better capture this complexity, it is crucial to improve the integration of hydrodynamic and ecological components, as this can enhance the accuracy of future phytoplankton bloom predictions (Palmer et al., 2015; Rousso et al., 2020; Tyler et al., 2016). This is typically achieved through process-based or data-driven modelling approaches (Rousso et al., 2020).

1.3.1 Process based vs data driven

Process-based or data driven are both valid approaches to simulate chl-a in lakes. A data-driven approach relies on statistical techniques to identify patterns and relationships in data without requiring knowledge of system processes. Whilst a process-based approach, processes are described by mathematical equations (Rousso et al., 2020).

A data driven model is trained to reproduce past patterns and uses a fitted algorithm to estimate parameters based on historical data (Izadi et al., 2021). The accuracy of simulations and forecasts depends on the desired output. In a process-based approach, historical data are used to calibrate the parameters within processes and to set initial and boundary conditions within the model. As the model uses equations that represent real-world processes, it can simulate deterministic, and probabilistic forecasts or predictions (Cuddington et al., 2013).

Table 1.3 Different aspects of modelling compared between data-driven vs. Process-based approaches.

	<i>Data-Driven</i>	<i>Process-based</i>
<i>Definition</i>	Uses statistical, AI, or machine learning techniques to find patterns in data.	Uses known physical, chemical, or logical rules to model processes.
<i>Flexibility</i>	More flexible and adaptable to changing conditions and can handle large, complex datasets	Less flexible. Requires modifications when conditions change.
<i>Interpretation</i>	Outputs are directly linked to defined processes, making them more interpretable and suitable for explaining system behaviour and cause–effect relationships.	Outputs are directly linked to defined processes, making them more interpretable and suitable for explaining system behaviour and cause–effect relationships.
<i>Generalisation</i>	Can generalise well across systems if trained on diverse and representative datasets (e.g. multiple lakes via Earth observation). However, performance may degrade outside the range of training data and may fail to capture unobserved processes.	Generalises established processes across systems, allowing application beyond observed conditions. However, transferability may be limited by site-specific parameterisation and data requirements.

<i>Computational power</i>	High: Big data, deep learning, real time analytics Low: simple statistical models, pretrained models	High: 2D and 3D Low: 1D or lower.
<i>Data dependency</i>	Strongly dependent on the availability, quality, and representativeness of historical data.	Can operate with limited data if system processes are well defined, but calibration data remain critical for reliable performance.
<i>Use cases</i>	• Short-term bloom forecasting and early warning systems • Pattern recognition in large datasets • Systems with high data availability, but poorly understood processes • Rapid model deployment across many sites	• Scenario analyses under changing conditions (Climate change impacts) • Mechanistic understanding of processes • Testing management interventions/hypotheses • Long-term projection

The comparison of a data driven or process-based approach (Table 1.3) highlights the need for careful consideration to fit the specific purpose of modelling. The data-driven approach needs less information on processes but needs more historical data of the explained variable and has been shown to be better suited for short-term forecasting (Rousso et al., 2020). A process-based approach generally has been shown to be more useful in long-term future predictions whereas a data-driven approach might outperform for short-term prediction (Rousso et al., 2020).

1.3.2 Modelling on different scales

Independent of the modelling approach of choice, the dimensionality of the model determines the complexity captured and consequently the runtime. The dimensionality of the model influences the constraints to a set of variables or spatial axis and are generally referred to as one-, two- or three-dimensional models. The one-dimensional models require the least computational power with a runtime of seconds to minutes (Ishikawa et al., 2022). When modelling lakes, the one dimension usually refers to a vertical spatial dimension, which is

dominated by the seasonal changes in stratification, oxygen, nutrient and plankton dynamics in the water column (Hipsey et al., 2019; Rouso et al., 2020; Schladow & Hamilton, 1997). In a data-driven approach one-dimensional could also mean, using one variable, for example temperature to simulate chl-a growth.

Two- or three-dimensional models simulate more spatial components (horizontal and/or width) or variables (species growth, nutrients, oxygen), which is more computationally intensive with runtimes of minutes up to days (Ishikawa et al., 2022). Whilst, the number of dimensions can be important for specific research questions, studies have shown that all three dimensions are able to provide valuable information on the lake system (Ishikawa et al., 2022).

Next to model dimensions, the spatial and temporal scale of the variable being modelled is an important consideration. An ideal scenario would involve having readily accessible information on all waterbodies at any given time, whereby comprehensive modelling of each lake or reservoir enables stakeholders to obtain relevant data on demand. However, the implementation of such an approach on a global scale would necessitate certain generalisations and simplifications within the models (Janssen et al., 2019; Tigli et al., 2025). For example, modelling only a single section of a waterbody allows for detailed complexity, but limits the generalisability across the whole waterbody, catchments, or larger spatial scales. Thus, the choice of spatial scale and model dimensionality (1D, 2D, or 3D) must align with the specific modelling objectives (Ishikawa et al., 2022; Rouso et al., 2020). In this study, the focus is on climate change impacts on lake-specific, surface-dominated algal blooms. Therefore, a process-based, one-dimensional vertical model that considers individual waterbodies sequentially is selected. This approach balances the need for physical realism, generalisability, and practical constraints related to data availability and computational resources.

1.1.1 Models for algal bloom forecasting

Process-based models have been widely used to explore the effect of climate change on algal bloom dynamics in lakes and reservoirs. Commonly used models are: PCLake(+) (Janse, 2005; Janssen et al., 2015, 2017, 2019), MyLake (Saloranta & Andersen, 2007), DYRESM-CAEDYM (Hamilton & Schladow, 1997; Schladow & Hamilton, 1997; Trolle et al., 2008), PROTECH (Elliott, 2021) and FABM-GOTM (Bruggeman & Bolding, 2014). Among the various modelling frameworks considered, the General Lake Model coupled with the Aquatic EcoDynamics (GLM-AED) module (Hipsey et al., 2019) demonstrated the greatest suitability

for this study. The one-dimensional, process-based structure of GLM effectively balances process complexity and computational efficiency (Hipsey et al., 2019), while maintaining sufficient physical realism and accommodating practical data requirements. This makes it particularly well suited for modelling lake-specific algal blooms under climate change. Additionally, the model's flexibility to incorporate custom algal bloom species and generate a wide range of output variables enhances its utility for water management applications. Finally, the user-friendly interface and operational capabilities within R facilitate ease of model execution and visualisation. For these reasons, the GLM framework was selected for the modelling work presented in this thesis. Further details and comparisons with alternative models are provided in Appendix A and in the following section.

1.3.3 GLM-AED

The GLM-AED model is a one-dimensional hydrodynamic model for enclosed aquatic ecosystems (Hipsey et al., 2019). Numerous studies have applied GLM-AED to assess the impacts of climate change and to model algal bloom dynamics across diverse lake systems, highlighting both the strengths and limitations of the model under varying conditions. Several have examined how climate change influences lake thermal structure and phytoplankton dynamics. For instance, Deng et al., (2024) applied GLM-AED to an Australian lake to investigate responses to RCP scenarios and water scarcity. Their results showed projected increases in surface water temperature, longer stratification periods, and higher chl-a concentrations under future climate conditions. Similarly, (Fadel et al., 2019) demonstrated good model performance in Karaoun Reservoir, with substantial changes in stratification dynamics and phytoplankton structure under warming. In Germany, Bueche et al., (2017) found GLM-AED to be effective for simulating ice cover and water temperatures. Bucak et al., (2018) and Ladwig et al., (2021) extended these applications by coupling GLM-AED to catchment models in Turkey and the USA, respectively, to account for both climate and land-use changes. In Lake Mendota, Ladwig et al. (2021) found that the lake's heat budget was primarily driven by meteorological conditions, implying that summer anoxia will likely worsen under future warming.

A growing body of research has assessed the sensitivity and performance of GLM-AED across different environments. Bruce et al., (2018) evaluated the model across 32 globally distributed lakes, focusing on the sensitivity of key parameters related to heat exchange and mixing. Their study identified both strengths in model performance and areas needing

parameter adjustment for improved accuracy. In subtropical reservoirs, Soares & Calijuri, (2021) conducted a sensitivity analysis and found that while temperature sensitivity patterns were consistent across sites, chl-a responses were more site-specific.

Model comparison studies have also played a key role in understanding the utility of GLM-AED. Wang & Wang, (2021) compared its predictive performance to an Artificial Neural Network (ANN) and reported that the ANN achieved lower RMSE and MAE values for chl-a, suggesting potential advantages of data-driven approaches. Meanwhile, Ishikawa et al., (2022) compared the hydrodynamics of GLM to 2D and 3D hydrodynamic models and found that all models could reproduce seasonal temperature and stratification patterns, although the dimensionality of models may affect their suitability for specific applications.

Some researchers have focused on the role of climate variability and extreme events in shaping bloom dynamics. Krinos et al., (2019) investigated how uniform versus variable warming scenarios affected cyanobacterial biomass in Lake Mendota. They found that incorporating interannual variability in air temperature led to a much wider range of predicted biomass outcomes, emphasising the importance of both the magnitude and variability of warming in long-term bloom forecasting. Similarly, Mesman et al., (2020) assessed GLM's performance during short-term extreme weather events, concluding that while the model remains useful, increased uncertainty must be acknowledged under these conditions.

Algal bloom responses to combined climate and nutrient drivers have also been explored. Ward et al., (2020) used a 31-year simulation with GLM-AED to evaluate chl-a responses to air temperature and phosphorus loading. Their results showed that while median summer chl-a increased with air temperature, annual peak concentrations were more strongly controlled by prior external phosphorus loads, illustrating the need to consider both climate and nutrient inputs in bloom predictions. Similarly, Wang & Boegman, (2021) scaled initial conditions in GLM-AED based on management scenarios to simulate water quality in western Lake Erie, demonstrating the model's utility in applied lake management contexts. Fenocchi et al., (2019) used GLM-AED for long-term projections of water chemistry and phytoplankton succession, cautioning that model reliability decreases over extended timeframes and that interpretation of phytoplankton results requires particular care.

Together, these studies demonstrate that GLM-AED is a widely used and versatile tool for simulating physical and ecological processes in lakes under both current and future conditions. The wide range of prior applications, from sensitivity testing to scenario

forecasting, highlights both its strengths and the need for careful parameterisation and validation. Importantly, while many studies have examined individual lakes or focused on short-term forecasts or broad-scale comparisons, gaps remain in understanding how GLM-AED performs across varying climatic zones and integrated climate scenarios. As well as under data-scarcity and lower data quality. GLM-AED will be a valuable tool to demonstrate the value of lake ecosystem modelling for understanding the effect of climate change on algal bloom dynamics in different water body types and regions.

While physical processes in lakes, such as temperature and stratification, are relatively well understood and can be modelled with a reasonable degree of accuracy, simulating algal blooms is considerably more complex. Algal dynamics are governed by a complex interplay of physical, chemical, and biological factors, including nutrient availability, light conditions, species-specific growth traits, grazing pressure, and internal feedback mechanisms. As a result, modelling algal blooms carries greater uncertainty and presents more challenges than modelling lake physics alone. This complexity partly explains why fewer studies have focused on projecting algal responses to climate change, compared to those examining thermal structure. Nonetheless, this gap highlights a clear research need for work aimed at improving algal bloom modelling under future climate scenarios.

1.3.4 The challenges of modelling

Statistician George E. P. Box famously stated, ‘All models are wrong, but some are useful’, highlighting the fundamental truth that all models are simplifications of reality and can never be entirely accurate. However, despite their inherent limitations, models remain valuable tools that aid in understanding, predicting, and making informed decisions about complex ecological systems.

Confidence in model outputs poses a significant challenge for water management. The utility of models lies in their ability to inform decision-making processes, particularly for forecasting future ecological conditions. However, for models to be effectively integrated into management strategies, water managers must have sufficient trust in their outputs or, at the very least, be able to quantify the associated uncertainty. Forecasting without quantified uncertainty risks reducing models to mere speculative predictions (Carey et al., 2022). Recognising this, uncertainty quantification is a critical consideration in environmental

modelling. Although this thesis primarily focuses on model development and application, it lays the foundation for incorporating rigorous uncertainty analysis in future work.

Collaboration between water management authorities and academic institutions has the potential to enhance the accuracy and reliability of bloom modelling. Water managers often possess extensive datasets and resources but may lack the necessary tools or expertise to integrate these data into comprehensive predictive models. Academic research can bridge this gap by developing and refining models that better capture chl-a dynamics with greater precision and certainty.

If improvements in modelling techniques can enhance the accuracy and reliability of chl-a forecasts, water managers will be better equipped to take proactive measures to mitigate future water quality impairments. Much like meteorological forecasting, advanced aquatic ecosystem models could provide probabilistic estimates of future water quality conditions in lakes and reservoirs, enabling informed and timely management decisions (Carey et al., 2022)

Errors in modelling are particularly evident during the processes of calibration and validation. This is especially true for process-based model, which require numerous parameters to be set or calibrated. The challenge in modelling chl-a dynamics stems from the complexity and variability of the underlying ecological processes, which are not only specific to individual lakes but can also fluctuate within a single waterbody. Parameters such as phytoplankton growth rates and nutrient uptake rates are difficult to derive directly from the literature or empirical measurements. As a result, these parameters must often be estimated or calibrated, introducing further sources of uncertainty.

The success of calibrating models to simulate algal bloom dynamics depends critically on both the quantity and quality of available data. While large datasets can provide valuable information, poor data quality may still hinder accurate representation of ecological processes. On the other hand, limited datasets risk missing key system dynamics if important ecological signals are not captured by in situ measurements. Although process-based models typically require less data than purely data-driven approaches, they still rely on enough reliable data to generate meaningful results. What constitutes ‘enough’ data varies depending on the specific system being studied, the model’s intended application, and the level of confidence required in its predictions (Refsgaard et al., 2007). This highlights the need to

better understand the interplay between data quantity, quality, and model performance in algal bloom forecasting.

1.4 Earth observation

Reliable and extensive datasets are essential for calibrating accurate process-based ecological models (Rousso et al., 2020), yet obtaining high-frequency, large-scale measurements remains a significant challenge. Technological advancements and improved sampling techniques have led to the establishment of high-frequency monitoring stations equipped with sensors in some lakes (Carey et al., 2022). Deploying such systems across many waterbodies, or even within a single catchment, is currently not feasible given the cost and logistical constraints. Satellite Earth observation (EO) provides an alternative high-frequency measurement tool with regional to global coverage. Earth observation or remote sensing has emerged as a powerful tool, offering a cost-effective means of collecting environmental data at relatively high frequency (daily to every few days, cloud permitting) and over large spatial scales (Klemas, 2012; Rousso et al., 2020).

Remote sensing has been utilised for decades. As early as the 1960s, the first meteorology-focused satellite systems were launched into space. Since then, satellite technology has evolved significantly (McCabe et al., 2017; Q. Zhao et al., 2022). Early systems primarily captured panchromatic and/or red-green-blue (RGB) or red-green-near-infrared (NIR) imagery (De Wulf et al., 2007). Modern satellites, however, employ multi- and hyperspectral visible to near-infrared (VNIR) bands, multiband thermal imaging, multi-channel microwave emissions, as well as radar and lidar techniques.

Most space agencies provide satellite data to end-users in five distinct levels, with the raw data at Level 0, to more advanced, aggregated environmental products at Level 4. In more detail, Level 0 refers to the unprocessed, spectro-radiometric data acquired directly by the satellite sensor. Level 1 data are radiometrically calibrated and generally include geometric corrections, for optical data, this means quantised at-sensor radiances that have been corrected for sensor-specific effects. Level 2 products consist of derived geophysical variables such as bottom-of-atmosphere reflectance, which have been corrected for atmospheric effects and are therefore more directly representative of surface conditions. Level 3 data are georeferenced and Level 4 products go a step further and often involve

spatial or temporal aggregation. The level of data used in a project depends on its specific objectives and whether additional processing (e.g. atmospheric correction) is intended.

1.4.1 Aquatic remote sensing of inland waters

Oceanographers recognised the potential for monitoring chl-a and temperature using remote sensing as early as the launch of the NASA Earth Resources Technology Satellite (later renamed Landsat-1) in 1972. In contrast, the adoption of remote sensing techniques by limnologists progressed more gradually (Bukata, 2013). Oceanographers came up with the first bio-optical ocean model as early as 1975 (Gordon et al., 1975). This model used the water-leaving reflectance(ρ_w), typically derived from remote sensing reflectance ($R_{rs}(\lambda)$) times P_i , to determine water quality parameters.

Limnology following that up around the 1980's (Bukata et al., 1981a; Bukata et al., 1979; Bukata et al., 1981b; Jerome et al., 1983) with a bio-optical model that enabled the extraction of chl-a, suspended particulates, and coloured dissolved organic carbon in inland water bodies using a single full-spectrum measurement. That work has continued well into the 2000s, enabling remote monitoring of optically complex waters, and has made it possible to generate time-series data on changing water quality in inland lakes and coastal regions (Bukata, 2013).

Monitoring inland waters via remote sensing presents several unique challenges. Inland waters are optically complex, and the inversion of water-leaving reflectance is an inherently ill-posed problem, complicating the retrieval of bio geophysical parameters. For example, problems like sun-glint (Harmel et al., 2018) result in reflectance in addition to that of the water column and present challenges for the atmospheric correction (Moses et al., 2017). Atmospheric correction is also more difficult over inland waters due to the continental nature of the overlying atmosphere and typically higher concentrations of aerosols (Gordon, 1978), which introduce greater variability than over open oceans. Finally, the proximity of land introduces adjacency effects (Santer & Schmechtig, 2000), further compounding atmospheric correction and reducing the accuracy of remote sensing observations. As well as their relatively small spatial extent compared to oceans makes it difficult to extract enough usable pixels (Beck et al., 2016).

Effective monitoring requires high spatial, temporal, and spectral resolution which are demands that are difficult to meet simultaneously with current satellite technologies (Serafy et al., 2021). The launch of the Copernicus Sentinel missions, beginning with Sentinel-1A in 2014, marked a significant advancement in Earth observation capabilities (Thépaut et al., 2018). Of relevance for inland water quality monitoring are the Ocean and Land Colour Instrument (OLCI) aboard the Sentinel-3A and -3B satellites, which offers a spatial resolution of 300 meters, and the MultiSpectral Imager (MSI) on Sentinel-2, which provides finer resolution ranging from 20 to 60 meters. The spatial resolution of the latter is particularly suited for assessing smaller inland waterbodies. Sentinel-2 MSI has been successfully used to retrieve chl-a concentrations in lakes ranging from 0.5 to over 1,000 km² (Ansper & Alikas, 2018; Sakuno et al., 2019) and continues to be applied in diverse aquatic environments worldwide (Qin et al., 2025; Salls et al., 2024; D. Zhao et al., 2024).

1.4.2 Deriving chlorophyll a

Deriving chl-a using satellite data from top-of-atmospheric radiances (Level 1) has two important steps: atmospheric correction and application of appropriate ‘in-water’ retrieval algorithms. Atmospheric correction removes attenuation effects caused by active atmospheric constituents, such as aerosol and molecular scattering and absorption by water vapour, ozone, oxygen and carbon dioxide (Gao et al., 2009). Atmospheric correction highly impacts the surface reflectance quality, next to atmosphere and surface characteristics and sensor design (Okin & Gu, 2015).

The chl-a algorithms derive the chl-a values from water-leaving or remote sensing reflectance. These algorithms tend to be either (semi-) empirical or (semi-) analytical. Empirical models estimate chl-a using statistical relationships between reflectance data and in situ measurements, without making explicit assumptions about the underlying optical properties of the water. In contrast, analytical models are based on radiative transfer theory and derive chl-a by inverting reflectance data to retrieve inherent optical properties. Empirical approaches have evolved to incorporate machine learning and artificial intelligence techniques (Cao et al., 2020), enabling more flexible and potentially more accurate estimations under a wider range of conditions. Some of the algorithms can be calibrated using the available in situ chl-a data, improving the model fit and subsequently the chl-a derivation.

To further improve algorithms that do not inherently take the optical water properties into account, optical water types can be derived beforehand to make them work on a more global transferable scale. (Neil et al., 2019; Spyrakos et al., 2018). Optical water types (OWTs) are a classification system based on satellite-derived remote sensing reflectance (R_{rs}), grouping waters into distinct types with similar optical characteristics, e.g. ranging from very clear to highly turbid conditions (Spyrakos et al., 2018). The classification and calibration of OWTs can support the development of more robust and flexible approaches for chl-a retrieval. OWT schemes (e.g. Jackson et al., 2017; Moore et al., 2014; Spyrakos et al., 2018) enable the optimisation of algorithms for specific water types and facilitate the selection of the most appropriate algorithm for a given water body or even individual water pixels. This targeted, blended approach has been shown to retrieve chl-a (Jackson et al., 2017; Moore et al., 2014), particularly in optically complex inland and coastal waters where concentrations can range from near-zero in clear conditions to over 100 mg m^{-3} in highly turbid systems, necessitating tailored calibration strategies.

1.4.3 Challenges and uncertainties

Despite considerable advances in Earth observation techniques for monitoring inland water quality, substantial challenges and uncertainties remain, particularly in relation to data accuracy and retrieval. One of the most critical sources of uncertainty is atmospheric correction, which directly influences the accuracy of remote sensing reflectance ($R_{rs}(\lambda)$) used in chl-a retrieval (Pereira-Sandoval et al., 2019). Within this process, estimating aerosol contributions introduces the greatest variability (Pahlevan et al., 2021), which can differ widely across space. These uncertainties are further compounded by the influence of local climate and the proximity of inland waters to land, which creates complex land–atmosphere interactions.

Additional challenges stem from adjacency effects caused by surrounding land or vegetation (Santer & Schmechtig, 2000), the highly variable composition of optically active water constituents (Werther et al, 2022a), and errors introduced during observational data processing (Burggraaff, 2020a). Algorithmic retrieval of chl-a concentrations is also subject to model-specific assumptions and uncertainties, many of which are rarely quantified (Werther et al, 2022b). These assumptions may not hold when applied to novel or uncharacterised observations, particularly given the wide range of chl-a concentrations

sometimes reaching up to 350 mg m⁻³ in inland waters (Gitelson et al., 1993) and the highly non-linear spatial variability of associated biophysical parameters.

Taken together, these sources of uncertainty underscore the critical need for rigorous quality control in EO-derived datasets before they are integrated into modelling frameworks.

Whether through data filtering, bias correction, or uncertainty flagging, identifying best practices for managing EO data uncertainty remains an open and important area for future research.

1.4.4 Remote sensing and modelling

Remote sensing offers a valuable tool for addressing data gaps in global waterbodies, providing high-frequency observations that can be used to complement modelling efforts and validate ecological models, as demonstrated in previous studies (Hunter et al., 2010; Li et al., 2020; Serafy et al., 2021).

While remote sensing offers a means of monitoring, it may not be sufficient on its own to fully capture the complexity of underlying ecological processes (Shen et al., 2012) as well as future projections. Numerical models provide a means to extend observations to short- and long-term forecasts; however, their accuracy is often limited by insufficient or inconsistent data inputs. The potential to harness remote sensing data to enhance process-based ecological models, thereby improving our understanding and forecasting of algal dynamics, remains relatively underexplored. Recent studies have highlighted the promise of using satellite in machine learning approaches in marine systems (Anderson et al., 2016; Yñiguez & Ottong, 2020) as well as in combination with hydrological modelling (Xu et al., 2014). However, little progress has been made in effectively integrating satellite data into ecosystem process-based models, particularly in a way that improves their predictive capacity or captures system complexity. Key challenges include how model performance is affected by the unknown uncertainty of satellite observations, and how best to filter and quality-assess remote sensing-derived chl-a data prior to its use in modelling workflows. Addressing these challenges will be crucial for improving model accuracy and advancing our ability to assess the impacts of algal blooms under future climate scenarios. Moreover, it will determine whether satellite Earth observation data can be used to support the calibration of lake ecosystem models allowing their application to water bodies where monitoring is currently limited or absent.

1.5 Research gaps and objectives

In this thesis, the primary aim is to improve the forecasting of algal blooms to provide tools for future freshwater management strategies, particularly in preparing for the challenges posed by climate change. Algal blooms themselves, although not always directly harmful, can have significant indirect consequences that threaten freshwater systems. These consequences are likely to become more severe as freshwater systems face the pressures of a changing climate. By improving our future climate bloom forecast, we can better prepare for and mitigate their impacts, ensuring the sustainability of freshwater resources in the long term. This thesis aims to provide valuable insights into how we can improve predictive models using novel tools like remote sensing, considering climate scenarios, waterbody characteristics, and other relevant factors, to better inform management strategies and policy decisions.

The current lack of future simulation and spatial monitoring in algal bloom management calls for a cost-effective and spatially transferable approach. A process-based modelling approach could be the solution help future simulation but will need reliable data availability for set up. To relieve data-scarcity a high-frequency, low-cost monitoring of chl-a using low uncertainty remote sensing can be used and used to inform models. This work aims to combine modelling and remote sensing approaches to improve future algal bloom simulates, whilst addressing the key gaps of model data availability and remote sensing data uncertainty. The three data chapters each support the overarching aim of improving algal bloom forecasting to aid management under climate change. The first focuses on data scarcity, exploring how limited in situ observations affect model reliability. Thus, advancing our understanding of how data quantity and quality affect our ability to model algal bloom dynamics. The second addresses remote sensing uncertainty, evaluating how data quality impacts model performance and can actively be filtered out for model improvement. As well as explore the use of satellite Earth observation data for supporting the calibration of lake ecosystem models, allowing these models to be applied in water bodies lacking adequate monitoring. The third examines climate change impacts, using future scenarios to assess shifts in bloom dynamics across UK waterbodies. Furthermore, this chapter will illustrate how lake ecosystem modelling can enhance our understanding of climate change effects on algal bloom behaviour across

different water bodies and regions. Together, these chapters highlight key challenges and opportunities in developing more robust and scalable forecasting tools.

1.6 Thesis structure

Chapter 1 introduced the core concepts explored in this thesis, including algal blooms and their ecological impacts, the GLM-AED lake model, the use of satellite remote sensing for chl-a detection, and the influence of climate change on freshwater systems.

Chapter 2 investigates the minimum data requirements for effective algal bloom modelling. While models are increasingly used in lake management, many practitioners hesitate to apply them in data-limited settings. This chapter explores whether certain data types (e.g., meteorological, in-lake) are more influential than others, and assesses how reduced data frequency for both model forcing and calibration affects performance. The findings can guide water managers in optimizing monitoring strategies or determining whether modelling is feasible in their specific context.

Chapter 3 focuses on the integration of satellite remote sensing in algal bloom modelling. It presents a framework for quality-controlling satellite-derived chl-a time series and evaluates the uncertainty of these datasets for use in lake model calibration. The chapter tests whether these processed satellite products can enhance GLM-AED model outputs. This is particularly relevant for eutrophic systems with limited traditional monitoring data and presents a novel method for remote sensing integration.

Chapter 4 uses the newly calibrated lake models to simulate the effects of future climate scenarios across a gradient of UK lakes. By applying consistent modelling under different climatic and morphological contexts, the chapter evaluates how lakes such as Esthwaite Water, Loch Leven, and Alton Water might respond to climate-driven stressors. The results highlight spatial variability in bloom risk and can inform future management priorities.

Each of these core chapters (Chapters 2–4) is structured as a stand-alone manuscript. Chapter 3 is currently under peer review, while the others are written with the intention of publication. Chapter 4 will be used to inform management strategies for Anglian Water who manage the Alton Water Reservoir. Chapter 5 provides a general discussion, synthesising insights from all chapters and reflecting on their implications for freshwater management and policy.

Chapter 2: The crucial role of data frequency in modelling algal blooms: lessons from Esthwaite Water

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Abstract

Algal blooms pose significant risks to aquatic ecosystems, meaning accurate modelling and forecasting of their abundance over time essential for effective lake management. This study investigates how the frequency of calibration and driving data influences the performance of process-based models in predicting algal abundance (chlorophyll-a) and detecting blooms in Esthwaite Water (UK). High-frequency calibration data, meteorological inputs, and inflow records from this well-monitored lake are systematically reduced to assess the effects of data scarcity and to identify the minimum data requirements for reliable model performance. The General Lake Model, coupled with the Aquatic EcoDynamics (AED) model, is employed with progressively lower-frequency inputs to simulate algal bloom dynamics, making use of the full chlorophyll-a concentration range and evaluate bloom detection capabilities at the WHO threshold of 24 mg m^{-3} . The results emphasise the importance of high-frequency calibration data, with errors in chlorophyll-a estimates increasing substantially when calibration data frequency is reduced. While daily meteorological data improved chlorophyll-a predictions by smoothing high-frequency noise, hourly data enhanced bloom prediction. Due to bloom thresholds being lake specific, we have assessed the effect of the three data

sources at different bloom thresholds below and above the WHO threshold, showing that meteorology will always be the most influential data source, however, inflow may become more important at extreme (low or high) thresholds. These findings highlight the importance of prioritising calibration data frequency and selecting appropriate driving data frequencies to optimise model performance for both chlorophyll-a estimation and bloom prediction.

2.1 Introduction

Water bodies across the world have increasingly been experiencing problems with algal blooms (Beaulieu et al., 2013; Fang et al., 2022; Ma et al., 2023; Paerl & Huisman, 2008). Impacts from anthropogenic factors and climate change exhibited increases in frequency and intensity of blooms. These blooms, defined as rapid increases in algal biomass, can have significant ecological (Paerl & Otten, 2013) economic (Kouakou & Poder, 2019; Wurtsbaugh et al., 2019) and health (Carmichael, 2012) impacts. As a proxy for algal biomass, water managers frequently measure chlorophyll-a (chl-a), a pigment indicative of algal biomass. Currently, most of the algal bloom monitoring is done using *in situ* chl-a sampling, which are costly, time-consuming, labour-intensive, and only giving opportunity to react when a bloom is happening.

A desire from water management towards a more proactive approach in the form of short- and long-term prediction of algal bloom dynamics has highlighted the value of modelling tools (Isles & Pomati, 2021; Richardson et al., 2018; Wang & Wang, 2021). According to the European Water Framework Directive (European Parliament & of the European Union, 2000), the phytoplankton based assessment should include species composition, species abundance or biomass, and the frequency and intensity of phytoplankton blooms, all which can be done using modelling approaches.

Several modelling approaches exist that can simulate and prediction algal blooms or biomass, of which Machine learning, Statistical and process-based approaches are the most common. Among these tools, process-based numerical models such as the General Lake Model (GLM) coupled with the Aquatic Eco-Dynamics model (AED) (Hipsey, 2022; Hipsey et al., 2019), seem promising due their lower need for driving data and more process true approach to prediction. The model's simplicity, freely available code, one-dimensional structure, compatibility with high-frequency sensor data, and moderate computational requirements (Hipsey et al., 2019; Trolle et al., 2014) make it an accessible yet powerful tool for algal bloom simulation.

GLM-AED represents hydrodynamic and ecological processes mathematically, making it well-suited for hindcasting and forecasting chl-a dynamics (Bruce et al., 2018; Bueche et al., 2017; Lofton et al., 2023; Mesman et al., 2020). Previous studies have successfully used GLM-AED to simulate temperature (Bruce et al., 2018; Bueche et al., 2017), dissolved oxygen, total phosphorus, nitrate, ammonium, and chl-a (Fadel et al., 2019; Fenocchi et al., 2019; Krinos et al., 2019; Soares & Calijuri, 2021; Ward et al., 2020).

A major challenge in chl-a modelling is the limited availability of observational data, as in situ monitoring remains sparse across many water bodies. Accurate modelling requires two data types: driving data, to simulate physical and biogeochemical processes, and calibration data, to constrain parameter uncertainty and improve model performance (Jackson et al., 2000). The frequency of sampling usually is high enough when all system-relevant signals are recorded (Isles & Pomati, 2021), but this is not always easily quantified. Therefore, it is unclear whether both data types require equally frequent sampling, or whether limited resources could justify prioritising one over the other.

Several studies have highlighted data scarcity as a significant challenge in ecological modelling, offering various strategies to address these issues (Latombe et al., 2011; Ritzema et al., 2010; Wang et al., 2025). However, few studies quantify the impacts of data scarcity on model performance and usability (Pluchinotta et al., 2024). For example, (Derot et al., 2020) demonstrated that lower temporal resolution negatively affects the forecast performance of chl-a in coastal areas when using machine learning models. Similarly, (Daugaard et al., 2024) maintained consistent data point numbers across their analyses, ensuring that higher-frequency datasets did not inherently contain more data. Their findings, based on empirical dynamic modelling, also indicated that reduced sampling frequency worsened forecast accuracy. Although both studies discussed driving data frequency, neither investigate frequency of calibration data, typically needed for process-based models.

As process-based modelling is becoming more prominent, the effect of lower frequency calibration data needs to be investigated. Therefore, we aim to not only examine the effect of sampling frequency on the driving data but also investigate the frequency of calibration data. Specifically, if GLM-AED can still produce reliable algal bloom simulations using low-frequency data, or is high-resolution temporal data essential for accurate forecasting like stated in previous work? As the reliance on modelling tools increases for informing environmental policy and management strategies, understanding the implications of data frequency and model

calibration becomes crucial to ensuring that these tools remain robust and applicable under varying data availability conditions.

While the focus here is on biomass, particularly the specific increase in algal bloom days, another challenge arises in establishing a consistent definition of an algal bloom. Visual indicators like surface scums are easily recognisable, but numerical thresholds for bloom detection vary considerably across waterbodies are often highly system-specific (WFD-UKTAG, 2014; World Health Organization, 2021). From a health problems perspective, the World Health Organization (WHO) defines three concentration levels for *chl-a* associated with cyanobacteria: Vigilance Level (3 to 12 mg/m³), Alert Level 1 (12 to 24 mg/m³), and Alert Level 2 (greater than 24 mg/m³) (World Health Organization, 2021). These ranges can be specified further by determining the species of cyanobacteria, which determines the level of cyanotoxins at which they are harmful. The cyanobacteria Microcystin is the most common in Esthwaite Water, the which puts the WHO chl-a threshold in the upper section of the range with chl-a concentrations of greater than 24 mg/m³ causing Alert Level 1, indicating high-risk conditions for cyanobacterial blooms.

However, not every lake has the resources to determine species or has the necessary data to define what constitutes a bloom, making it difficult to establish such thresholds consistently. From a modelling perspective, adopting a fixed threshold could facilitate the integration of model outputs into decision-making processes. However, the variability in threshold values introduces a key question: Does the threshold influence a model's ability to accurately detect bloom events across diverse systems? This is especially relevant in the context of low-frequency data, where infrequent sampling may obscure finer temporal variations, further complicating the accurate detection of bloom events.

In this study we aim to:

1. Evaluate the criticality of driving and calibration data frequency in modelling efforts, including the feasibility of using lower-frequency data to produce reliable outputs.
2. Asses the model accuracy at thresholds set by the WHO and compare with accuracy at other thresholds.
3. Investigate the adaptability of GLM-AED to forecast algal blooms across diverse lake systems with varying data constraints.
4. Provide actionable recommendations for water managers on prioritising data collection, selecting optimal bloom thresholds, and enhancing modelling strategies for effective decision-making.

2.2 Methods

2.2.1 Case study lake

Esthwaite Water is a small (0.96 km²), shallow (mean depth 6.9 m) eutrophic lake situated in the English Lake District with a high monitoring frequency of fortnightly data (Mackay et al., 2012, 2014; Mortimer, 1942) It lies within the Windermere catchment and has a drainage area of approximately 17 km². The catchment is predominantly a mix of pasture, woodland, and agricultural land. The lake receives inflow primarily from Black Beck and drains southward into Windermere via Cunsey Beck.

Over 55% of the lake is less than 5 m deep, facilitating seasonal thermal stratification during spring and summer, followed by mixing in winter, classifying it as a Monomictic lake. Esthwaite Water is one of the most nutrient-rich lakes in Cumbria, with recurring phytoplankton concentrations exceeding 100 mg/m³ (Maberly et al., 2011; Madgwick et al., 2006). The 75th percentile (P75) of the chl-a concentration range in Esthwaite Water is 25.7 mg m⁻³. Its eutrophic status reflects a long history of phosphorus enrichment, primarily from agricultural runoff and localised point sources.

2.2.2 Long-term monitoring data

In situ chl-a

Fortnightly chl-a measurements (January 2016 to December 2022) (n = 156) (Talling, 1974) were provided by the UK Centre for Ecology & Hydrology (UKCEH) as part of an ongoing long-term monitoring dataset. Chl-a was extracted from a known volume of water from a 0-5m integrated sample filtered onto a Whatman GF/C filter on the day of sampling and frozen for later analysis. Filters were defrosted and extracted in hot methanol, measured spectrophotometrically and absorbance values converted to chl-a following the protocol of Talling (1974). These data were used for calibration of GLM-AED.

GLM-AED data

Lake morphometry data (latitude, longitude, depth, area, elevation) were provided by UKCEH (Mackay et al., 2014; Spears et al., 2012). Hourly meteorological forcing data (including shortwave radiation, longwave radiation, air temperature, relative humidity, wind speed, rainfall, and snowfall) were extracted from the fifth ECMWF atmospheric reanalysis (ERA5) (Hersbach et al., 2020) via the Copernicus Climate Data Store for the period 2016 to 2022.

Inflow from the main tributary, Black Beck, was estimated using daily outflow data from Cunsey Beck, obtained from the UK National River Flow Archive (Talling, 1974). Given the relatively stable water level in Esthwaite Water, inflow and outflow were assumed to be in balance. Water chemistry data for the inflow, including temperature, pH, phosphate (PO_4), nitrate (NO_3), ammonium (NH_4), and silicate (SiO_4), were provided by the UK Centre for Ecology & Hydrology (UKCEH) at fortnightly intervals and linearly interpolated to a daily resolution for model input.

2.2.3 Design of model experiments: data frequency effects

The GLM-AED model was used to evaluate how the temporal resolution of both driving and calibration data influences simulation accuracy of bloom detection. This included varying the frequency of meteorological driving data (such as hourly versus daily), inflow nutrient data (fortnightly, monthly, and seasonally focused sampling), and calibration datasets (fortnightly to seasonal chl-a observations). The experiment aimed to assess the extent to which temporal aggregation affects model performance and parameter estimation, particularly for dynamic processes like phytoplankton growth.

Driving data scenarios

Fourteen different driving data scenarios were considered for the period 2016 to 2022, consisting of frequency-combinations from two pathways: Meteorology and Inflow. The frequency of meteorological data was reduced from hourly to daily to reflect the typical resolution available from meteorological models in most UK regions. All variables in the dataset (including shortwave and longwave radiation, air temperature, relative humidity, wind speed, rainfall, and snowfall) were aggregated simultaneously by computing daily means.

Timestamps were first converted to date-time format to ensure accurate temporal alignment during aggregation, resulting in a consistent daily time series for use in model forcing. Inflow nutrient data (phosphorus, nitrogen, and silica) were resampled to seven different temporal resolutions: fortnightly, monthly, and seasonally (spring, summer, autumn, winter), as well as during the growing season. For the seasonal and growing season scenarios, nutrient concentrations were sampled fortnightly within the specified period and monthly during the remainder of the year, simulating targeted high-frequency monitoring during critical periods. In all scenario's, inflowing discharge was retained at a daily resolution to maintain an accurate water balance. Nutrient concentrations were then linearly interpolated to a daily time

step to align with the discharge data and ensure continuity for model input. Because meteorological and inflow data simultaneously drive the model, each with seven possible temporal resolutions, a total of fourteen unique input combinations were generated for simulation (Table 2.1).

Table 2.1 Overview of each driving data scenario used in the model simulations. The column n indicates the total number of observations across the full time series, with the value in parentheses representing the fraction of the maximum frequency (Frequency factor). The indicator of each scenario is DrivingInflow_DrivingMeteorology. The frequency factor column is the multiplied frequency factor from the inflow and meteorology data in brackets.

Indicator	Inflow	n	Meteorology	n	Frequency factor
<i>FN_H</i>	Fortnightly	120 (1)	Hourly	61367 (1)	1
<i>GS_H</i>	Growing Season	88 (0.73)	Hourly	61367	0.73
<i>SU_H</i>	Summer	75 (0.63)	Hourly	61367	0.63
<i>WI_H</i>	Winter	74 (0.62)	Hourly	61367	0.62
<i>AU_H</i>	Autumn	72 (0.6)	Hourly	61367	0.6
<i>SP_H</i>	Spring	70 (0.58)	Hourly	61367	0.58
<i>MO_H</i>	Monthly	57 (0.48)	Hourly	61367	0.48
<i>FN_D</i>	Fortnightly	120	Daily	1828 (0.029)	0.029
<i>GS_D</i>	Growing Season	88	Daily	1828	0.023
<i>SU_D</i>	Summer	75	Daily	1828	0.018
<i>WI_D</i>	Winter	74	Daily	1828	0.018
<i>AU_D</i>	Autumn	72	Daily	1828	0.017
<i>SP_D</i>	Spring	70	Daily	1828	0.017
<i>MO_D</i>	Monthly	57	Daily	1828	0.014

Calibration data scenarios

Four calibration scenarios were developed based on the highest available frequency of in situ chl-a measurements, sampled fortnightly ($n = 156$ observations per year). This dataset was systematically reduced to simulate limited monitoring resources, resulting in three additional scenarios: monthly, growing season (spring and summer), and summer-only sampling, each with progressively fewer observations per year (Table 2.2).

It is important to distinguish between the implementation of growing season and summer scenarios for driving data and calibration data. For calibration, these scenarios are strictly

limited to observations within the specified periods (spring–summer or summer only), meaning data outside these windows are excluded. In contrast, for the driving data (nutrient inflow), a continuous monthly baseline is maintained across the full year, with fortnightly sampling applied during spring and summer. This difference is illustrated in Figure 2.1.

Table 2.2 Calibration data frequencies used in the model. Each frequency represents a different temporal resolution of chlorophyll-a observations used for model calibration. The column n indicates the total number of observations across the full time series, with the value in parentheses representing the fraction of the maximum frequency. These varying observation frequencies are used to evaluate model performance under different data availability scenarios.

Indicator	Chl-a	n
FN	Fortnightly	156 (1)
MO	Monthly	78 (0.5)
GS	Growing Season	76 (0.48)
SU	Summer	51 (0.33)

Table 2.3 The possible calibration and driving data scenario combinations. With each scenario consisting of Calibration_DrivingInflow_DrivingMeteo.

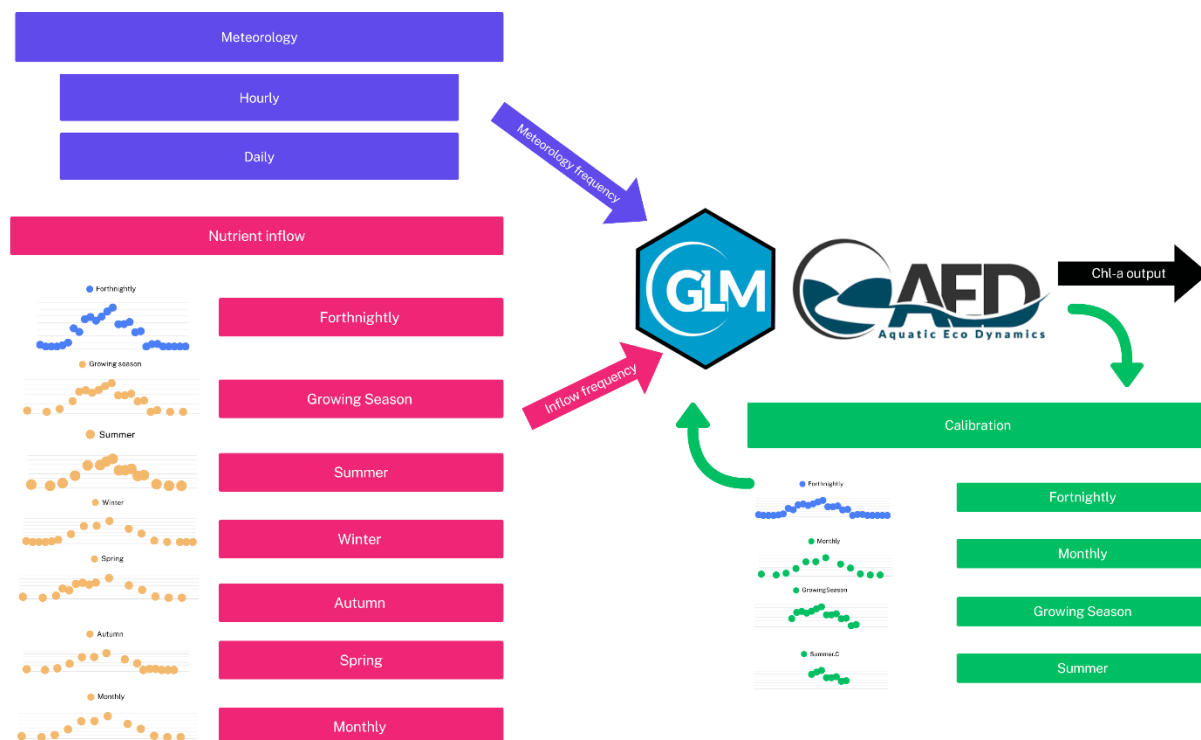


Figure 2.1 Flowchart showing the integration of meteorological forcing, nutrient inflow, and calibration data into the GLM-AED model under different sampling strategies. Each coloured block denotes a specific temporal resolution (e.g., fortnightly, monthly, growing season, summer, winter, autumn, spring, hourly, daily) applied to one of the input data streams. Combining these frequency options across all inputs results in 56 unique model scenarios. For nutrient inflow and calibration data, example time series are provided to illustrate how the different sampling frequencies are represented in practice.

All the calibration and inflow scenarios together, result in 56 unique combinations (Table 2.3).

Driving

<i>Inflow</i>	Meteorology	Fortnightly (FN)	Monthly (MO)	Growing Season (GS)	Summer (SUM)
<i>Fortnightly (FN)</i>	Hourly (H)	FN_FN_H	MO_FN_H	GS_FN_H	SU_FN_H
<i>Growing Season (GS)</i>	Hourly (H)	FN_GS_H	MO_GS_H	GS_GS_H	SU_GS_H
<i>Summer (SU)</i>	Hourly (H)	FN_SU_H	MO_SU_H	GS_SU_H	SU_SU_H
<i>Winter (WI)</i>	Hourly (H)	FN_WI_H	MO_WI_H	GS_WI_H	SU_WI_H
<i>Autumn (AU)</i>	Hourly (H)	FN_AU_H	MO_AU_H	GS_AU_H	SU_AU_H
<i>Spring (SP)</i>	Hourly (H)	FN_SP_H	MO_SP_H	GS_SP_H	SU_SP_H
<i>Monthly (MO)</i>	Hourly (H)	FN_MO_H	MO_MO_H	GS_MO_H	SU_MO_H
<i>Fortnightly (FN)</i>	Daily (D)	FN_FN_D	MO_FN_D	GS_FN_D	SU_FN_D
<i>Growing Season (GS)</i>	Daily (D)	FN_GS_D	MO_GS_D	GS_GS_D	SU_GS_D
<i>Summer (SU)</i>	Daily (D)	FN_SU_D	MO_SU_D	GS_SU_D	SU_SU_D
<i>Winter (WI)</i>	Daily (D)	FN_WI_D	MO_WI_D	GS_WI_D	SU_WI_D
<i>Autumn (AU)</i>	Daily (D)	FN_AU_D	MO_AU_D	GS_AU_D	SU_AU_D
<i>Spring (SP)</i>	Daily (D)	FN_SP_D	MO_SP_D	GS_SP_D	SU_SP_D
<i>Monthly (MO)</i>	Daily (D)	FN_MO_D	MO_MO_D	GS_MO_D	SU_MO_D

The expected ranking of the different frequencies (Figure 2.2) is based on their multiplied frequency factors (Table 2.1, Table 2.2, Table 2.3). This expected ranking will be used to compare to final rankings based on error metrics.

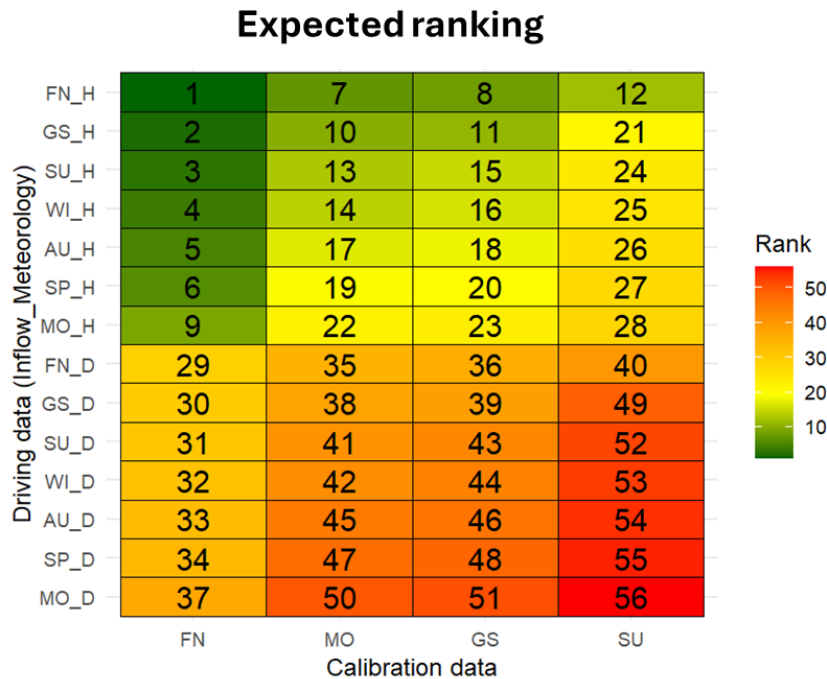


Figure 2.2 Expected model performance ranking based on observation frequency. Frequencies with more frequent sampling are expected to provide stronger calibration and thus receive higher rankings.

The best model fit was determined through comparison of the surface chl-a simulated by GLM-AED and in situ chl-a in the even validation years.

Two frequently used metrics: the Mean Absolute Error (MAE) and the Median Symmetric Accuracy (MdSA; Morley et al., 2017), which quantifies the median error. The MdSA was calculated as follows:

$$MdSA = (e^{\text{median}(\left[\log\left(\frac{Y_{est}}{Y_{true}}\right)\right])} - 1) * 100$$

The Y_{true} is the chl-a data from the *in situ* validation years, with Y_{est} being the modelled chl-a range.

Statistics

To assess the relative influence of different frequency data sources on model performance, an analysis of variance (ANOVA) was conducted. The independent variables included the temporal resolution of meteorological data, inflow nutrient data, and calibration frequency, while the dependent variables were model performance metrics: mean absolute error (MAE) and median symmetric accuracy (MdSA) of chl-a predictions. The ANOVA tested whether

variation in these data sources led to statistically significant differences in model errors across the data combinations. A low p-value (< 0.05) indicated that the corresponding data source had a significant effect on model performance, highlighting it as a key contributor to uncertainty or model sensitivity. This analysis helped identify which data types and resolutions were most influential in driving predictive accuracy, thereby guiding future data collection priorities for ecological modelling under resource constraints.

Bloom detection

For each data frequency scenario (Table 2.3) in situ chl-a measurements were merged with model-simulated chl-a output, retaining only dates where both datasets were available.

Whilst the focus in this research is on the WHO organisation bloom threshold of 24 mg m^{-3} , a range of bloom thresholds, from 4 to 44 mg m^{-3} in 2 mg m^{-3} increments, were evaluated. All threshold values were classified as Below WHO (4 to 22 mg m^{-3} , $n=10$), Above WHO (26 to 44 mg m^{-3} , $n=10$) or WHO (24 mg m^{-3} , $n=1$). For each threshold, both simulated and in situ chl-a values were classified as 'Bloom' if they exceeded the threshold, and 'No Bloom' if they fell below it.

Bloom detection performance for each scenario was evaluated using the F1-score, the harmonic mean of precision and recall. Precision was defined as the number of true positives (instances where both the model and in situ data indicated a bloom) divided by the total number of blooms predicted by the model. Recall was calculated as the number of true positives divided by the total number of in situ bloom observations. The F1-score provides a balanced measure of the model's ability to accurately identify bloom events.

$$F1 = 2 \frac{\text{precision} * \text{recall}}{\text{precision} + \text{recall}}$$

The F1 scores per threshold and scenarios were used to see model performance across a range of thresholds as well as what scenario influences performance the most. An Anova test was used to determine the cause of the variance in the F1 scores per threshold classification (Above, Below, WHO).

2.2.4 GLM-AED model and calibration

The General Lake Model coupled with the Aquatic EcoDynamics module (GLM-AED) was configured to simulate the physical and biogeochemical dynamics of Esthwaite Water. The GLM component simulates lake stratification, mixing, and temperature dynamics, while AED adds modules for nutrients, phytoplankton, oxygen dynamics, and sediment interactions.

The model setup included both required configuration blocks, (*glm_setup*, *morphometry*, *time*, and *init_profiles*) and additional optional modules such as *light* (for underwater irradiance), *mixing* (turbulence schemes), *WQ_setup* (water quality), *sediment* (sediment processes), *output*, and *debugging*. Boundary condition inputs included meteorological forcing, inflow, and outflow files. The AED configuration incorporated modules for oxygen dynamics, nutrient cycling (carbon, nitrogen, phosphorus, silica, and organic matter), two phytoplankton groups (diatoms and cyanobacteria), tracers, and non-cohesive sediment processes. Default parameterisations were adopted unless stated otherwise in Table 2.4 (Hipsey, 2022; Hipsey et al., 2019). Full parameterisation files are available on https://github.com/maudsiebers/GLM_AED_Waterbodies_PhD_Thesis.

Calibration approach

Model calibration was conducted using in situ water temperature and chl-a data provided by UKCEH. Thermal calibration targeted two physical parameters: the wind scaling factor (*fwind*) and the light extinction coefficient (*K_w*). These parameters were automatically adjusted using the built-in calibration tool in the GLM-R package to minimise the mean absolute error (MAE) between observed and modelled temperature profiles. This procedure resulted in an MAE of 0.99 °C and a median symmetric accuracy (MdSA) of 8.23% for the surface temperature.

Ecological calibration focused on two phytoplankton functional groups, diatoms and cyanobacteria, selected to reflect distinct ecological strategies and seasonal bloom dynamics. The maximum growth rates for both groups were manually calibrated to match observed chl-a concentrations, which served as the primary performance metric. A parameter sweep was performed across biologically plausible values (0.5 to 5 day⁻¹) for each group, using MAE and MdSA in chl-a as error metrics on the calibration period. Each parameter was sampled in 10 evenly spaced steps, resulting in a 10 × 10 grid of growth rate combinations (*n* = 100). Calibration and best-fit selection were carried out using data from the even years (2016, 2018, 2020, 2022), while model validation was conducted on the odd years (2017, 2019, 2021) to evaluate predictive skill against independent data.

Recalibration scenarios

Calibration was performed separately for each scenario. Due to manual nature of this calibration, the model was run for the 14 distinct driving data scenarios (

Table 2.1), with each run applying the 10x10 grid of phytoplankton growth rates to generate 100 model runs per scenario, totalling 1,400 simulations. The four calibration scenarios chl-a concentrations (Four calibration scenarios were developed based on the highest available frequency of in situ chl-a measurements, sampled fortnightly ($n = 156$ observations per year). This dataset was systematically reduced to simulate limited monitoring resources, resulting in three additional scenarios: monthly, growing season (spring and summer), and summer-only sampling, each with progressively fewer observations per year (Table 2.2).

It is important to distinguish between the implementation of growing season and summer scenarios for driving data and calibration data. For calibration, these scenarios are strictly limited to observations within the specified periods (spring–summer or summer only), meaning data outside these windows are excluded. In contrast, for the driving data (nutrient inflow), a continuous monthly baseline is maintained across the full year, with fortnightly sampling applied during spring and summer. This difference is illustrated in Figure 2.1.

Table 2.2), were subsequently used on the calibration period to determine the best fit scenario (MAE, MdSA), resulting in a 56 calibrated, one for each of the calibration driving data combinations (Table 2.3). The decision to only pick the best run instead of a range of best runs stems from the finding that top five runs for each scenario exhibit only a minimal increase ($\pm 10\%$) in MdSA, ensuring that selecting the best run does not present a distorted or unrealistic view.

Table 2.4 An overview of the parameters withing GLM-AED used for calibration and their range or default value as well as their assigned value.

Symbol	Description	Range or Default	Assigned Value
<i>Kw</i>	Light extinction coefficient (m-1)	-	0.81
<i>Wind_factor</i>	Scaling factor to adjust the windspeed data provided by in the meteorology file	1	0.70523
<i>R_growth_diatom</i>	Phytoplankton max growth rate at 20C (day-1)	0.5 to 5	2.8
<i>R_growth_cyano</i>	Phytoplankton mac growth rate at 20C (day-1)	0.5 to 5	1.1

2.2.5 Management recommendations

Management recommendations were developed by translating model outputs into implications for water quality monitoring and bloom forecasting under data-limited conditions. This process involved two main components.

First, model results from recalibration and sensitivity to input data frequency were systematically evaluated to identify aspects of model performance relevant to water management, such as robustness to reduced monitoring resolution and uncertainty in chlorophyll-a estimates.

Second, these findings were contextualised through engagement with experts associated with each waterbody. Interactions took place through meetings and focused on aligning model outputs with real-world monitoring practices, management priorities, and system-specific characteristics (e.g., stratification behaviour, dominant water uses).

This combined approach enabled the development of waterbody-specific recommendations that account for both model behaviour and practical management constraints.

2.3 Results

2.3.1 Esthwaite Water highest frequencies

The calibration of the model, performed on hourly data, resulted in a visually good of fit for surface temperature (Figure 2.3A). Despite no massive visual difference, the goodness of fit metrics were slightly better for daily than hourly. With and MAE of 1.03 C using hourly meteorology data and 0.98 C for daily, similarly for MdSA (10.87% and 9.92%). Interestingly, the R^2 is higher for hourly (0.98) compared to Daily (0.97), but again very minimally different.

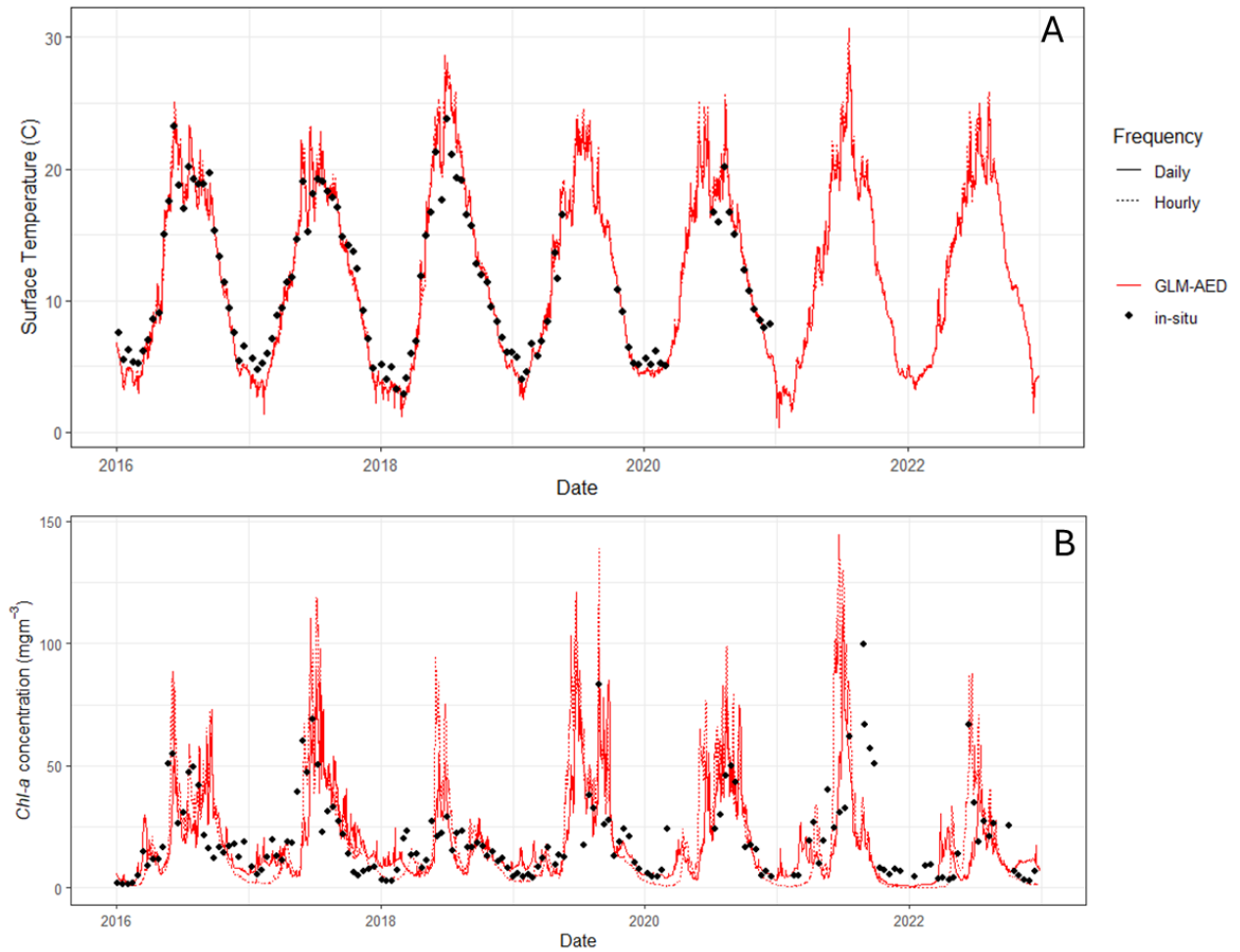


Figure 2.3 In-situ temperature vs model temperature (A) and in-situ chl-a vs model chl-a of the whole timeseries validated for the whole times series.

Chl-a again shows a visually good fit with the in-situ values (Figure 2.3B), with this time a larger difference between daily and hourly meteorology frequencies. With and MAE of 11.7 mg m^{-3} using hourly meteorology data and 10.7 mg m^{-3} for daily, similarly for MdSA (83.4% and 62.7%). Interestingly, the R^2 is higher for hourly (0.4) compared to Daily (0.31).

2.3.2 The effect of frequency

Calibration data

The highest frequency driving data is achieved using hourly meteorology and fortnightly inflow data (FN_H). Using that scenario as the basis, fortnightly (FN) and summer (SU) calibration frequency result in the same growth rates and thus the same low errors (MAE and MdSA) and therefore the same ranking (Four calibration scenarios were developed based on the highest available frequency of in situ chl-a measurements, sampled fortnightly ($n = 156$ observations per year)). This dataset was systematically reduced to simulate limited monitoring resources, resulting in three additional scenarios: monthly, growing season (spring

and summer), and summer-only sampling, each with progressively fewer observations per year (Table 2.2).

It is important to distinguish between the implementation of growing season and summer scenarios for driving data and calibration data. For calibration, these scenarios are strictly limited to observations within the specified periods (spring–summer or summer only), meaning data outside these windows are excluded. In contrast, for the driving data (nutrient inflow), a continuous monthly baseline is maintained across the full year, with fortnightly sampling applied during spring and summer. This difference is illustrated in Figure 2.1.

Table 2.2). The ranking of the fortnightly calibration was expected and indicates that a higher frequency calibration data results in lower combined errors compared to lower frequency calibration data. However, an equal response in summer was not expected. This could however be due to summer having the most phytoplankton peaks and therefore coincidentally picking the same growth rates to fit those peaks compared to Fortnightly.

Table 2.5 Model errors under 4 changing calibration data scenarios with hourly meteorology and fortnightly inflow data sorted from smallest to largest based on ranked position MAE and MdSA. The underscored combination is the highest data frequency.

Calibration_Inflow_Meteorology	MAE	#	MdSA	#	Expected rank	Final position
<u>FN_FN_H</u>	14.1	1	69.8	2	1	1
SU_FN_H	14.1	1	69.8	2	4	1
MO_FN_H	14.6	3	65.8	1	2	3
GS_FN_H	15.0	4	195.2	4	3	4

Whilst showing minor differences in MAE, the growing season (GS) frequency had a massive increase in MdSA compared to the three other calibration scenarios.

Driving data frequency

The high frequency calibration data scenario (FN) was the basis to compare the fourteen different driving data scenarios (Table 2.6). The findings show a completely different pattern to the expected ranks, with the expected number 1, placed second to last at the 13th position based on the error metrics. The top 4 positions show no real pattern when it comes hourly or daily meteorology being the favourite, however monthly inflowing data seems to be in position 2 and 3, despite being ranked 7th and 14th in the expected ranking. Overall, we see a more than 2 mg m⁻³ decreased in MAE and approximately 15 % in MdSA compared to the

expected 1 rank, with the highest frequency data. Which makes us wonder if the inflowing data is correct.

Table 2.6 Model errors under 14 driving data scenarios calibrated to fortnightly chl-a data sorted from smallest to largest based on ranked position MAE and MdSA. The underscored combination is the highest data frequency.

Calibration_ Inflow_ Meteorology	MAE (mg m⁻³)	#	MdSA (%)	#	Expected rank	Final position
FN_WI_D	11.9	1	55.2	2	11	1
FN_MO_H	13.1	5	53.8	1	7	2
FN_MO_D	12.3	2	63.0	7	14	3
FN_SP_H	13.2	7	57.1	3	6	4
FN_SU_H	13.2	6	62.2	6	3	5
FN_GS_D	12.9	4	65.5	9	9	6
FN_AU_D	13.4	10	61.7	5	12	7
FN_SP_D	12.7	3	71.4	12	13	8
FN_SU_D	13.3	9	64.0	8	10	9
FN_WI_H	16.3	14	58.7	4	4	10
FN_GS_H	13.6	11	66.2	10	2	11
FN_AU_H	13.3	8	78.9	13	5	12
<u>FN_FN_H</u>	14.1	12	69.8	11	1	13
FN_FN_D	15.1	13	79.3	14	8	14

Combined effect

The MAE and MdSA were considered across all combination, however due to showing a similar result, we focus further on the MdSA, which is a good fit for your data characteristics and scale-invariant and more robust to outliers than MAE.

A range of MdSA's was found from 53.8 % to 221.1% (Figure 2.4). The calibration data visually show the most impact, with the highest frequency of calibration generally staying the lowest, with occasional agreement of the MO and 2 instances of lower MdSA by the MO calibration.

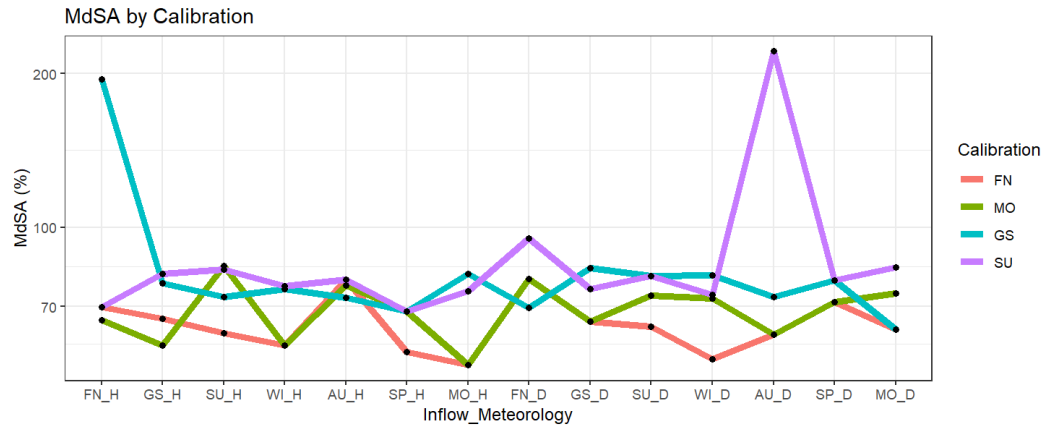


Figure 2.4 MdSA scores grouped by calibration data frequency. Calibration datasets are grouped by their sampling frequency: Fortnightly (FN), Monthly (MO), Growing Season (GS), and Summer (SU), to assess how data availability influences model skill. The x axis shows the different driving data combinations.

Hourly meteorology driving data has out of 28 possible combinations 7 values below 15, with Daily having 8. For the inflow, out of the 7 different frequencies only the daily frequency has 4 rankings under 15. The FN inflow driving data performs as one of the worst with no rankings below 15, showing inflow driving data to influence the model negatively, e.g. the less data the better.

In nine out of fourteen driving data combinations, FN calibration resulted in error rankings between 1st and 15th place, whilst in lower calibration frequencies of MO, GS and SU only six, one and zero combinations fall below 15 (Figure 2.5). This highlights that the calibration data does follow the expected trend and has influences on the model output.

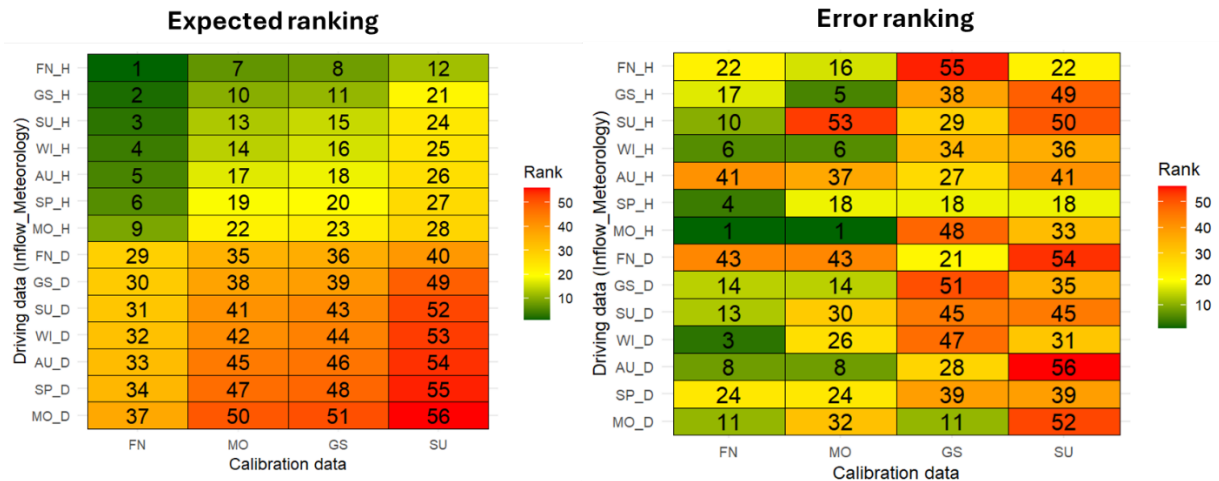


Figure 2.5 Expected ranking of the frequencies versus the found ranking. Left: Heat map of expected ranking based on the frequency factor per combination of data frequencies, with green being the highest frequency. Right: Heat map of differences between found ranking based on combined MAE and MdSA error metrics (number in black) and the expected ranking, with red being a decrease and green an increase in rank. The y axis shows the driving data frequency combinations, the x axis the calibration data frequencies.

An ANOVA was conducted to evaluate the influence of varying the temporal resolution of calibration, meteorological forcing, and inflow data on model performance, measured by the

MdSA of chl-a simulations. None of the main effects or interactions were statistically significant at the 0.05 level.

Among the main effects, calibration frequency explained the most variance in MdSA (Sum Sq = 5528.8, $F(3,18) = 2.36$, $p = 0.106$), though this was not statistically significant. Inflow frequency also contributed moderately (Sum Sq = 4645.2, $F(6,18) = 0.99$, $p = 0.460$), while the effect of meteorological resolution was negligible (Sum Sq = 197.6, $F(1,18) = 0.25$, $p = 0.621$).

Interaction effects between factors were also non-significant. The largest interaction sum of squares was observed for Calibration $\times$ Inflow (Sum Sq = 10741.4, $F(18,18) = 0.76$, $p = 0.713$), suggesting that variability in MdSA is not strongly driven by combined effects of forcing frequencies.

These results indicate that the temporal resolution of calibration, meteorological, and inflow data had no statistically significant impact on model accuracy as measured by MdSA, although calibration frequency showed a trend toward a potential effect.

2.3.3 Bloom detection at the WHO threshold

Bloom detection at the WHO threshold, expressed with the F1 score, resulted in a clear difference between daily and hourly meteorology frequency (Figure 2.6), where the hourly frequency results in F1 scores of about 0.05 higher compared to daily frequency. The calibration seems to matter much less, similarly the inflow driving data shows only minor differences which do not indicate any pattern.

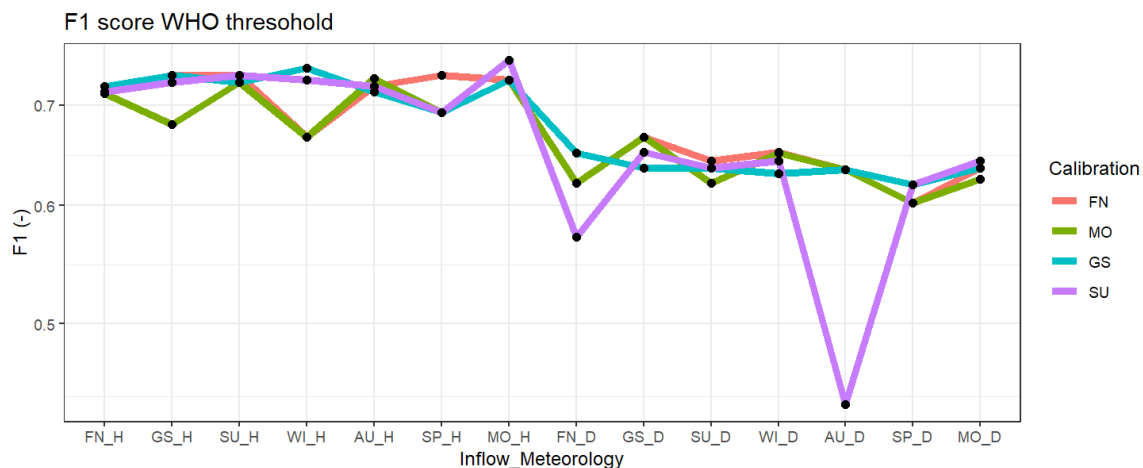


Figure 2.6 F1 scores grouped by calibration data frequency for the WHO threshold. Calibration datasets are grouped by their sampling frequency: Fortnightly (FN), Monthly (MO), Growing Season (GS), and Summer (SU), to assess how data availability influences model skill. The x axis shows the different driving data combinations.

The ranking results for bloom detection at the WHO threshold of 24 mg m^{-3} , therefore, also show larger influences based on meteorology driving data, with a 15 out of the 1 to 15 rankings fall within the hourly meteorology frequency (Figure 2.7). Whilst showing less of a distinct pattern, both summer and monthly inflow driving data frequency the most consistent pattern of all hourly meteorology driving data combinations falling in lower end of 1 to 15 range.

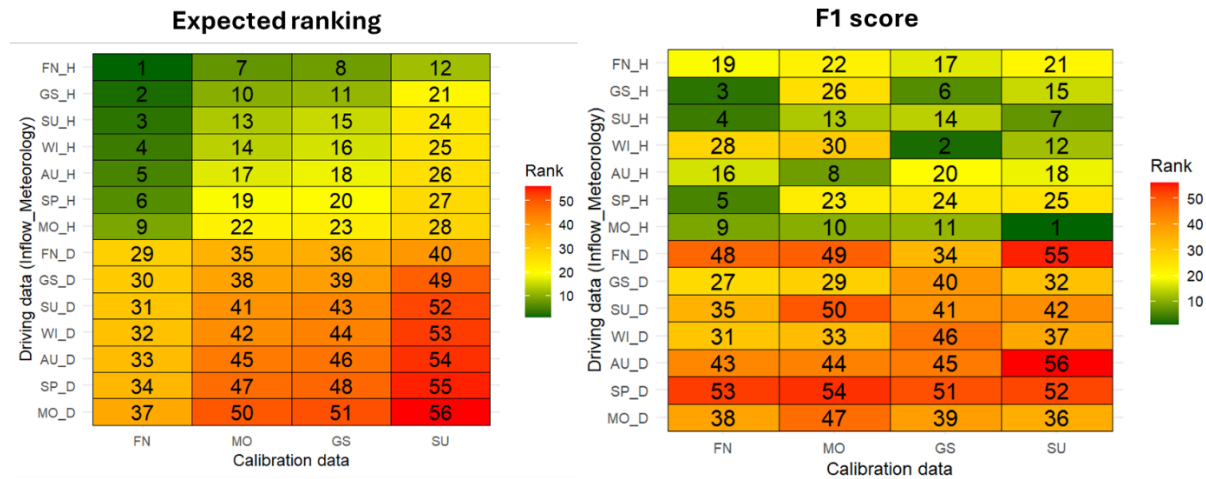


Figure 2.7 Comparison between expected rankings based on calibration data frequency (left) and actual model performance as indicated by F1 scores (right), using the WHO chlorophyll-a threshold (24 mg/m^3) for bloom classification. Lower calibration frequency is expected to yield lower model performance; this table contrasts that expectation with the observed F1-based rankings to assess consistency and highlight potential discrepancies.

The best performance of bloom detection ($F1 = 1$) falls in the MO_H combination of driving data similarly to the MdSA for the whole chl-a range, only this time with a summer calibration data which was originally expected to rank 23rd. This is not completely unsurprising, as this may result in a more bloom focused calibration that generally appear more prominent in summer. The F1 score ranking compared to the expected ranking does have a better overlap compared to the MdSA ranking.

The ANOVA analysis revealed a strong and statistically significant effect of meteorological resolution on bloom frequency ($F(1,18) = 123.38, p < 0.001$), indicating that the temporal resolution of meteorological data is a critical driver of modelled bloom occurrence. This factor alone explained most of the variance in F1 (Sum Sq = 0.117, compared to a residual sum of squares of 0.017), underscoring its importance.

In contrast, calibration frequency ($F(3,18) = 0.89, p = 0.465$), inflow resolution ($F(6,18) = 1.46, p = 0.247$), and all interaction terms were not statistically significant. These results

suggest that variation in calibration or inflow resolution did not meaningfully affect model estimates of bloom frequency, either alone or in combination with other factors.

Overall, this analysis highlights the dominant influence of meteorological data resolution on modelled bloom frequency, with other factors contributing comparatively little to model variance in this output.

As we know the threshold of the WHO is not waterbody specific, therefore a range of thresholds below (4 to 22 mg m⁻³) and above (26 to 44 mg m⁻³) were tested for their F1 scores. The WHO threshold showed a large significant effect of meteorology frequency on the F1 score, with no significant effects from inflow and calibration data frequency.

Thresholds below and above found similar results, however with significant variance caused by inflow data as well (Figure 2.8). The effect of meteorology and inflow data is much more evenly distributed between the two sources at lower thresholds, compared to at WHO and above, where meteorology is by far the dominant effect.

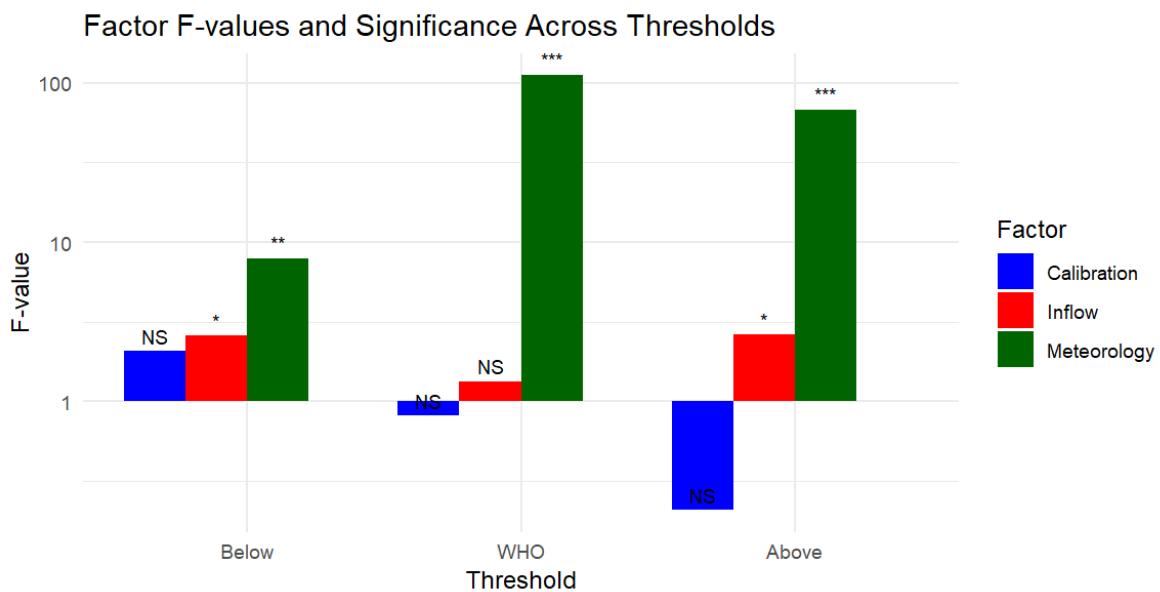


Figure 2.8 F-values (ratio of variance between groups to variance within groups) and significance levels per threshold per data group. (*** = 0, ** = 0.01, * = 0.05, NS = Not significant)

Overall, we see that meteorology has the largest significant effect on bloom detection, whilst calibration has the largest, albeit non-significant, effect on capturing the whole chl-a range according to the MdSA goodness of fit metric. We see inflow frequency has a minor effect on both the F1 and MdSA, however it tends to be negative, showing less data is better results, indicating possibly the inflowing data not being up to modelling standards. This could have implications for monitoring strategies in data-scarce waterbodies.

2.4 Discussion

This study showed that lake ecosystem modelling can be improved by optimising data collection decision. Despite potentially being more costly and labour intensive to increase monitoring frequencies for modelling purposes, it is still a more user friendly approach to improve modelling outputs than adjusting inherent model structures. With our findings and lessons learned from Esthwaite Water we aim to supply a practical route to enhancing model outputs for algal biomass simulation and bloom detection in waterbodies across the UK, potentially the globe.

2.4.1 Validation of using GLM-AED

The temperature validation of the original model (Figure 2.3) showed strong agreement between observed and modelled temperature, with MAEs of 1.03 °C (hourly) and 0.98 °C (daily), and R^2 values of 0.98 and 0.97, respectively. These values align well with those reported by Ward et al. (2020) for GLM-AED models, which showed MAEs ranging from 1.05 to 1.21 °C and R^2 values between 0.81 and 0.99. Similarly, our RMSE values (1.28–1.30 °C) were in line with, or lower than, those reported in other studies (Bruce et al., 2018; Bueche et al., 2017, 2020; Krinos et al., 2019; Ward et al., 2020).

For chl-a, our model achieved R^2 values between 0.31 and 0.40, which are higher than the 0.12–0.19 reported by Ward et al. (2020) but lower than the 0.69 found for the PROTECH model (Gray et al., 2019). Our R^2 is consistent with findings by Weng et al. (2020), highlighting variability in model performance across systems. MAEs for chl-a were substantially higher in our case (10.7–11.7 mg/m³) compared to Ward et al. (0.95–1.08 mg/m³), likely due to differences in trophic state, Lake Sunapee being oligotrophic with lower chl-a concentrations (5 mg/m³). Our chl-a RMSEs (16.3–18.9 mg/m³) closely matched those reported by Krinos et al. (2019) (16.9 mg/m³) and were much lower than those in Weng et al. (2020).

Across the different data frequency scenarios, our best GLM-AED chl-a outputs yielded MAEs ranging from 11.9 to 24.4 mg/m³. These values are comparable to those from other systems, such as Karaoun Reservoir (14.47–18.03 µg/L; (Fadel et al., 2019)) and Lake Erie (18.23 µg/L; Q.(Q. Wang & Wang, 2021)). The Median Symmetric Accuracy (MdSA) of 53.8% to 221.1 % supports the model's reliability, even though this metric is not commonly reported in GLM-AED literature. It indicates that the median absolute percentage error is just over

half (for 53%) of the observed value, which aligns with other studies where RMSEs and MAEs often approach or exceed half the mean chl-a concentration ((Fadel et al., 2019; Wang & Wang, 2021; Weng et al., 2020)). Given the lake-specific nature of chl-a dynamics, such variability in model performance metrics is expected and reinforces the need for context-specific evaluation.

2.4.2 Relative importance of calibration and driving data

The relative importance of driving data (Meteorology and Inflow) and calibration data depends on the modelling objective. Our results highlight that calibration data is the most critical factor in determining the model's predictive performance for chl-a estimates, with MdSA values being drastically lower using high frequency calibration data as opposed to low frequency calibration data. Next to that, calibration data frequency showed a higher explained variance and nearly significant impact ($F = 2.36$, $p = 0.106$).

In other fields, like crop-modelling (He et al., 2017), forest remote sensing (Lindgren et al., 2022) and computer science (Watson et al., 2021) the importance of calibration has already been explained. However, compared to the importance of driving data the result was still partly unexpected, as usually driving data is expected to represent temporal dynamics and are typically critical for simulating lake responses. Calibration data, while essential for parameter tuning, is not expected to have such a dominant role in influencing the model's response to new inputs. However, our findings reinforce the notion that an accurate baseline, achieved through high-frequency calibration data, is essential before driving data can effectively contribute to model predictions. When the foundation provided by calibration data is flawed, the impact of driving data becomes negligible.

Whilst the contributions of higher frequency inflow and meteorology data resulted in a smaller variance compared to calibration data, we do need to state, that without good driving data, even the best calibrated model will not run, which is why it is still essential to have good driving data, despite making more impact improving your calibration data.

We speculate that the marginal effect of inflow data frequency could indicate a few things. The most obvious being that our inflowing data, even at the highest frequency, is not accurately describing what goes into the system. Which would explain why the lowest MdSA and F1 scores were found using the lowest frequency inflow data (Monthly), i.e. the model

performing better with less inflow data. The approximation of these inflowing nutrients is from a measuring station at the outflow of Esthwaite Water, likely resulting in too low or too late nutrient concentration patterns. Another possible reasoning, which could also be the case in combination with flawed data, is that chl-a concentrations or blooms are not reacting to the inflowing nutrients as much due to a much larger impact of internal nutrient cycling, which has indeed been found to be a problem in Esthwaite Water (Mackay et al., 2012).

Despite these possible problems with the inflow, we have shown that outputs within reasonable accuracy according to literature can still be achieved with low frequency and low accuracy inflow data. As inflowing nutrients are generally one of the more difficult and costly data to monitor, knowing that lower frequency or accuracy of these nutrients still does the job is great for management monitoring schemes and gives options for lakes with less resources.

The meteorology frequency did not show an effect on the MdSA of the chl-a output, highlighting that driving data is needed, but frequency may not be as important. We do like to note, upon inspection of the timeseries of chl-a, hourly meteorology did seem to underestimate blooms ever so slightly more compared to daily meteorology, possibly indicating bloom growth rates to be influential based on day rather than hourly. With that, meteorology did have a large influence on bloom agreement (F1 scores). As temperature and light, are a few of the main drivers of algal growth and consequently blooms (Klemaš, 2012; Paerl et al., 2020), we anticipated meteorology would influence bloom dynamics, with higher temporal resolution yielding more accurate simulations. The ability to resolve diurnal variability in light availability, which plays a critical role in phytoplankton growth is likely better done using hourly data. Which better captures rapid fluctuations in irradiance, enabling more precise simulation of short-term growth responses. In contrast, daily meteorology inputs extrapolated to a diurnal cycle may obscure these fine-scale patterns, potentially missing bloom events.

2.4.3 Bloom detection vs. full chl-a concentration modelling

Full chl-a concentration modelling

When modelling the full range of chl-a concentrations, both calibration and driving data frequency had notable, but sometimes counterintuitive, effects.

For calibration data, higher-frequency inputs such as fortnightly or monthly observations resulted in lower model errors than seasonal subsets (e.g., growing season or summer-only

data). These results suggest that consistency and regularity in calibration data are more valuable than high-resolution or seasonally constrained inputs. Although increasing temporal resolution might still enhance model performance, the gains appear marginal beyond the fortnightly scale. A strategic approach could therefore involve using high-quality, frequent calibration data over a shorter period (e.g., 3 years) to support modelling over longer timescales (e.g., 100 years), if the calibration captures relevant variability. A possible cost effective method towards higher frequency chl-a calibration data could be the use of remote sensing (Klemas, 2012; Rousso et al., 2020).

Regarding driving data, the results were variable across input types. For meteorological data, daily inputs generally outperformed hourly ones in terms of minimising model error (e.g., MdSA). While it may be expected that higher-frequency inputs improve accuracy, hourly meteorological data often led to overestimation of chl-a peaks by over 10 mg/m³ more compared to daily in summer, whilst daily overestimated diatom peaks. This likely results from the disconnect between algal growth rates, which operate on daily scales, and the high variability captured in hourly weather data. Thus, daily meteorology strikes a better balance between temporal resolution and ecological realism.

For inflow data, higher-frequency inputs (e.g., daily or hourly) were consistently outperformed by lower-frequency data such as monthly inflows. Although in theory, high-resolution inflow data could enhance model performance, in practice, they may introduce noise or misalign with the ecological drivers of chl-a variability. This suggests that for chl-a modelling where inflow data is inaccurate, monthly inflow data may be sufficient, and perhaps even preferable.

Bloom detection

In contrast, the requirements for bloom detection diverged from those needed for continuous chl-a modelling. The frequency of calibration data had little to no influence on the F1 score, indicating that once the model is appropriately tuned, the ability to classify blooms above a threshold is not as sensitive to calibration frequency compared to driving data. While still essential for baseline model performance, calibration data play a less critical role in bloom detection than in continuous chl-a modelling.

On the other hand, driving data frequency, especially for meteorology, proved highly influential for bloom detection. Notably, using hourly meteorological data improved the F1 score by up to 0.05 compared to daily inputs, emphasising the importance of capturing short-

term weather dynamics (e.g., radiation spikes or temperature surges) that can rapidly trigger bloom events. This sensitivity highlights a trade-off: while continuous chl-a modelling benefits from smoothed daily inputs, bloom events require high-frequency meteorological data to be detected accurately.

For inflow data, the pattern again favoured lower-frequency inputs for bloom detection. Although inflow contributed significantly to the variance in bloom predictions, monthly inflows outperformed higher-frequency alternatives, and the contribution was sometimes negative, suggesting that too much detail can reduce signal clarity. These findings indicate that, like the full chl-a range modelling, coarser inflow data can still support robust bloom predictions.

2.4.4 Lessons from Esthwaite Water for water managers

The following recommendations are derived from exploring the effects of driving on calibration data frequency on chl-a simulations and bloom detection performance. These findings were further contextualised through discussions with experts familiar with Esthwaite Water, which helped align model-based insights with practical monitoring constraints and management priorities.

Align Strategy with Modelling Goal: Clearly define whether your objective is to model the full range of chl-a concentrations or to detect bloom event, as these goals require different data strategies.

Results showed that continuous chl-a modelling was relatively robust to lower-resolution meteorological and inflow inputs, if calibration data were consistent. In contrast, bloom detection performance was highly sensitive to meteorological resolution, with hourly data significantly improving bloom detection (F1 scores).

For continuous chl-a modelling, focus on consistent calibration data and daily meteorology. Both meteorology and inflow can often remain low-resolution unless nutrient pulses are proven to be a dominant driver of blooms.

For bloom detection, prioritise hourly meteorology. Adjust the importance of inflow based on bloom thresholds and catchment dynamics (Figure 2.7). Calibration remains necessary but was found to be less influential than meteorological resolution for classification performance.

Prioritise Calibration and Meteorological Inputs: When the goal is to model both the full chl-a range and bloom detection, use recent, multi-year chl-a datasets at fortnightly or monthly resolution for calibration. This frequency supports accurate model tuning without overfitting. An hourly meteorology significantly improves classification accuracy for bloom detection and still gives reasonable results for the chl-a concentration range should be used when available to optimise results for both goals.

Optimise Inflow Data Use: Results showed that monthly or seasonal inflow data were generally sufficient for both chl-a modelling and bloom detection. In some cases, higher-frequency inflow data reduced model performance, likely due to mismatches between measured flow locations and actual nutrient delivery to the lake. As such, higher-frequency inflow data should only be used when they accurately represent ecologically relevant inputs for the system.

2.5 Conclusion

This study demonstrated that both the choice and frequency of data inputs critically influence model performance in freshwater systems. By simulating data constraints, we evaluated the feasibility of using lower-frequency data while maintaining reliable outputs, and assessed model accuracy across different bloom thresholds, including those set by the WHO.

Our results highlight the importance of aligning data strategies with specific modelling objectives. For continuous chl-a concentration modelling, consistent calibration data and daily meteorological inputs are most effective. In contrast, accurate bloom detection requires higher-frequency meteorological data, with inflow data being more influential in certain contexts, especially at extreme bloom thresholds.

The adaptability of the GLM-AED model across diverse data environments further supports its application in both data-rich and data-scarce lakes. These findings provide actionable guidance for water managers, informing decisions on data collection priorities, data needs at bloom thresholds, and model applicability. By tailoring data availability and monitoring to specific modelling goals, managers can enhance the accuracy, relevance, and efficiency of forecasting efforts like GLM-AED across a range of lake systems and data availabilities.

Chapter 3: Improving algal bloom modelling in eutrophic lakes by calibrating the General Lake Model with satellite remote sensing products

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Abstract.

Accurate forecasting of algal blooms in lakes can support effective freshwater management. However, observational datasets for calibrating and validating algal bloom forecasting models such as the General Lake Model - Aquatic Eco Dynamics (GLM-AED) are often scarce, which impedes robust model calibration and forecasting ability. Satellite remote sensing can help fill these gaps by offering high-frequency, large-scale measurements of phytoplankton chlorophyll-a concentration (mg m^{-3}), but satellite chl-a products often carry high uncertainty. Here we introduce a novel approach to quantify uncertainty in satellite chl-a based on conformal prediction, with the aim of integrating robust chlorophyll-a products into

GLM-AED. Using Sentinel-2 imagery from two eutrophic lakes in the UK, Esthwaite Water and Loch Leven, we obtain remotely sensed chlorophyll-a with low systematic signed percentage bias (-1.22% and 0.38) and moderate median symmetric accuracy (15.87 and 43.02%) using Polymer atmospheric correction. We effectively flag potentially uncertain chlorophyll-a estimates (coverage factor: 75.6 - 81%). Integrating the screened remotely sensed chlorophyll-a estimates improved GLM-AED algal bloom forecasts by 50% in Loch Leven and 13% in Esthwaite Water, with the greater improvement in Loch Leven attributed to its higher initial model errors. In contrast, incorporating unscreened chlorophyll-a estimates into GLM-AED increases validation errors on average by 32%.

Our findings show that process-based model predictions can substantially benefit from incorporating additional satellite-derived chlorophyll-a estimates. At the same time, they highlight a crucial need for robust uncertainty quantification to support downstream applications such as algorithm validation, biological monitoring in data-scarce regions, and water management decision-making.

Moreover, because conformal prediction is model-agnostic and satellite-derived chlorophyll-a products are globally accessible, our study paves the way for large-scale, well-calibrated bloom forecasting through process-based models.

Keywords: Algal bloom forecasting, lake modelling calibration, earth observation, conformal prediction

3.1 Introduction

Algal blooms, defined as high accumulation of phytoplankton or cyanobacteria in aquatic systems, have become a pressing issue in lakes and reservoirs worldwide (Beaulieu et al., 2013; Feng et al., 2024; Paerl & Huisman, 2008). Blooms can appear swiftly under favourable conditions driven by warm temperatures (Jöhnk et al., 2008; Paerl & Huisman, 2008), abundant nutrients (Beaulieu et al., 2013) and stable water column conditions, such as thermal stratification (Bormans et al., 2005). These complex and interconnected drivers highlight the dynamic and often unpredictable nature of algal blooms.

Process-based models, like the General Lake Model (GLM) coupled with the Aquatic Eco Dynamics model (AED) (Hipsey, 2022; Hipsey et al., 2019), have the capabilities to resolve algal bloom dynamics and their temporal heterogeneity. GLM-AED can simulate temperature (Bruce et al., 2018; Bueche et al., 2017; Mesman et al., 2020), dissolved oxygen, total phosphorus, nitrate, ammonium and a proxy for algal biomass, phytoplankton chlorophyll-a concentration (chl-a) (Fadel et al., 2019; Fenocchi et al., 2019; Krinos et al., 2019; Soares & Calijuri, 2021; Ward et al., 2020). While GLM-AED demonstrates the potential to simulate algal blooms, its effectiveness remains contingent on the availability of high-quality observational datasets.

Meteorological and hydrological data, such as air temperature, wind speed, solar radiation, inflow rates, and nutrient concentrations, are essential for driving the GLM-AED model and can often be obtained from models or in situ sensors at relatively low cost. In contrast, chl-a measurements, which are used for calibrating or validating phytoplankton dynamics within the model, are expensive and labour-intensive to collect, as they rely on laboratory analysis. This leads to limited spatial and temporal coverage of consistent chl-a observations across lakes.

This scarcity of in situ chl-a measurements limits our ability to model algal dynamics, including forecasting of blooms through process-based models and widens the gap between advances in hydrodynamic and ecological lake modelling. To close the observation gap between physical and biological variables, satellite remote sensing of lakes could provide direct estimates of water constituent concentrations such as chl-a (Bukata et al., 1974; Morel, 1980). In particular, the Sentinel-2 (S2) MultiSpectral Instrument (MSI) constellation provides high spatial resolution imagery (10 – 60 m) with a short revisit cycle of 2-3 days, with the A,B and C satellites in orbit (10-day nominal global coverage).

However, the estimation of chl-a through S2 MSI is subject to various sources of uncertainty including the necessary correction for atmospheric disturbances (Warren et al., 2019), adjacency effects of the surrounding environment (Santer & Schmechtig, 2000), complex water constituent compositions (Werther, et al., 2022a) and errors in observational processing schemes (Burggraaff, 2020b). Algorithmic approaches for chl-a retrieval are subject to model-specific uncertainties, and only a handful of methods explicitly quantify them (Werther, et al., 2022b). As multiple sources of uncertainty are inherent within aquatic remote sensing, accurately quantifying uncertainty in satellite-derived products for downstream uses, such as an input to GLM-AED, is pivotal to reliable modelling (Werther & Burggraaff, 2023). To enable the use of satellite-derived chl-a products for improved GLM-AED calibration and validation, we introduce an approach rooted in conformal prediction (CP) (Vovk et al., 2005). Using a separate baseline dataset, CP evaluates how closely new chl-a estimates conform to established patterns. CP not only produces well-calibrated, spatially explicit uncertainty estimates but also offers a data-driven threshold for filtering unreliable observations. Although CP is well established in applied machine learning and terrestrial remote-sensing tasks, such as estimating canopy height and identifying tree species (Fontana et al., 2023; Papadopoulos, 2008; Singh et al., 2024), its application in aquatic remote sensing is only indirect (Waczak et al., 2024). Here, we apply CP to a range of S2 MSI chl-a retrieval approaches and illustrate how its model-agnostic design allows seamless integration with these approaches.

We hypothesise that incorporating MSI-derived chl-a estimates into the GLM-AED model will enhance both its calibration and estimation accuracy relative to using only in situ chl-a measurements. This assumption is driven by evidence from prior research suggesting that satellite-based observations can refine ecosystem models (Deng et al., 2024; Hedger et al., 2002). We also hypothesise that filtering MSI chl-a estimates through CP-derived uncertainty thresholds will result in greater levels of improvement than relying on unfiltered estimates, given that discarding highly uncertain observations may prevent error propagation.

Accordingly, this study addresses the following questions:

- (1) To what extent can chl-a be accurately estimated from MSI data over two eutrophic lakes for integration into the GLM-AED model?
- (2) How effective is the conformal prediction method in filtering MSI-derived chl-a estimates?
- (3) Does incorporating these filtered chl-a estimates into the calibration of GLM-AED improve the accuracy of algal bloom forecasting and detection?

3.2 Methods

3.2.5 in situ data

Study lakes

Two freshwater lakes in the United Kingdom (UK) were used as case study sites (Figure 3.1). Esthwaite Water is a small (surface area of 0.96 km²), shallow (mean depth 6.9 m), eutrophic lake located in the English Lake District (Mackay et al., 2012, 2014; Mortimer, 1942). Loch Leven is a comparably larger (surface area 13.3 km²) and shallower (mean depth 3.9 m) eutrophic lake in lowland Scotland (Carvalho et al., 2012). Both lakes have a long history of algal blooms consisting of cyanobacterial and diatom species (Maberly et al., 2011; May & Spears, 2012) with mean annual chl-a values of 18.5 mg m⁻³ in Esthwaite Water and 25.1 mg m⁻³ in Loch Leven (Carvalho et al., 2012; Maberly et al., 2011; Madgwick et al., 2006; Spears et al., 2012). In addition, both lakes have been studied using Earth observation (Hedger et al., 2002; Hunter et al., 2010; Liu et al., 2021).

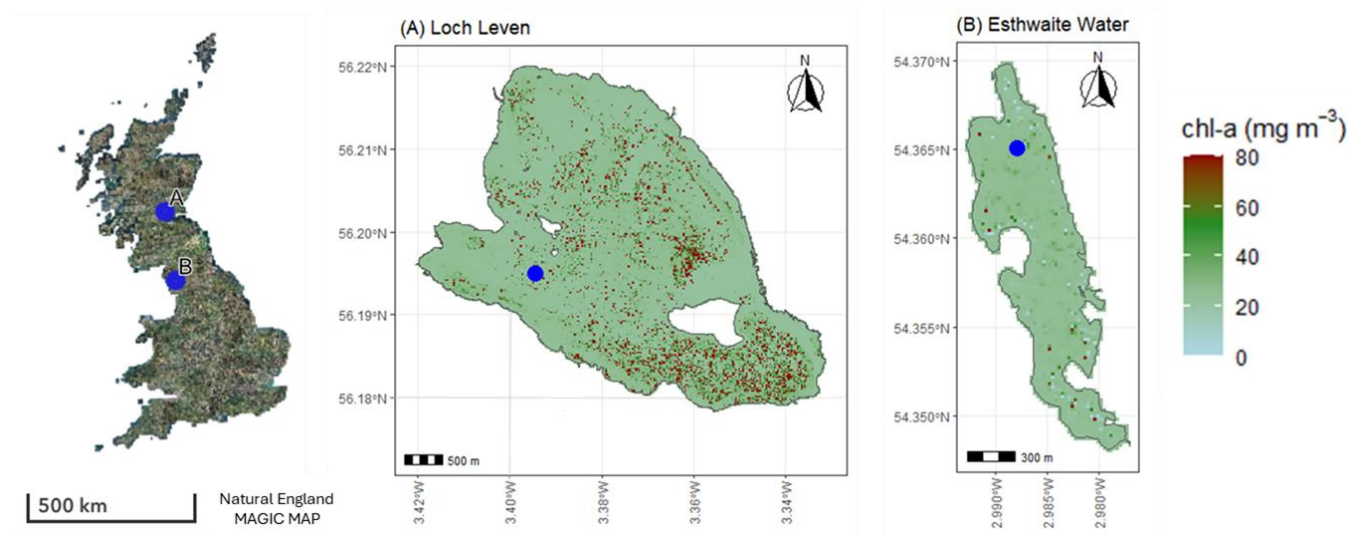


Figure 3.1 MSI chl-a maps of Loch Leven (A) and Esthwaite Water (B) and their respective locations in the UK, using Polymer atmospheric correction and lake-optimised Gurlin et al. (2011) on 2016-06-09 (A) and 2016-07-19 (B). The blue points indicate in situ sampling sites.

Chlorophyll-a concentration

Fortnightly in situ chl-a for Esthwaite Water (n = 156) (Feuchtmayr et al., 2021, 2024, 2025) and Loch Leven (n = 145) (Dudley et al., 2013; Taylor et al., 2021, 2022a, 2022b, 2023) were extracted for the period January 2016 to December 2022 from an ongoing long-term monitoring programme by the UK Centre for Ecology & Hydrology (UKCEH) (Figure 3.1).

Samples were unavailable or could not be collected in June and July 2019 and March to July 2020 due to the Covid-19 pandemic. For Loch Leven, chl-a data were only available until November 2021.

For both lakes, chl-a was determined by filtering a known volume of water from a 0-5m integrated sample onto a Whatman GF/C filter on the day of sampling with the filter then frozen for later analysis. Filters were defrosted and extracted in a faster hot methanol method for Esthwaite Water and a slower cold methanol for Loch Leven, which reduces thermal degradation. These were measured spectrophotometrically with absorbance values converted to chl-a following the protocols of Talling (1974) for Esthwaite Water by and Rice et al. (2017) for Loch Leven.

GLM-AED driving data

Latitude, longitude, depth, area and elevation for each lake were provided by UKCEH (Mackay et al., 2014; Spears et al., 2012). Hourly shortwave radiation, longwave radiation, air temperature, relative humidity, windspeed, rain and snow were obtained from ERA 5 simulations for 2016 to 2022 for the respective pixel (latitude-longitude $0.25^\circ \times 0.25^\circ$ grid) in which the lake coordinate falls (Hersbach et al., 2018). For the same period, daily lake inflow or outflow data were obtained from the UK National River Flow Archive for the main inflowing rivers (Esthwaite Water: Black Beck; Loch Leven: North Queich, South Queich and Greens Burn) or the outflow. In both lakes, outflow was assumed to be equal to the inflow. Fortnightly water temperature and chemistry in situ measurements (pH, phosphorus, nitrate, ammonia and silica) were provided by UKCEH and linearly interpolated to provide daily resolution.

3.2.6 Satellite data processing

S2 MSI images were atmospherically corrected to derive surface water remote-sensing reflectance ($R_{rs}(\lambda)$), followed by a valid pixel identification to exclude non-water pixels using IdePix (Identification of Pixel features) (Skakun et al., 2022). We then assessed the spatial homogeneity of the water surface area around the fortnightly sampling locations in Esthwaite Water and Loch Leven. We used thirteen inland water Optical Water Types (OWTs) defined in Spyarakos et al. (2017), representing clusters of water bodies with similar optical characteristics, to inform chl-a retrieval algorithm selection for each lake (Atwood et al., 2024; Eleveld et al., 2017; Liu et al., 2021; Neil et al., 2019). Finally, we quantified the

uncertainties associated with MSI chl-a estimates through CP, resulting in filtered MSI chl-a to calibrate the GLM-AED model.

Atmospheric correction and valid pixel identification

S2 MSI tiles (30UVF for Esthwaite Water and 30VVH for Loch Leven) were processed using three different atmospheric correction algorithms: Atmospheric Correction for OLI ‘lite’ (ACOLITE) (Vanhellemont & Ruddick, 2016), POLYnomial-based approach of MERIS data (Polymer) (Ramon et al., 2011) and Case 2 Regional CoastColour atmospheric correction (C2RCC) (Brockmann et al., 2016) for the period of 2016 and 2024. A 3x3 MSI pixel grid around the respective in situ coordinate was extracted for match-up generation with the fortnightly in situ sampling following the match-up protocol of Concha et al. (2021). We excluded pixels flagged as invalid due to cloud (including ambiguous, sure, and a buffer) or cloud shadow, snow/ice, bright, coastline land, white and glint risk.

Spatial homogeneity test and S2 matchups

A spatial homogeneity test was conducted to identify MSI scenes affected by high spatial R_{rs} variability within 3x3 kernels of valid pixels (Zibordi et al., 2018). Spatial coefficient of variation (CV), defined as the ratio of the standard deviation to the mean, was calculated for the 560 nm band (Zibordi et al., 2018). Pixel kernels with a CV greater than 0.25 (25%) were deemed to have high spatial variability and removed from the dataset.

Remote sensing algorithm calibration and validation

The resulting MSI scenes were matched with in situ chl-a within a +/- 3-day range of the in situ sampling date following previous studies (Ansper & Alikas, 2018; Ruddick et al., 2019). A 3-day window resulted in significantly more match ups (± 50 matchups) than a 1 (± 22) or 2 (± 34) day window. For all valid R_{rs} (λ) an OWT membership score was calculated by estimating of the spectral angle (Kruse & Lefkoff, 1994; Liu et al., 2021) and the OWT with the highest similarity score was assigned (Spyrakos et al., 2017), resulting in one OWT (table 3.1) per pixel. The OWTs were assigned to one of three clusters based on common cluster characteristics (Table 3.1; Neil et al., 2019). Cluster A represents the most transparent water (in terms of biomass and turbidity), B represents moderately transparent water conditions associated with mesotrophic status and C represents turbid and/or hypereutrophic conditions.

Table 3.1 Optical Water Types (OWT), characteristics, trophic status, and clustering. The table summarises the characteristics and trophic status of different OWTs based on their reflectance features and associated water quality properties. Each OWT is categorised into a trophic status (hypereutrophic, meso-eutrophic, or oligotrophic) and assigned to a cluster (A, B, or C).

OWT	Dominant characteristics	Trophic status	Cluster
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1	Hypereutrophic waters with scum of cyanobacterial bloom and vegetation like R_{rs} .	Hypereutrophic	B
2	Diverse reflectance shape, marginal dominance of pigments and CDOM over inorganic suspended particles	Meso-eutrophic	B
3	Clear waters	Oligotrophic	A
4	Turbid waters with high organic content	Meso-eutrophic	B
5	Sediment-laden waters	Meso-eutrophic	B
6	Balanced effects of optically active constituents at shorter wavelength	Hypereutrophic	C
7	Highly productive waters with high cyanobacteria abundance and elevated reflectance at the red/near-infrared spectra	Hypereutrophic	C
8	Productive waters with cyanobacteria presence and with R_{rs} peak close to 700 nm	Hypereutrophic	C
9	Optically neighbouring to OWT2 but higher R_{rs} at shorter wavelength	Oligotrophic	A
10	CDOM rich waters	Hypereutrophic	C
11	High in CDOM with cyanobacteria presence and high absorption efficiency by NAP	Meso-eutrophic	B
12	Turbid, moderately productive waters with cyanobacteria presence	Meso-eutrophic	B
13	Clear blue water	Oligotrophic	A

Chlorophyll-a algorithms

Nine widely used chl-a algorithms (Table 3.2) were evaluated for the case study lakes.

Algorithms 1 to 7 are empirical band-ratio and (semi-) analytical algorithms, 8 and 9 are probabilistic neural networks. All algorithms use multispectral $R_{rs}(\lambda)$ in selected bands as input (Table 3.2).

Algorithm parameters were optimised for the case study conditions within each OWT cluster (Table 3.1) using a nonlinear fit for algorithms 3, 4 and 6 and a linear model fit for algorithm 5, because global algorithm coefficients often fail to generalise effectively to individual lakes (Werther, et al., 2022b). Algorithms 1, 2 and 7 have fixed parameters, and the two probabilistic algorithms (8 and 9) are calibrated based on large-scale application and therefore cannot be optimised.

Table 3.2 Chl-a estimation algorithms used in this study. Ranges are adjusted based on findings of Odermatt et al. (2012)

Name	Abbreviation	Used bands	Chl-a application range (mg m ⁻³)	Reference
1 Two Band MERIS	Gil2band	665, 708	0-80	(Gilerson et al., 2010)
2 Three Band Meris	Gil3band	665, 708 and 753	0-80	(Gilerson et al., 2010)
3 Ocean Colour 2-band	OC2	490,560	0.012-15	(O'Reilly, 2000)
4 Ocean Colour 3-band	OC3	443,490,560	0.012-15	(O'Reilly, 2000)
5 Moses 2-band	Moses	665,708	10-100	(Moses et al., 2009)
6 Gurlin 2-Band	Gurlin	665,708	2.3-200.8	(Gurlin et al., 2011)
7 Gons05	Gons	665,708, 783	0-100	(Gons et al., 2002)
8 Bayesian Neural Network based on Monte Carlo Dropout	BNN	All bands (443 – 783)	0-68	(Werther, et al., 2022b)
9 Mixture Density Network	MDN	All bands (443 – 783)	0-1000	(Pahlevan et al., 2020)

MSI estimates in oligo-mesotrophic lakes with low to moderate chl-a concentrations are particularly susceptible to inaccuracies in satellite-derived retrievals (Neil et al., 2019; Werther et al., 2022a). To address this, we introduce a separate classification, “BNN < 10,” which uses the Bayesian Neural Network (BNN) approach by Werther et al. (2022b). This approach targets lakes with chl-a below 10 mg m⁻³ in OWTs 2, 3, 4, 5, and 9, providing estimates that carry a BNN-specific uncertainty below 60%. Whenever these BNN-based low uncertainty estimates are available, they take precedence over other algorithm values. The algorithm performance for each OWT cluster was assessed using three widely used metrics: the Pearson correlation coefficient (R), to measure the strength of the linear relationship between in situ and MSI chl-a estimates; the mean absolute error (MAE); and the Median Symmetric Accuracy (MdSA), which quantifies the median error between in situ chl-a and estimated chl-a (Morley et al., 2018), and is commonly used in remote sensing literature (Pahlevan et al., 2020; Werther, et al., 2022b):

$$MdSA = (e^{\text{median}(\lceil \log(\frac{y_{est}}{y_{true}}) \rceil)} - 1) \times 100 \quad (1)$$

and the Symmetric Signed Percentage Bias (SSPB), which evaluates whether an algorithm systematically over- or under-estimates chl-a (Morley et al., 2018):

$$SSPB = \text{sign}\left(\text{median}\left(\log\left(\frac{y_{est}}{y_{true}}\right)\right)\right) \left(e^{\lceil \text{median}(\log(\frac{y_{est}}{y_{true}})) \rceil} - 1\right) \times 100 \quad (2)$$

In which Y_{est} represent the estimated chl-a concentrations from the model, algorithm or MSI and Y_{true} represents the in situ chl-a concentrations. The best-performing algorithms were identified for each OWT cluster and subsequently combined to calculate MAE, MdSA, and SSPB values over the whole chl-a range. These metrics facilitated the selection of the optimal OWT-clustered chl-a algorithm and atmospheric correction combination for each lake.

3.2.7 Conformal prediction uncertainty quantification

Conformal prediction (CP) (Angelopoulos & Bates, 2023); Vovk et al., 2005) was adapted here to quantify uncertainty in MSI-derived chl-a estimates (Figure 3.2). We used a *non-conformity percentage* as a proxy for uncertainty, based on the idea that the uncertainty associated with a new MSI chl-a retrieval relates to how the chl-a retrieval error compares with those of the reference observations. In this context, error is the non-conformity score (α_i) defined as the absolute error between an MSI chl-a estimate and its corresponding match up in situ measurement.

The absolute error for MSI chl-a estimates with corresponding in situ observations (matchups) was calculated and the dataset was split into two sets: conformity (reference dataset) and test (new observations). In the CP framework, the terms conformity and test are used instead of calibration and validation to avoid confusion with their traditional use in chl-a algorithms and GLM-AED model tuning. While these dataset splits may appear similar, their functions differ: calibration and validation involve adjusting and evaluating model parameters, whereas conformity and test assess the consistency of new data without modifying the model. The terminology reflects these distinct roles.

One year was assigned as the test set, while the remaining years (six for Esthwaite Water and five for Loch Leven) formed the conformity set (Figure 3.2). As noted previously, not all MSI chl-a estimates had corresponding in situ chl-a measurements (i.e., no match-up); these estimates were assigned to the test set. Their absolute errors for these observations were estimated using the following procedure:

1. Identifying the three in situ chl-a measurements closest in time (day of the year).
2. Averaging these measurements by weighting same-year observations twice to account for inter-annual variability.
3. Calculating the absolute difference between the MSI estimate and this weighted average.

We then sorted the non-conformity scores from the conformity set ($\alpha_{conformity}$) in ascending order. For each test observation, we determined the position of its non-conformity score ($\alpha_{test,i}$) within the sorted conformity set and calculated its percentile rank, termed the non-conformity percentage.

Prediction intervals were derived using the 5th and 95th percentiles of $\alpha_{conformity}$ and scaled by the ratio of $\alpha_{test,i}$ to the median of $\alpha_{conformity}$ to accommodate varying uncertainty levels. Calibration quality was evaluated using a coverage factor, i.e. the proportion of intervals that successfully encompassed the interpolated in situ chl-a values, including those without a direct match-up (Saranathan et al., 2024; Werther, et al., 2022a; Yao et al., 2019). An automatic rejection threshold ($\hat{q}$) was set at the 90th percentile of $\alpha_{conformity}$: if a test sample's non-conformity percentage exceeded this threshold, it was classified as an outlier. Additionally, to illustrate the impact of uncertainty filtering, a stricter manual threshold of 50% was applied, resulting in three filtering scenarios for MSI-derived chl-a estimates: All Earth Observations (EO) (no filtering), High NC (filter out values above 90%) and Low NC (filter out values above 50%).

The conformal prediction process was executed in folds that resampled the data, ensuring that each year served as the test set once so that every MSI chl-a estimate received a non-conformity percentage. For estimates appearing in multiple folds, the final non-conformity percentage was computed as the average across folds.

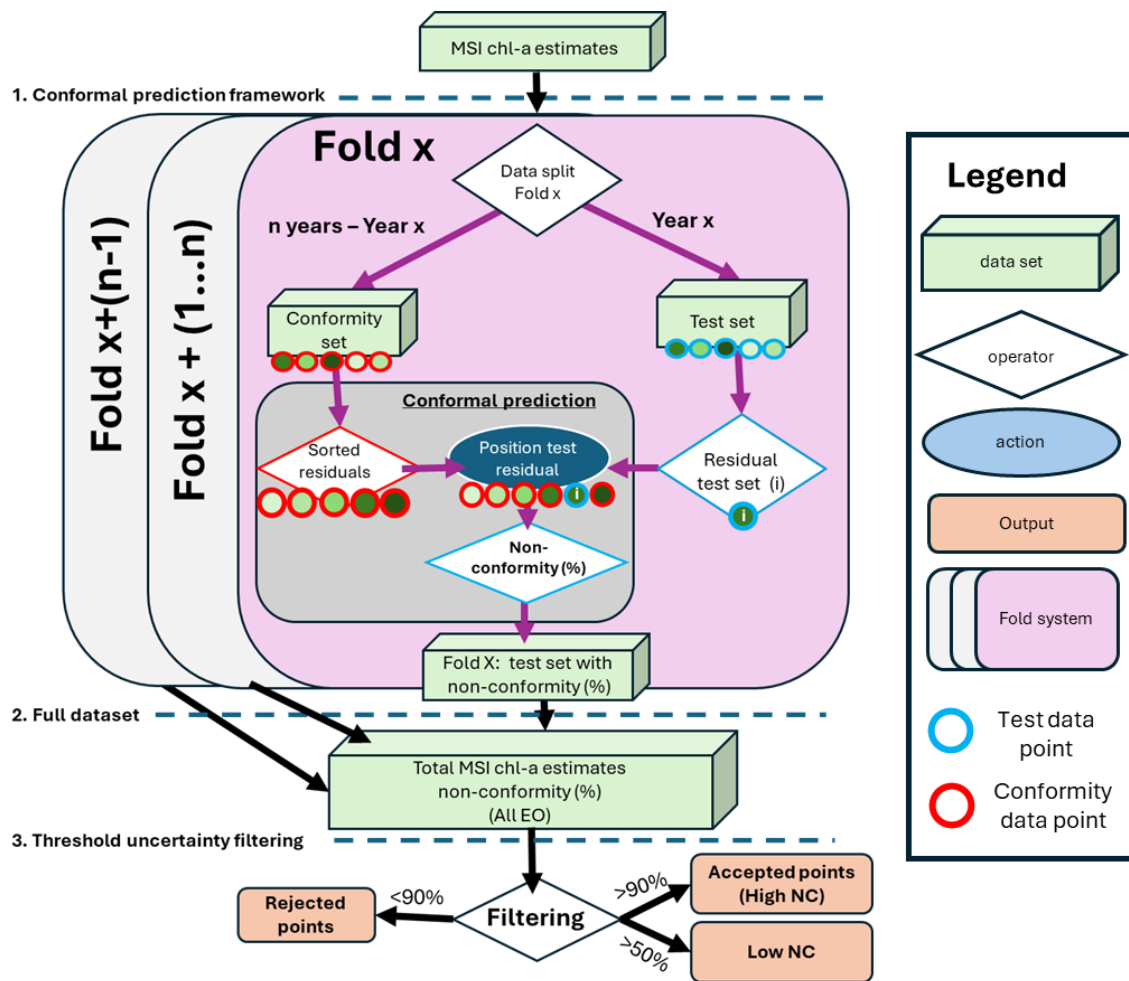


Figure 3.2 Overview of the conformal prediction approach developed based on Angelopoulos & Bates (2023) and Vovk et al. (2005).

Our CP approach includes two adaptations to quantify uncertainty in satellite-derived chl-a estimates. First, rather than splitting data into three sets (training, calibration, and test) as required by typical CP applications in machine learning settings (Angelopoulos & Bates, 2023; Singh et al., 2024; Waczak et al., 2024), we leverage the fact that most chl-a algorithms used in this study are semi-analytical or empirical. These methods do not require training; hence, we partition the available dataset directly into a calibration set and an evaluation (test) set.

Second, exchangeability, a key assumption for the validity of CP (Angelopoulos & Bates, 2023; Singh et al., 2024; Vovk et al., 2005), requires that the order of observations does not affect their joint distribution. To approximate this condition in our dataset, we split the dataset by year rather than using random sampling. This approach naturally accounts for seasonal variations by ensuring that observations within each year are drawn from the same underlying

distribution, which is essential for the CP guarantees to hold. Our CP implementation is publicly available on GitHub (see the Code Availability section).

3.2.8 GLM-AED recalibration

The GLM-AED model was applied to Esthwaite Water and Loch Leven to simulate chl-a concentrations. Each lake was manually calibrated by adjusting key parameters within realistic ranges: the light extinction coefficient (K_w , 0.1–1.5 m⁻¹), which affects light penetration and thermal stratification, and the wind factor (f_{wind} , 0–2), which scales wind speed and influences mixing and surface cooling.

Sensitivity analyses identified the maximum growth rates of phytoplankton groups (R_{growth}) as key parameters for optimisation. These parameters were found to offer the greatest potential for improving model performance but are difficult to determine accurately from existing literature. For this study, two functional phytoplankton groups were defined: one representing diatom and the other cyanobacteria, as these were identified as the dominant bloom-forming taxa in the databases of the two lakes. A systematic parameter calibration was conducted to optimise the maximum growth rates for cyanobacteria (R_{cyano}) and diatoms (R_{diatom}). A total of four hundred combinations of the two parameters were evaluated using a 20x20 grid, with simulations run for the period 2016 to 2022. This approach allowed for the identification of parameter combinations that produced the best agreement with in situ chl-a dynamics. For Esthwaite Water (R_{diatom} : 0.06 – 2.8, R_{cyano} : 0.26 – 1.16) and Loch Leven (R_{diatom} : 0.1 – 4, R_{cyano} : 0.1 – 4) the growth rate ranges were thus lake-specific and ensured that the parameter space was representative of the ecological conditions in each system. GLM-AED model calibration was conducted on even years (2016, 2018, 2020, and 2022), while validation was performed on odd years (2017, 2019, and 2021) following the method used by Essou et al., (2016) and as suggested by Xu, (2021) for hydrological models due to its spatial and temporal varying data quality and to consider climatic trends. For each of the 400 runs, the MdSA and the Mean Absolute Error (MAE):

$$MAE = \frac{\sum_{i=1}^n |y_i - x_i|}{n}, \quad (3)$$

were calculated using the calibration years. The top three runs for each scenario, based on these metrics, were selected for further validation. GLM-AED model validation was conducted by calculating the MdSA and MAE based on the model-derived surface chl-a and in situ chl-measurements.

Evaluation scenarios

GLM-AED model calibration was undertaken using seven different scenarios. These scenarios were based on the different uncertainty filtering scenarios of the MSI-derived chl-a estimates per lake (Table 3.3).

Table 3.3 The seven different evaluation scenarios used for model recalibration. Each scenario has a letter (a-g), a Name and a column explaining which chl-a data is part of that scenario. Non-Conformity is later abbreviated as NC and Earth Observation as EO (Scenario e, f and g).

SCENARIO	NAME	DESCRIPTION
a	In situ	All available in situ chl-a values
b	All Earth Observation	All MSI chl-a estimates
c	High Non-Conformity	MSI chl-a estimates with a non-conformity score $\leq 90\%$
d	Low Non-Conformity	MSI chl-a estimates with a non-conformity score $\leq 50\%$
e	In situ + All EO	a + b
f	In situ _ High NC	a + c
g	In situ + Low NC	a + d

The seven scenarios allow us to evaluate three key aspects. First, they assess whether using MSI chl-a estimates enhances the calibration of GLM-AED (scenario a). Second, they examine whether filtering MSI chl-a estimates further improves GLM-AED accuracy (comparison of scenarios b, c, and d). Third, they evaluate whether a calibration approach that incorporates in situ and MSI chl-a estimates is more effective than one that relies solely on MSI chl-a estimates (comparison of scenarios b, c, and d versus e, f, and g).

Algal bloom agreement

In situ and model-derived chl-a were labelled as 'Bloom' if they exceeded 25 mg m^{-3} . The threshold is based on Alert level 2 ($>24 \text{ mg m}^{-3}$) for cyanobacteria of the World Health Organization (World Health Organization, 2021). To evaluate the model's alignment with in situ chl-a bloom occurrences (*Bloom agreement*) for each scenario, instances in which in situ chl-a values and GLM-AED chl-a outputs simultaneously indicated a bloom, were counted ($N_{correct}$) and divided by the total number of bloom instances in the in situ chl-a ($N_{observed}$):

$$Bloom \text{ Agreement } (\%) = \left(\frac{N_{correct}}{N_{observed}} \right) * 100. \quad (4)$$

The bloom agreement percentage per scenario, per lake provides insight into the impact of filtered MSI chl-a estimates on bloom forecasting.

3.3 Results

3.3.9 MSI spatial homogeneity

Polymer derived reflectance produced the lowest spatial variability ($n=105$, $n=172$ scenes with $CV < 0.25$) in Esthwaite Water and Loch Leven, when compared to the atmospheric correction algorithms ACOLITE ($n=100$, $n=97$) and C2RCC ($n=87$, $n=153$).

The difference in spatial variability across the atmospheric correction methods is an inherent indicator of their limitations. The most spatially variable scenes ($CV > 0.25$) in Esthwaite Water and Loch Leven were removed. Match-ups were available for approximately 25% of scenes in Loch Leven (Polymer = 47, C2RCC = 39, ACOLITE = 24) and 36% of scenes in Esthwaite Water (Polymer = 37, C2RCC = 29, ACOLITE = 40).

3.3.10 Optical Water Type classification

All OWTs, except 10, were observed at least once across all atmospheric correction approaches and lakes, but their relative frequencies varied strongly across the different atmospheric correction methods (Figure 3.3). Polymer and C2RCC aligned in that they excluded certain OWT classes (1, 5, 7 and 8 for Esthwaite Water, and 1 and 7 for Loch Leven), whilst ACOLITE observes classes 1 in Esthwaite Water and 5 in both lakes (Figure 3.3). C2RCC and Polymer show highest representation of clusters A and B with cluster C being absent in C2RCC. ACOLITE shows equal representation of clusters A, B and C in Esthwaite Water. In Loch Leven, ACOLITE assigns most scenes to cluster B, showing ACOLITE to be the outlier.

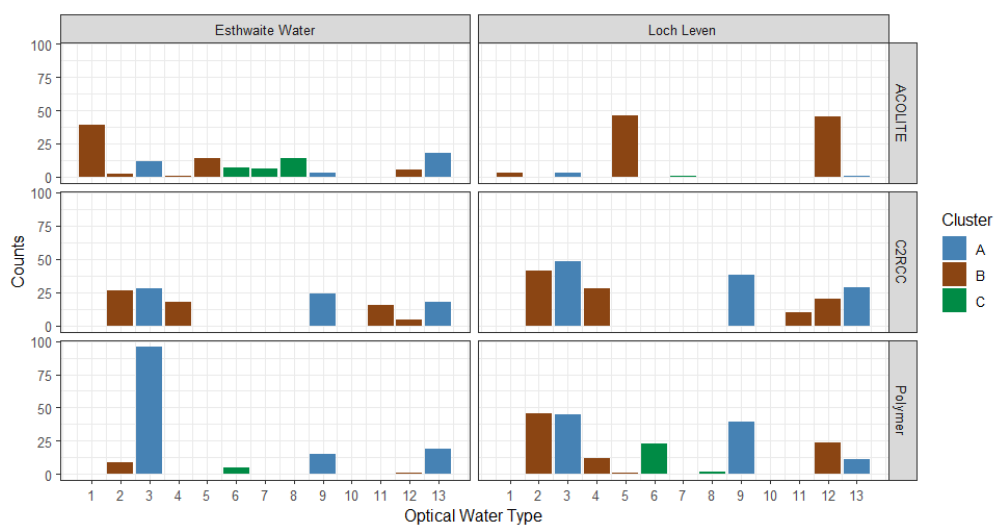


Figure 3.3 Total number of images per Optical Water Type, per lake and, per atmospheric correction method. The colours represent the different OWT clusters: A (clear), B (intermediate), and C (turbid), providing a visual distinction of the distribution of individual OWT across the different clusters.

3.3.11 MSI chl-a estimation

The MSI chl-a retrieval resulted in higher R values in Esthwaite Water compared to Loch Leven and a better visual fit (Figure 3.4). Moderate chl-a range (10- 40 mg m⁻³) of Loch Leven was inadequately retrieved by the chl-a algorithms. The OWT cluster-based optimisation improved the retrieval for both lakes compared to the non-optimised MSI chl-a estimates (grey triangles, figure 3.4), which showed up to 50% lower R values, 3.8 times higher MdSA's and 16 times higher SSPB values.

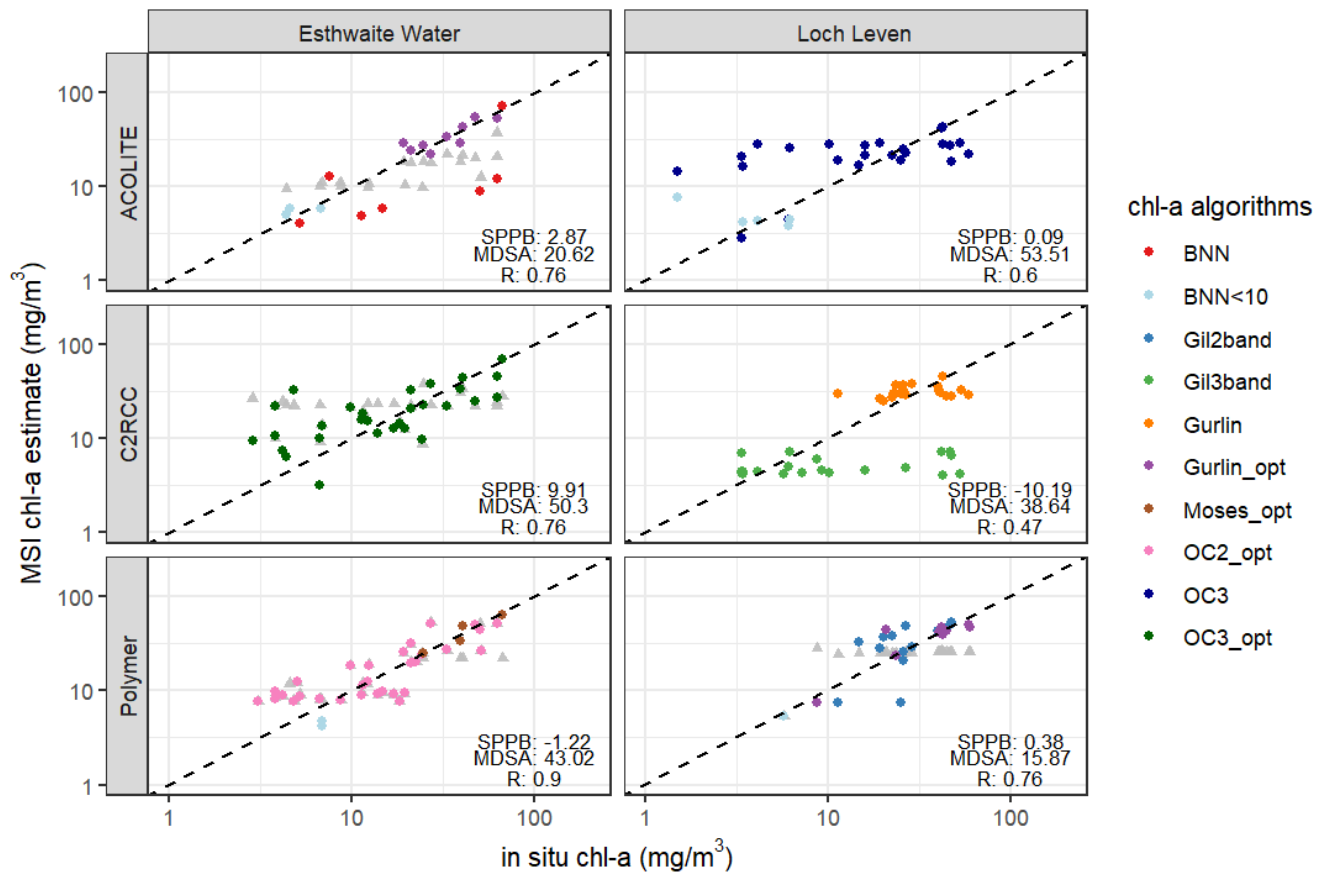


Figure 3.4 Performance of the best-performing chl-a algorithms for each lake and atmospheric correction method across OWT clusters A, B, and C (one per cluster). Coloured points indicate optimised algorithms; grey triangles represent non-optimised algorithms, highlighting performance differences under varying conditions. Evaluation metrics include the Pearson correlation coefficient (R), Median Symmetric Accuracy (MdSA), and Symmetric Signed Percentage Bias (SSPB).

The diversity between atmospheric correction methods was visible in the error metrics of the chl-a retrieval results (Figure 3.4). The C2RCC SSPB was 3 to 10 times higher compared to Polymer and ACOLITE, with the MdSA (higher) and R (lower) metrics deterioration as well. The ACOLITE SSPB for Loch Leven and MdSA for Esthwaite Water were observed to be the

lowest. However, Polymer outperforms across the remaining error metrics and therefore the better choice.

3.3.12 Uncertainty quantification

The uncertainty quantification using CP resulted in an expected range of non-conformity scores for MSI chl-a estimate from 0 to 100%. A rejection rate (non-conformity > 90%) of +/- 29 % was observed with 29 MSI chl-a estimates in Esthwaite Water and 26 in Loch Leven (Figure 3.5).

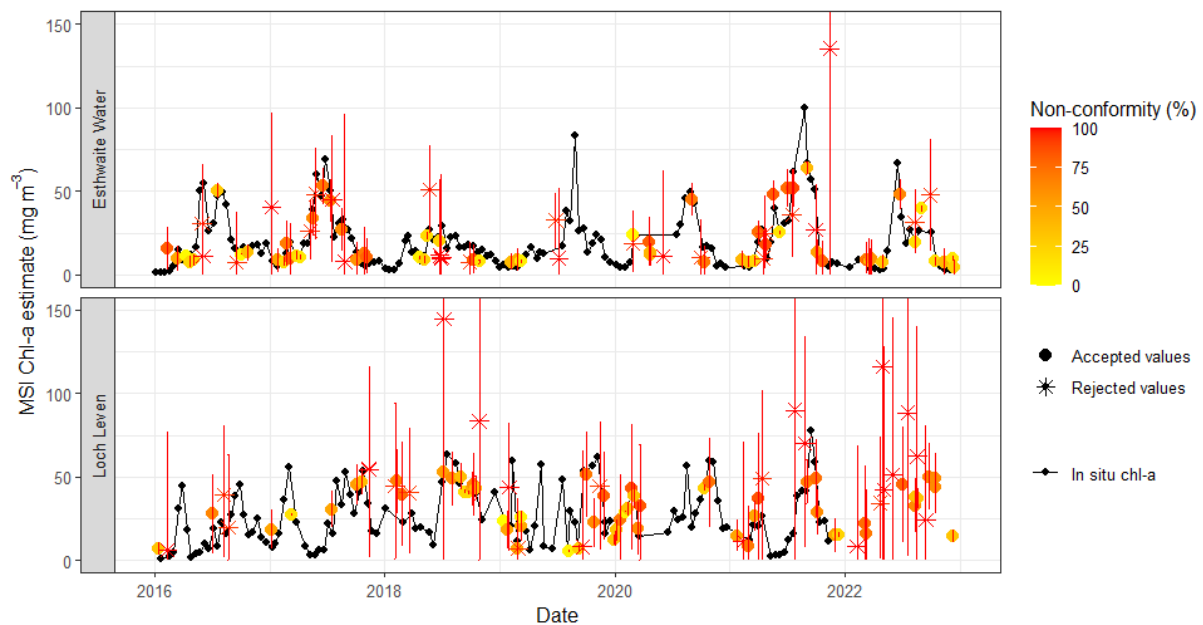


Figure 3.5 Non-conformity quantification of the MSI chl-a estimates, along with their corresponding prediction intervals. In situ chl-a values are shown in black, with MSI chl-a estimates coloured based on their conformity. Rejected estimates, where non-conformity exceeds 90%, are marked displayed as an asterisk and accepted estimates are represented as points. The data is separated by lake to illustrate the variability in conformity.

Removal of rejected values resulted in a significant reduction of the MdSA from 53.83% to 36.55 % in Esthwaite Water (MAE: 9.2 to 4.95) and in Loch Leven from 39.17% to 24.93% (MAE: 12.6 to 7.65). Adjusting the rejection rate further to 50% (Low NC) changed the MdSA of Esthwaite Water minimally from 36.55 % to 37.33 % (MAE: 4.95 to 3.81). However, reduced it significantly for Loch Leven from 39.17% to 16.21% (MAE: 7.65 to 5.38). The coverage factor is lower for Esthwaite Water (75.58%) than for Loch Leven (80.95%), indicating that the uncertainty percentages in Loch Leven were slightly better calibrated than those for Esthwaite Water.

3.3.13 GLM application

Esthwaite Water resulted in lower errors between in situ and GLM-AED compared to Loch Leven. An overestimation of the chl-a peaks by 25 mg m⁻³ in Esthwaite Water and 50 to 75

mg m⁻³ in Loch Leven was observed in all scenarios. A detailed description of the model validation of the full temporal range can be found in Appendix B, which was not included in the publication.

Calibration scenarios relying solely on MSI chl-a estimates (b, d, f) consistently reduced the MdSA in Loch Leven compared to scenarios using in situ data. In Esthwaite Water, the scenario d resulted in a reduction in MdSA, making it the sole scenario to demonstrate a decrease across both lakes (Figure 3.6).

Scenarios combining MSI chl-a estimates and in situ chl-a (c, e, g) resulted in decreased or equal MdSA values in 5 out of 6 cases, with g showing no change for either lake. In Esthwaite Water, High NC + In situ (e) was the only scenario involving in situ data that reduced the MdSA.

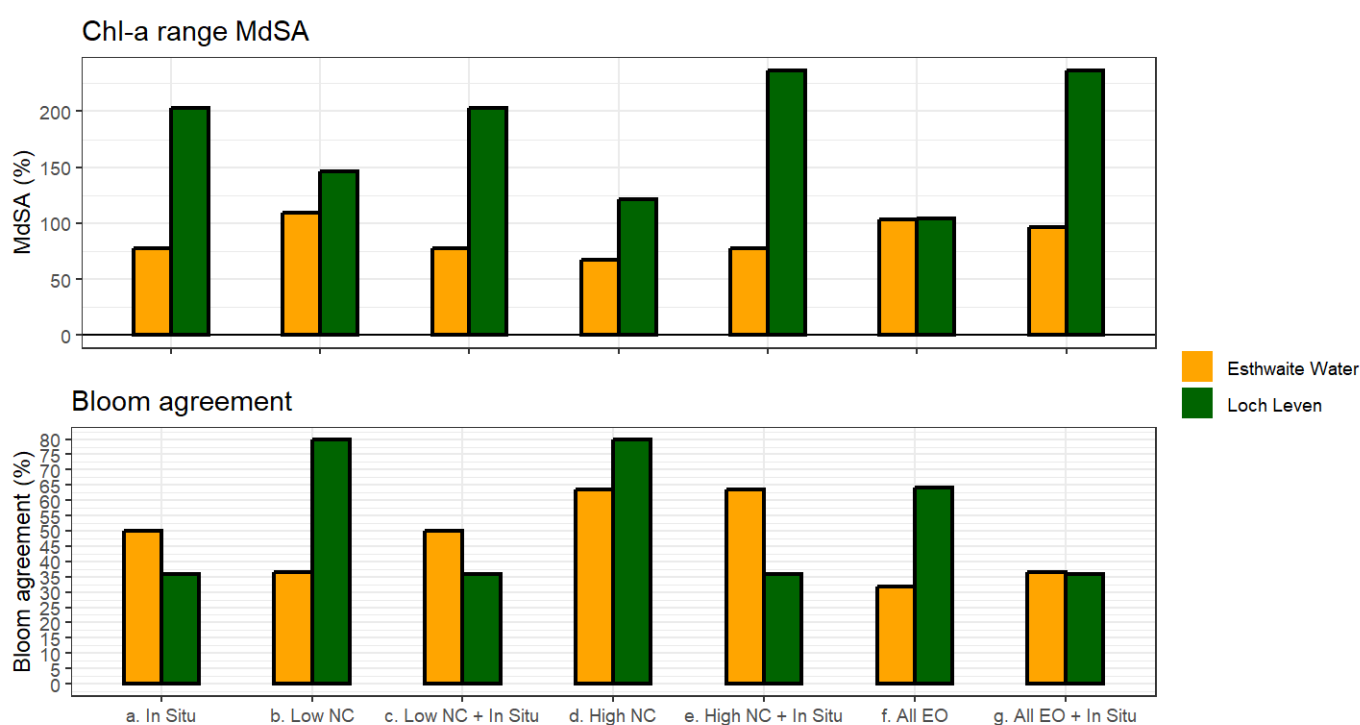


Figure 3.6 Median Absolute Scaled Error (MdSA, %) of the full chl-a range for each scenario and lake (A-G) shown on the left. On the right, the percentage of bloom agreement between in situ chl-a concentrations and the GLM-AED scenario outputs (A-G) is displayed. Both figures highlight the accuracy and agreement of chl-a estimations across different scenarios and lakes.

Calibration using in situ (a) captured fifty percent of blooms in Esthwaite Water and 36% in Loch Leven (Figure 3.6). In Loch Leven, the MSI chl-a estimate scenarios increased bloom agreement up to 80% (b and d) and 64% (f). Esthwaite Water bloom agreement increased in two scenarios (d and e) up to 63.6%, making the High NC scenario the best performing across the lakes.

Despite improving the MdSA in both lakes, the All EO scenario (f) resulted a significant decrease in bloom agreement to 31% in Esthwaite Water and reduced improvement in Loch Leven.

3.4 Discussion

The GLM-AED model chl-a output for Loch Leven and Esthwaite Water is line with the current literature. For comparison with (Fenocchi et al., (2019) who report errors in terms of nMAE, the MAE of 19.73 mg m⁻³ for Loch Leven and 12.61 mg m⁻³ for Esthwaite Water correspond to a normalised MAE values of 88.3% and 56.5%, respectively. These values are in line with the nMAE of 56% ± 24% found in Fenocchi et al (2019) for a range of different lakes. Loch Leven exhibits a larger error compared to Esthwaite Water, with higher MAE, nMAE, and MdSA values, reflecting greater challenges in accurately representing this lake as well as the differences between lakes characterised by the same model.

3.4.14 MSI derived chl-a

The MSI derived chl-a also reported higher errors in Loch Leven, compared to Esthwaite Water across atmospheric correction and chl-a algorithms. This reoccurring finding across different data sources can be explained by the shallower nature of Loch Leven resulting in more dynamic clear and turbid states (Scheffer & Van Nes, 2007).

Overall, MSI-derived chl-a estimates achieved reasonable accuracy across the two case study lakes using the Polymer atmospheric correction (R: 0.76–0.90; MdSA: 15.67%–43.02%). Optimal performance required the combined use of OWT clustering, appropriate atmospheric correction, and careful selection of chl-a retrieval algorithms.

3.4.15 Uncertainty quantification through conformal prediction

The high coverage factor (75 – 80%) and improved error metrics after CP filtering showed that the approach is an effective tool for quality control of MSI derived chl-a concentrations. While some inaccuracies were observed, particularly chl-a estimates showed high nonconformity scores despite being close to in situ measurements, these variations provided valuable insights into the dataset. The anomalous climatic conditions of 2017, the fifth warmest year since 1910 (Royal Meteorological Society, 2018), likely contributed to these discrepancies, alongside the limited number of in situ matchups available for that period. Understanding these factors helps refine the CP approach and improve uncertainty estimates.

Importantly, since these errors occurred at chl-a values below 30 mg m⁻³, their impact on bloom detection outcomes remained minimal.

The uncertainty estimates from our CP approach align with those reported in previous studies. For instance, Saranathan et al., (2023) reported uncertainties of 10 to 45 % for chl-a using Mixture Density Networks, while Werther et al. (2022b) found uncertainties ranging from approximately 30% to 80% for chl-a over oligotrophic and mesotrophic lakes, depending on prior atmospheric correction and lake characteristics. Similarly, global chl-a estimates by Liu et al. (2021) yielded comparable uncertainty ranges, suggesting that our findings reflect common capabilities of chl-a estimation via Sentinel-2 MSI.

A wide range of uncertainty quantification methods for chl-a retrieval exist (IOCCG, 2019), but in practice are often built on machine learning–based approaches (e.g., Saranathan et al., 2024) techniques tailored to specific models or optical water types (e.g., Lui et al, 2021), and uncertainty propagation calculations (e.g., Xi et al., 2021). These methods are usually not model agnostic, therefore not easily transferrable. In contrast, CP fills a critical gap by providing uncertainty estimates for any chl-a algorithm, provided a sufficient dataset is available, even for algorithms originally published without uncertainty metrics.

3.4.16 Incorporation of MSI derived chl-a

Calibration using MSI chl-a estimates filtered using the High NC scenario produced significant reductions in MdSA, demonstrating two key points. First, MSI chl-a estimates can improve the calibration of the chl-a model; second, filtering these estimates prior to downstream use is not only beneficial but necessary to prevent calibration deterioration. Although we expected that combining MSI chl-a estimates with in situ data would yield even better results, our findings indicate that the combined use provided no additional model improvement or bloom agreement. We speculate that the in situ observations are dominated by low chl-a values (<25 mg m⁻³), whilst the MSI estimates show an even distribution after matchups. In addition, satellite estimates are constrained to surface chl-a values only, whilst in situ tends to be a mixed sample from 0 to 5 m which could result in a more diluted sample. As no negative effects were observed when combining the two sources, structured integration of chl-a values creates potential for further enhancement.

The High NC scenario improved bloom agreement in both lakes, while scenarios that incorporated unfiltered MSI chl-a estimates (All EO, scenarios B and E) or in situ data (scenarios F and G) showed diminished or no improvements. This indicates that filtering MSI

chl-a estimates is essential for optimising their predictive utility, and we propose filtering based exclusively on the High NC scenario metric of rejected values.

3.4.17 Towards large-scale algal bloom forecasting

Despite the merits of each method, neither GLM-AED nor EO alone would be able to support large-scale algal bloom forecasting. GLM-AED's capacity to estimate bloom events is often constrained by limited calibration datasets, especially for regions lacking consistent in situ observations. Meanwhile, EO platforms can only provide near-real-time or retrospective measurements, heavily dependent on clear-sky conditions. Consequently, relying on GLM-AED alone risks calibration inaccuracies, and solely using EO forfeits the ability to forecast. The combined use offers a novel pathway for scaling algal bloom forecasting to a global level. Its core strength lies in leveraging complementary capabilities: GLM-AED grounds bloom estimation in physical principles constrained by hydrodynamic forcing parameters, while satellite observations, such as those derived from Sentinel-2 MSI, provide spatially extensive estimates of chl-a based on bio-optical relationships.

A critical first step for broad application of this combined approach is establishing a robust hydrodynamic foundation in GLM, ensuring that water balance and temperature/oxygen profiles are accurately modelled prior to refining chl-a calibration. In cases where hydro-meteorological observations are lacking, consistent input variables (e.g. inflow, outflow, meteorological drivers) can be derived from large-scale reanalysis products, such as the Modern-Era Retrospective Analysis for Research and Applications, Version 2 (MERRA-2) (Gelaro et al., 2017) or ERA-5 for atmospheric drivers and Soil and Water Assessment Tool (SWAT) (Arnold et al., 1998) for flow and nutrients. These often have broad spatial coverage and high temporal resolution, thereby overcoming observational scarcity and provide reliable forcing conditions for the model.

Whilst Bruce et al., (2018) demonstrated multi-lake applications of GLM, no parallel large-scale study using GLM-AED with EO datasets has been completed. A logical next step would be to apply the approach developed in this study across a broader set of lakes globally, moving toward large-scale algal bloom forecasting. However, scaling up to the global level presents substantial challenges. These include the selection and adaptation of atmospheric correction models, the lack of globally validated in situ datasets, differences in satellite mission coverage, and the absence of a globally consistent Sentinel-2 water-leaving

reflectance product for inland waters. Atmospheric correction performance is highly sensitive to the OWT encountered (Pahlevan et al., 2021), which complicates algorithm transferability. The European Space Agency Lakes Climate Change Initiative (CCI) project is a key initiative in this space, aiming to generate consistent global-scale water quality products from satellite data, and has been successfully used for variables including chl-a (Caroni et al., 2025). Our results further show that even among two eutrophic lakes, optimal chl-a algorithm performance and GLM model behaviour differ substantially. This highlights a core limitation of global process-based modelling: either lakes must be parameterised individually, requiring considerable effort, or generalised models must be accepted with reduced confidence in their outputs. Addressing this trade-off will be crucial for the development of robust, global-scale bloom forecasting systems.

As reanalysis datasets improve and satellite product accuracy increases, near-real-time and broad-scale monitoring and forecasting will become a more feasible option for lake management.

3.5 Conclusions

This study demonstrates that integrating MSI chl-a estimates, when quality-filtered using CP, significantly enhances GLM-AED model calibration and algal bloom detection. The ability to quantify uncertainties in remote sensing-derived chl-a, alongside reductions in validation model errors and significant improvements in bloom agreement, underscores the value of this approach and the broader role of remote sensing in ecological modelling.

The negative impact of unfiltered MSI chl-a estimates on model performance highlights the necessity of quality filtering methods such as CP to minimise downstream errors. These findings emphasise the potential of CP-filtered MSI chl-a estimates for improving bloom forecasting and supporting more informed lake management decisions. This approach provides a robust framework for integrating EO-based water quality data into predictive models, with applications extending beyond algal blooms. Future research could explore its effectiveness across different water systems, EO datasets, and modelling techniques, further validating its role in ecological forecasting.

3.6 Code, model and data availability.

The code for the conformal prediction framework is available on:

https://github.com/maudsiebers/Conformal_prediction_Framework

GLM-AED is freely available. In this work Version 3.1.9 of the GLM-AED was downloaded and executed in RStudio. For running and visualisation purposes the packages ‘glmtools’ (<https://github.com/robertladwig/glmtools>) and ‘GLM3r’ (<https://github.com/robertladwig/GLM3r>) were installed from GitHub.

Data for lakes is freely available from the UK Lakes Portal (<https://uklakes.ceh.ac.uk>), managed by the UK Centre for Ecology & Hydrology (UKCEH). For additional data requests, enquiries can be made directly to UKCEH. These are the published datasets of relevance for Esthwaite Water: (Feuchtmayr et al., 2021, 2024, 2025) and Loch Leven (Dudley et al., 2013; Taylor et al., 2021, 2022a, 2022b, 2023)

Sentinel-2 data is publicly available through multiple platforms, with the primary source being the Copernicus Open Access Hub (<https://dataspace.copernicus.eu/explore-data/data-collections/sentinel-data/sentinel-2>). Additional access points include ESA’s Sentinel Hub, Google Earth Engine, NASA Earthdata Search, and AWS Open Data, each offering various tools for visualisation and analysis.

3.7 Author contributions

MACS and MW conceptualised the study. MACS performed the analyses and written the first draft. Reviewing and editing was done with contributions from all co-authors. EM and LM provided in situ lake data. Acquisition and atmospheric correction performed by MB and MW.

3.8 Competing interests

The authors declare that they have not conflict of interest.

3.9 Acknowledgements

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Copernicus information or data it contains. The sampling and processing were supported by the Natural Environment Research Council award number NE/R016429/1 as part of the UK-SCAPE programme delivering National Capability.

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3.11 AI Use

During the preparation of this work the author(s) used Chat-GPT to improve language clarity and sentence structure. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Chapter 4: The effect of climate change on algal bloom dynamics across a latitudinal gradient in the UK

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Abstract

Climate change is projected to intensify freshwater algal blooms globally, yet the extent of this intensification as a function of latitude and waterbody type remains underexplored. This study used the process-based model GLM-AED to simulate chlorophyll-a concentrations and bloom duration across three contrasting UK waterbodies: Alton Water (Monomictic reservoir), Loch Leven (polymictic lake), and Esthwaite Water (Monomictic lake).

GLM-AED was calibrated using remote sensing and high frequency sensor data, after which it was run for a period of 2000 to 2100, using input data obtained from scenarios of multiple Shared Socioeconomic Pathways (SSPs), latitudinal positions, and climate model forcings. Results show that days with chlorophyll-a concentrations above 24 mg m⁻³ (bloom days) and mean chlorophyll-a concentrations are projected to increase across all waterbodies, with reservoirs and shallow lakes in northern latitudes showing the most pronounced changes, especially under high-emission scenarios (e.g., SSP5-8.5). While waterbody characteristics emerged as the dominant driver of variability, latitude and global climate models also significantly modulated bloom responses. In contrast, SSP scenario differences had comparatively smaller effects, indicating that local lake features and geographic position may

outweigh global emission trajectories in shaping near-term bloom risks. These findings underscore the need for targeted, lake-specific management strategies, particularly for reservoirs at northern latitudes ($>56^{\circ}\text{N}$), where significant climate-driven increases in water temperature and thermal stratification are expected to exacerbate algal blooms most strongly.

4.1 Introduction

Freshwater ecosystems such as lakes, rivers, and reservoirs provide a range of critical services including drinking water, irrigation, recreation, and support for biodiversity (McIntyre et al., 2016; Paetzold et al., 2010; Van Vliet et al., 2017). However, these systems are increasingly vulnerable to multiple stressors, among which climate change plays an escalating role.

Rising temperatures, shifting precipitation patterns, and changing seasonality associated with global climate change are altering the physical and ecological dynamics of freshwater systems (Adrian et al., 2009; Williamson et al., 2009). One major consequence is the increased frequency and severity of phytoplankton blooms, including harmful algal blooms (HABs), which are often triggered by elevated water temperatures and stable periods of thermal stratification (Paerl et al., 2020; Paerl & Paul, 2012). While nutrient enrichment remains a key driver for eutrophication, climate-related changes are now recognized as critical amplifiers of bloom risk across different geographic and climatic contexts (Moss et al., 2011; Wurtsbaugh et al., 2019).

HABs reduce water clarity, mostly consistent of cyanobacteria, deplete oxygen levels, and produce toxins that threaten aquatic life, public health, and economies (Carmichael, 2012; Chorus & Testai, 2021). The toxins (e.g. cyanotoxins) can lead to closure of recreational waters due to health risk for bathers. Next to that, taste and odour compounds can negatively impact the use of drinking water and algal biomass can blind media filters, increasing the cost of potable water production or lead to loss of supply. As bloom-forming species benefit from higher temperatures and longer water retention times, they are expected to gain a competitive advantage over other phytoplankton groups in a warming climate (Paerl & Otten, 2013; Visser et al., 2016). This trend is of particular concern in eutrophic and warming-prone regions (K. E. Havens & Paerl, 2015; Paerl & Huisman, 2008).

However, climate-driven responses in bloom dynamics vary significantly with geography (Adrian et al., 2009). Environmental factors such as temperature regimes, solar radiation, hydrology, and land use differ along latitudinal and longitudinal gradients, influencing how

lakes respond to climate pressures. For instance, in the Northern hemisphere, cyanobacterial dominance is currently more common in warmer, southern and mid-latitudes, but ongoing warming may shift bloom patterns northward (Richardson et al., 2018). In the United Kingdom, the north–south climatic gradient is particularly pronounced, with the north-west being wetter and cooler, and the south-east drier and warmer - a contrast that has become more marked over time (Mayes, 2000).

Process-based models, such as the one-dimensional General Lake Model coupled with the Aquatic Eco-Dynamics module (GLM-AED), offer a promising approach to simulating lake stratification, nutrient cycling, and phytoplankton dynamics under varying climate scenarios (Hipsey, 2022; Hipsey et al., 2019). These models allow for more nuanced scenario testing by integrating projected climate forcings with lake-specific characteristics, ultimately providing management-oriented insights into potential bloom risks.

This study investigates how climate change influences bloom dynamics across a latitudinal gradient in the UK, using a comparative modelling approach across multiple lakes from southern England to Scotland (51.9 to 56.2°N), (Figure 4.1). By capturing a range of climatic and limnological contexts, this research aims to identify region-specific vulnerabilities and anticipate how future climate scenarios may reshape bloom risks.

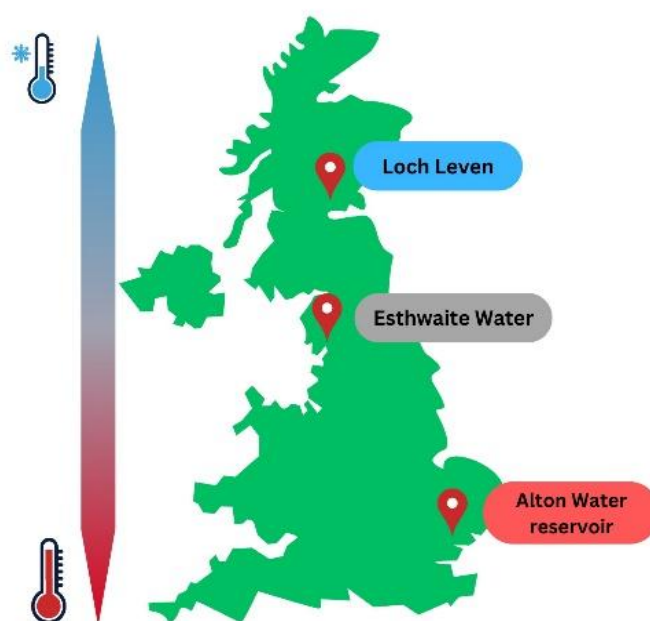


Figure 4.1 Temperature gradient across the United Kingdom. The location of the case study lakes is indicated with red pins; the colour indicates their location in the gradient.

To drive climate projections in this study, we incorporate combinations of Shared Socioeconomic Pathways (SSPs) and Representative Concentration Pathways (RCPs), which together provide a comprehensive view of future climate and development trajectories. RCPs represent different greenhouse gas concentration pathways, while SSPs outline various socioeconomic futures, which influence emissions and, consequently, climate outcomes (O'Neill et al., 2017). Specifically, this study utilises three SSP-RCP combinations: SSP1-2.6, SSP3-7.0, and SSP5-8.5. These scenarios span a broad spectrum of potential futures, from strong mitigation efforts to high-emission pathways, and allow us to assess how both global emissions and regional development may shape algal bloom risks.

Investigating waterbody responses across a latitudinal gradient will give insights into interactions between climate and waterbody type. These insights consequently provide a better mechanistic understanding and ultimately improve water management. For example, knowing whether stratified lakes are more susceptible to bloom conditions in northern latitudes in specific climate scenarios will highlight these waterbodies for more intensive water management to prevent future problems.

Thus, we present a novel approach that virtually relocates existing UK waterbodies across a latitudinal climate gradient to disentangle the effects of local climate from site-specific characteristics on algal bloom dynamics. Using three contrasting systems – Esthwaite Water (monomictic lake), Loch Leven (shallow polymictic lake), and Alton Water (monomictic reservoir)– we evaluate how latitude, waterbody traits, and climate scenarios interact.

Modelling real waterbodies ensures ecological realism while supporting spatial transferability across temperate freshwater systems (Figure 4.1). The study's aims are to:

- Quantify future changes in bloom magnitude and bloom duration and in these three UK lakes under various climate scenarios (SSP-RCP combinations).
- Assess the relative influence of waterbody characteristics, latitude, global climate models (GCMs), and socio-economic pathways (SSPs) on algal bloom dynamics.
- Examine the effect of geographic location by shifting each lake across a latitudinal gradient, isolating the role of climate from local drivers.
- Provide management-relevant insights into which types of waterbodies and regions may be most vulnerable to future algal blooms.

4.2 Methods

4.2.1 Case study lakes

Three different UK waterbodies, that regularly experience algal blooms, were used to assess the independent variables of waterbody design/characteristics as well as latitudinal and climate effects. These algal blooms consist mainly of diatom and cyanobacterial species. Two freshwater lakes and one drinking water reservoir in the United Kingdom were used as case study sites to represent a gradient across the UK (Figure 4.1). Esthwaite Water is a small (surface area of 0.96 km²), shallow but stratifying (mean depth of 6.9 m), eutrophic lake located in the English Lake District (Mackay et al., 2012, 2014; Mortimer, 1942). Loch Leven is a comparably larger (surface area of 13.3 km²) and shallower eutrophic lake in lowland Scotland, with a strongly mixed water column (mean depth of 3.9 m). Alton Water is a drinking water reservoir opened in 1987 in Suffolk, England with an area of 1.62 km², a mean depth of 5.8 meters and a maximum depth of 20 meters. Designed to address the water shortages in the Ipswich area, its catchment is primarily farmland. Alton Water a non-impounding reservoir (not reliant on natural inflows) dammed by a 20 m wall, with water pumped in from the nearby River Gipping.

Both natural lakes have a long history of algal blooms with mean annual chlorophyll-a (chl-a) concentrations of 18.5 mg m⁻³ in Esthwaite Water and 25.1 mg m⁻³ in Loch Leven (Carvalho et al., 2012; Maberly et al., 2011; Madgwick et al., 2006; Spears et al., 2012). Alton Water has been experiencing more severe algal blooms over the last 10 years, with mean annual chl-a values of 17 mg m⁻³. The reservoir operators have been actively working on reducing these using aeration, sonic buoys and ferric dosing. Whilst all three waterbodies regularly exceed the WHO Alert Level 2 chl-a concentration of 24 mg m⁻³ (World Health Organization, 2021), the waterbodies are expected to react differently to climate change due to their size, shape and external factors.

Table 4.1 Waterbody characteristics of Loch Leven, Esthwaite Water and Alton Water.

	LOCH LEVEN	ESTHWAITE WATER	ALTON WATER
LATITUDE	North	Central	South
COORDINATES	56.19 N°, -3.39 E°	54.36 N°, -2.98 E°	51.98 N°, 1.12 E°
MORPHOMETRY	Shallow and large	Medium depth and small	Deeper and small
SURFACE AREA	13.3 km ²	0.96 km ²	1.62 km ²
MEAN DEPTH	3.9 m	6.9 m	5.8 m
FUNCTIONALITY	Nature reserve	Nature reserve	Drinking water reservoir, recreational
MEAN ANNUAL LAKE TEMPERATURE	~10-13°C	~7 – 10.5°C	~8-15 °C
MEAN ANNUAL CHL-A CONCENTRATION	High (25.1 mg m ⁻³)	Moderate–high (18.5 mg m ⁻³)	Moderate (17 mg m ⁻³)
TROPHIC STATUS	Eutrophic	Eutrophic	Mesotrophic/Eutrophic
MAIN CATCHMENT LAND USE	Improved grassland and arable and horticulture	Improved grassland and broadleaved woodland	Arable and horticulture
MANAGEMENT	Extensive (nutrient input reduction, reed beds)	Eutrophication management	Water quality management for drinking water
LAKE TYPE	Shallow polymictic	Monomictic stratified	Monomictic

4.2.2 GLM-AED

The water bodies (Loch Leven, Esthwaite Water, Alton Water) were all implemented into the one-dimensional GLM-AED model. The model was configured to simulate the physical and biogeochemical dynamics of the three case study waterbodies. The GLM component simulates lake stratification, mixing, and temperature dynamics, while AED adds modules for nutrients, phytoplankton, oxygen dynamics, and sediment interactions.

The model setup included both required configuration blocks, (glm_setup, morphometry, time, and init_profiles) and additional optional modules such as light (for underwater irradiance), mixing (turbulence schemes), WQ_setup (water quality), sediment (sediment processes), output, and debugging.

Parameterisation and driving data

The waterbodies were parametrised using latitude, longitude, elevation, and depth-vs area relationship, which were provided by UKCEH (Mackay et al., 2014; Spears et al., 2012) for Loch Leven and Esthwaite Water and Anglian Water for Alton Water.

Boundary condition inputs included meteorological forcing, inflow, and outflow files. The AED configuration incorporated modules for oxygen dynamics, nutrient cycling (carbon, nitrogen, phosphorus, silica, and organic matter), two phytoplankton groups (diatoms and cyanobacteria), tracers, and non-cohesive sediment processes. Default parameterisations were adopted unless stated otherwise in Table 2.4 (Hipsey, 2022; Hipsey et al., 2019). Full parameterisation files are available on https://github.com/maudsiebers/GLM_AED_Waterbodies_PhD_Thesis.

4.2.3 Model calibration

Model calibration was conducted in four sequential steps:

1. Data preparation

Observational datasets were compiled and quality-controlled, including in situ water temperature and chlorophyll-a (chl-a) data, as well as satellite-derived chl-a from Sentinel-2 (MSI).

2. Thermal calibration

Physical model parameters were calibrated using temperature profiles/observations. Two key parameters were optimised: the wind scaling factor (*fwind*) and the light extinction coefficient (K_w) (Table 4.3). These parameters were automatically adjusted using the built-in calibration tool in the GLM-R package to minimise the mean absolute error (MAE) between observed and modelled temperature profiles.

3. Ecological calibration

Ecological calibration focused on two phytoplankton functional groups, diatoms and cyanobacteria, selected to reflect distinct ecological strategies and seasonal bloom dynamics. The maximum growth rates for both groups were manually calibrated to match observed chl-a concentrations, which served as the primary performance metric (Table 4.2).

A parameter sweep was conducted across biologically plausible ranges (Table 4.2), sampling 10 evenly spaced values for each group ($n = 100$ combinations). Model performance was evaluated using MAE and median symmetric accuracy (MdSA).

4. Validation

Model performance was assessed using independent datasets where available. Due to limited data availability for Alton Water, both 2022 and 2023 were used for validation, with results compared across years to ensure consistency in model behaviour.

Table 4.2 An overview of the parameters within GLM-AED used for calibration and their range or default value as well as their assigned value.

Symbol	Description	Range or Default	Assigned Value
<i>Kw</i>	Light extinction coefficient (m-1)	-	0.81
<i>Wind_factor</i>	Scaling factor to adjust the windspeed data provided by in the meteorology file	1	0.70523
<i>R_growth_diatom</i>	Phytoplankton max growth rate at 20C (day-1)	0.5 to 5	2.8
<i>R_growth_cyano</i>	Phytoplankton mac growth rate at 20C (day-1)	0.5 to 5	1.1

The initial models for Esthwaite Water and Loch Leven were calibrated using a combination of in situ chl-a measurements and Sentinel-2 (MSI) chl-a estimates (Esthwaite Water ($n = 70$) and Loch Leven ($n = 64$)) using conformal prediction according to Siebers et al., (2025). For this work in the Loch Leven data, the deepest point was excluded from calibration, as it represents a small proportion of the lake but had a disproportionate influence on model performance.

Alton Water benefited from higher-frequency observational data. Daily chl-a measurements from nine sensor buoys (2022–2023) were evaluated and filtered to retain spatially representative and reliable data. The resulting dataset was cross validated against other sensors operating concurrently to ensure consistency. Due to the higher temporal resolution,

ecological calibration for Alton Water was conducted exclusively using in situ sensor data and no satellite data was incorporated.

4.2.4 Future climate modelling

The effect of climate forcing on water quality variables across the UK were investigated by feeding climate forcing scenarios into the GLM-AED set up for each of the lakes. These climate forcings are taken from each of the waterbody latitudes resulting in northern (Loch Leven), central (Esthwaite Water) and southern (Alton Water) climate forcings (hereafter referred to as latitudes). To separate the effects caused by the different water body characteristics (Table 1), each waterbody modelled using all three of the latitude climate forcings, essentially simulating each waterbody at each of the latitudes, resulting in nine latitude x waterbody combinations (LWBC) (A-I) (Figure 4.2, Right).

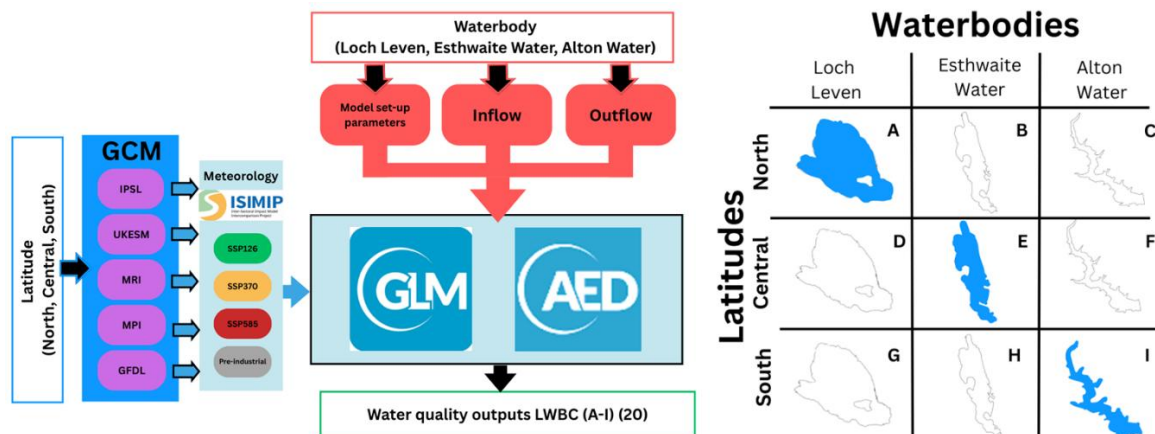


Figure 4.2 The future climate forecasting using GLM-AED. Left: the workflow. Right: The latitude Waterbody Combinations (LWBC) going into workflow on the left. Original location of the waterbodies in blue.

The waterbody includes the inflow and hydrogeology, making climate the only rematched input. The result is a comparison of climate forcing effects on different water bodies and different latitudes.

Climate forcing data

Daily meteorology information (shortwave radiation, longwave radiation, air temperature, relative humidity, windspeed, rain and snow) were obtained from climate simulations from the Inter-Sectoral Impact Model Intercomparison Project (ISIMIP). These include: (1) a pre-industrial control run covering 1650–2100, (2) historical simulations from 1850–2025, and (3) future climate scenarios spanning 2025–2100. Note that the pre-industrial control overlaps

with the start of the historical period but serves as a stationary baseline forcing (Lange & Büchner, 2021). Each period was extracted for the respective lake coordinates (Warszawski et al., 2014). Simulation round ISIMIP3b was used to gather five Global Climate Models (GCM) (GFDL-ESM4, IPSL-CM6A-LR, MPI-ESM1-2-HR, MRI-ESM2-0 and UKESM1-0-LL) and 3 SSPs with their coupled RCPs (ssp126, ssp370 and ssp585) available from ISMIP as well as a historical and pre-industrial control, henceforth referred to as SSPs (Figure 4.2). The future climate forecasting using GLM-AED. Left: the workflow. Right: The latitude Waterbody Combinations (LWBC) going into workflow on the left. Original location of the waterbodies in blue. Figure 4.2, left).

The climate scenarios used in this research are divided in Shared Socioeconomic Pathways (SSPs) which consider what humans will add to climate change (CO₂ etc.) and Representative Concentration Pathways (RCPs) which are the mitigation scenarios based on GHG emission and atmospheric concentrations, air pollutant emission and land use.

Flow data

The inflow data for each waterbody were individually prepared to match the time span of the climate forcing simulations. This study considers only the effects changes in temperature; changes in nutrient loading were not considered. To achieve this, constant nutrient and hydrological inputs were used.

For Loch Leven and Esthwaite Water, mean inflow values were derived from the UK National River Flow Archive using data from 2016 to 2022. The main inflowing rivers—Black Beck for Esthwaite Water, and the North Queich, South Queich, and Greens Burn for Loch Leven—were used to calculate mean inflows, with the assumption that outflow equals inflow to maintain mass balance.

In-situ water temperature and chemistry data (including pH, phosphorus, nitrate, ammonia, and silica) were provided by UKCEH, measured fortnightly and interpolated to a daily resolution. These values were then averaged by day-of-year across the 2016–2022 period, producing a repeating seasonal cycle. This average inflow, outflow, and chemistry dataset was repeated annually over the full simulation period (1850–2100 for Historical and Future scenarios, and 1650–2100 for the Pre-Industrial control).

The reservoir Alton Water was handled differently due to annual water level changes of up to 2.5 m. To reflect this variability, representative inflow and outflow patterns from four recent

years (2018–2022) were selected and repeated across the climate forcing periods. This approach captures high-use periods, seasonality of river abstraction and full reservoir recharge events, ensuring a realistic representation of operational dynamics.

5.2.3.3 The modelling framework

As evident in the workflow (Figure 4.2), GLM-AED is run based on nine LWBC (A-I). For each LWBC a waterbody, which is represented by the GLM-AED model via its parameterisation, in- and outflow, is ran with the meteorology from a different latitude. Such a latitude consisted of daily meteorology variables from five GCMs, with each GCM modelling three SSP scenarios and the pre-industrial control, ultimately resulting in 20 different outputs per LWBC and therefore a total of 180 runs were considered across the analysis for a varying number of years. The SSP scenarios consist of 250 years, with a historical component of 165 years (1850–2014), which is the same for each scenario, and a future component of 85 years (2015–2100). Similarly, the pre-industrial control simulation spans 450 years in total, representing a stationary climate under constant pre-industrial forcings, and is used to assess natural climate variability in the absence of anthropogenic influence.

4.2.5 Indicators of climate impact

Several water quantity and quality variables were extracted from the 180 runs, including Total surface chl-a concentration (mg m^{-3}), Lake Number (-) and Surface Water Temperature ($^{\circ}\text{C}$). For each of these variables the yearly mean of the 5 GCMs was considered for trend analysis, resulting in 36 trend lines (4 for each). The 36 runs are made up of 4 climate scenarios for each LWBC (SSP1-2.6, SSP3-7.0, SSP8-5.8).

Stratification days

The Lake Number was used to indicate whether the water column was mixed or stratified. The Lake Number shows whether the stratification in a lake will be stable or mixed by wind and is automatically calculated by GLM-AED per timestep. A Lake Number of 1 or lower indicates the wind influence to be strong enough to mix the water column, whilst a 1 or higher indicates a stratified water column to be more likely. The GCM mean number of days per year that are stratified were counted, resulting in several stratified days per year.

Surface water temperature

The waterbody surface temperature was used in multiple analyses, first to visualise the effect of climate forcing on the lake temperature by calculating the GCM annual mean surface

temperature. Secondly, cyanobacterial blooms favour higher temperatures and have been found to have elevated toxin release above a certain temperature threshold of 20 to 25 °C (Bowes et al., 2024; Paerl & Huisman, 2009; Walls et al., 2018). Therefore, we examined whether the number of days with lake temperatures above 25 °C were increasing, possibly indicating more toxic waters and a high abundance of cyanobacteria.

Total surface chl-a concentration and bloom days

The total surface chl-a concentration was averaged per GCM to obtain the annual mean chl-a concentration for each LWBC. Additionally, it was used to calculate the number of days exceeding the World Health Organization Alert Level 2 threshold ($>24 \text{ mg m}^{-3}$) (World Health Organization, 2021). Alert Level 2 indicates serious health problems occurring when the algal population is dominated by toxin-producing cyanobacteria.

4.2.6 Impact assessment and model validation

Quantitative differences

The effect of climate forcings on the LWBC was assessed by comparing changes in key variables over four time periods within the 21st century:

Current Century: 2000–2025

Early Century: 2026–2050

Mid Century: 2051–2075

End Century: 2076–2100

The significance of changes between these periods was used to determine when and to what extent climate forcings would impact each variable relative to the Current Century period.

Slope calculation

To quantify the magnitude of change, the slope of each variable from the beginning of the Current Century to the end of the century was calculated for the period 2000 to 2100 for each SSP scenario. This slope indicated the rate of change across the different LWBCs under each climate scenario and was calculated using a linear regression.

Model validation

The models were validated using the mean absolute error (MAE) and the Median Symmetric Accuracy (MdSA), which quantifies the median error between in situ chl-a and estimated chl-a (Morley et al., 2018):

$$MdSA = (e^{\text{median}\left(\left|\log\left(\frac{y_{est}}{y_{true}}\right)\right|\right)} - 1) \times 100 \quad (1)$$

Model validation was performed using the original model set-up, which excludes any SSP scenarios or latitude shifts. This set-up incorporates the observed inflow, outflow, and meteorological data for the three waterbodies considered in this study, allowing validation at their original locations. Additionally, the MAE and MdSA were evaluated across 180 simulation runs (20 combinations of GCMs and climate scenarios $\times$ 9 LWBCs) to assess the performance of the averaged flow and climate inputs, ensuring the error metrics remain within acceptable ranges reported in the literature.

4.1.1.1 Relative importance

To evaluate the relative importance of the factors influencing the outcomes, a linear model was fitted for each subset of data corresponding to the different time periods. The model incorporated latitude, waterbody, SSP, and GCM as predictor variables.

An Analysis of Variance (ANOVA) was then performed for each model to determine the proportion of variance explained by each factor. The ANOVA calculates the sum of squares for each factor and the proportion of explained variance, allowing for an understanding of which factors most influence changes in the variables across time.

To track how the importance of each factor evolved over time, the data was grouped by the specified time periods. For the SSP variance analysis, the "Pre-Industrial control" scenario was excluded, as it was not relevant for this analysis.

4.2.7 Recommendations for water management

Management recommendations were developed by translating model outputs into implications for water quality monitoring and bloom forecasting under changing climate conditions across different waterbody types and latitudes.

First, GLM-AED model outputs were systematically evaluated across all latitude–waterbody combinations, climate scenarios, and global climate models. This focused on identifying management-relevant patterns in chl-a concentrations, bloom duration, surface temperature, and stratification. Further analyses highlighted the relative influence of waterbody characteristics, latitude, and climate forcing, as well as key thresholds and system-specific responses.

Second, these findings were contextualised through engagement with site-specific water managers and experts (Anglian Water for Alton Water, UKCEH for Loch Leven and Esthwaite Water), ensuring alignment with local monitoring practices, operational constraints, and management priorities. This involved meetings with representatives of the water bodies throughout the process to discuss findings and recommendations.

This combined approach enabled the development of targeted, waterbody-specific recommendations that integrate model-based insights with practical management considerations.

4.3 Results

First, we investigated the effect of climate forcings on the waterbodies in their original locations, and then we examined the effect across latitudes (Section 4.3.4 Latitudinal effect).

4.3.1 Model validation

The model performed best for Alton Water ($R^2 = 0.47$), followed by Esthwaite Water ($R^2 = 0.31$), while Loch Leven showed limited predictive skill ($R^2 = 0.12$). This pattern was consistent across the error metrics, with Loch Leven exhibiting the highest RMSE (23.4 $\mu\text{g/L}$) and MdSA (115.8%), indicating larger deviations between simulated and observed values. In contrast, Esthwaite Water and Alton Water showed lower errors, suggesting more accurate model performance at these sites. In Loch Leven, GLM-AED performed better in earlier years compared to later years (Figure 4.3). Validation of the climate runs against the observes can be found in Appendix C.

Table 4.3 Validation error metrics comparing in situ and modelled chlorophyll-a concentrations. RMSE, MAE, MdSA, and R^2 are reported for each waterbody, based on the model using original input data and parameter settings.

Waterbody	RMSE	MAE	MdSA	R^2
Loch Leven	28.5	22	115.0	0.12
Esthwaite Water	16.4	10.7	62.7	0.31
Alton Water	26.0	11.0	81.7	0.47

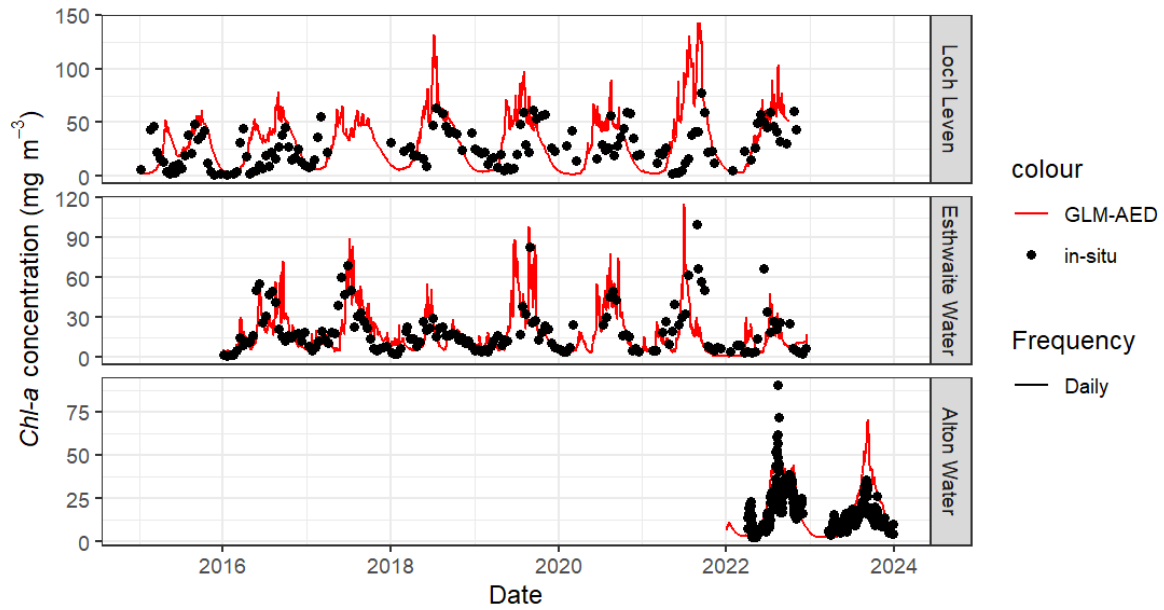
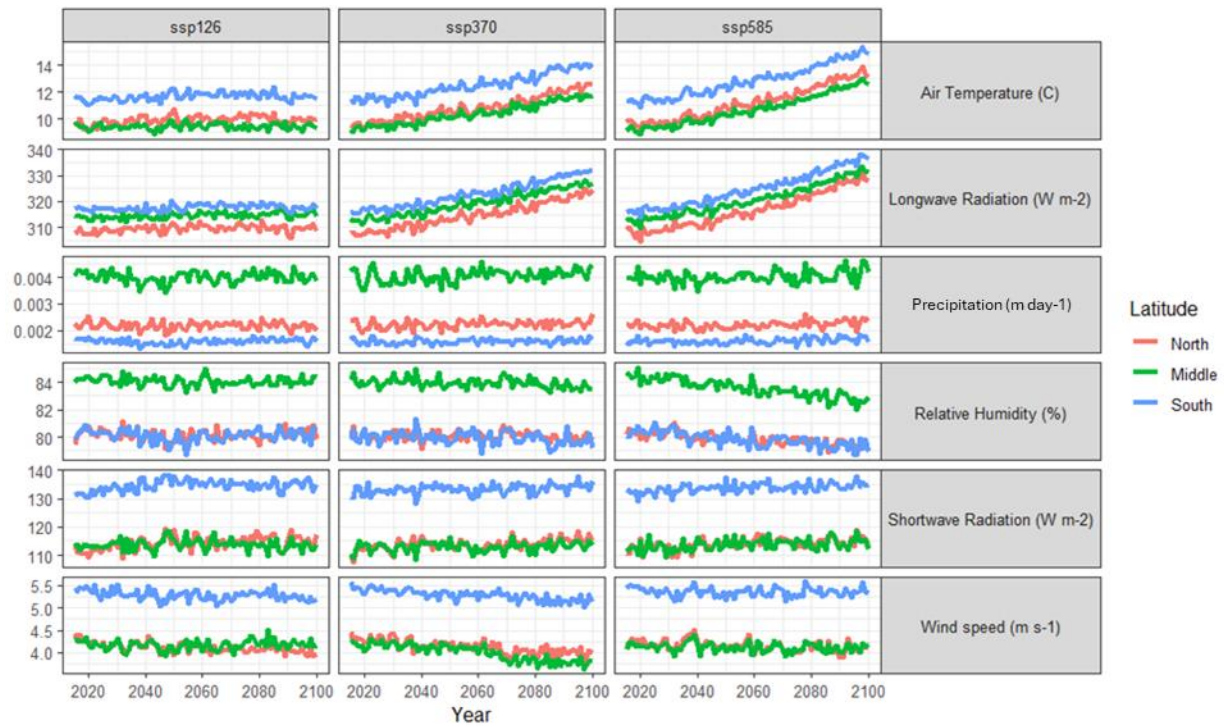


Figure 4.3 Model validation of chl-a concentrations for the three waterbodies using the original model set-up with default meteorological forcing and inflow data. In-situ chl-a (black dots) compared with modelled outputs (red line) over the full simulation period.

4.3.2 Climate forcings

The climate forcings averaged across 5 GCMs per latitude illustrate how the inputs to GLM-AED vary by SSP and latitude. The southern latitude showed increased air temperatures of approximately 2 °C between 2025 and 2100, and a much increased windspeed and (1 m/s) and shortwave radiation (20 W m⁻²), where the north and central agreed on lower values (Figure 4.4).

Figure 4.4 Mean annual SSP scenario inputs from five GCMs across different latitudes.



The central latitude dominated in precipitation with more than double the precipitation of the south and below double of the north. This also explained the 4% higher relative humidity in the central latitude. The climate projections variables all have significant slope ($p < 0.05$) for each SSPS and LWBC. With air temperature (0.013 year^{-1}) and longwave radiation increasing (0.07 year^{-1}) more rapidly, a slight increasing trend for shortwave radiation (0.02 year^{-1}) and a declining trend in relative humidity (-0.003 year^{-1}) and windspeed (-0.002 year^{-1}). Precipitation ($0.0000009 \text{ year}^{-1}$) change the least and stabilise in SSP585.

4.3.3 Climate forcing effects

Between 2000 and 2100, the three real LWBCs (A, E, and I) showed a change in surface temperature, with an increase of approximately $\sim 0.75 \text{ }^{\circ}\text{C}$ projected under SSP1-2.6, and larger increases of $2.6 \text{ }^{\circ}\text{C}$ and $3.2 \text{ }^{\circ}\text{C}$ projected under SSP3-7.0 and SSP5-8.5, respectively. Correspondingly, the number of stratification days, which was strongly influenced by surface temperature, also increased, with SSP1-2.6 indicating an extension of 13 days. SSP3-7.0 and SSP5-8.5 showed increases ranging from 17.4 to 43 days which was a 2.5 fold increase in stratification days.

Echoing these projected temperature increases, the model also projected a corresponding rise in chl-a concentrations toward the end of the century (Figure 4.5). Among the LWBCs, Loch

Leven displayed the widest range suggesting that chl-a projections are particularly sensitive to differences in GCM inputs. In contrast, Alton Water showed the narrowest range, indicating more consistent responses across GCMs.

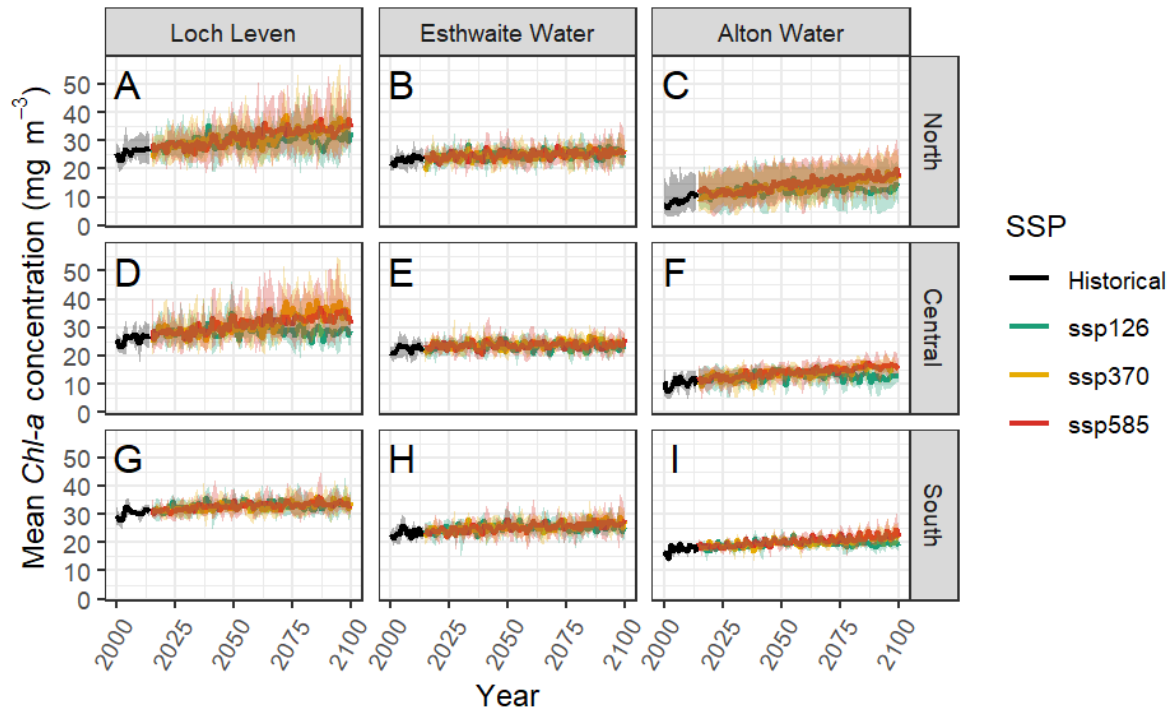


Figure 4.5 Mean annual chl-a concentrations across LWBCs, denoted by letters. Colours correspond to different Shared Socioeconomic Pathway (SSP) scenarios, with ranges showing the GCM outputs. Alton Water shows some clear 4 year oscillations, which are an artefact of the extrapolation technique used. The shade area shows the range of the GCMs.

Under the SSP1-2.6 scenario, projected mean annual chl-a concentrations significantly increased from 19 mg m⁻³ in Loch Leven, 21 mg m⁻³ in Esthwaite Water, and 16 mg m⁻³ chl-a in Alton Water in the historical period to 26.6 mg m⁻³, 23.3 mg m⁻³, and 18.8 mg m⁻³ chl-a respectively by 2100. Concentrations at the end of the century increased even further under SSP3-7.0 (31.3, 26.3, and 21.7 mg m⁻³ chl-a respectively) and SSP5-8.5 (30.3, 26.4, and 22.1 mg m⁻³). While Esthwaite Water also showed an upward trend in chl-a over the century, the rate of increase was more gradual than the steeper trajectories observed in Loch Leven and Alton Water.

Across all sites, the difference in chl-a concentration between the high-emission scenarios SSP3-7.0 and SSP5-8.5 was relatively minor (approximately 0.6 mg m⁻³), especially when contrasted with the larger difference to SSP1-2.6 (averaging 3.4 mg m⁻³) at the end of the century. This suggests that most of the increase in chl-a occurs between low- and mid-range emission scenarios, with marginal increases under the most extreme forcing.

In terms of bloom duration, the real LWBCs were projected to experience up to 45.4 additional bloom days per year by the end of the century under SSP5-8.5, with a similar increase of 46.7 bloom days in SSP3-7.0. A lower increase was observed with SSP1-2.6 of 18.5 bloom days.

Overall, chl-a concentrations and subsequently bloom days increased significantly in all three water bodies toward the end of the century indicating a strong response of phytoplankton bloom dynamics to climate forcing.

4.3.4 Latitudinal effect

The effect of the latitude of these climate impacts was investigated by running each of the waterbody models with the other two latitudes, negating any waterbody specific effects.

The LWBC from nine scenarios lettered A–I revealed that the northern latitude had the strongest impact on several lake response variables, with a few exceptions.

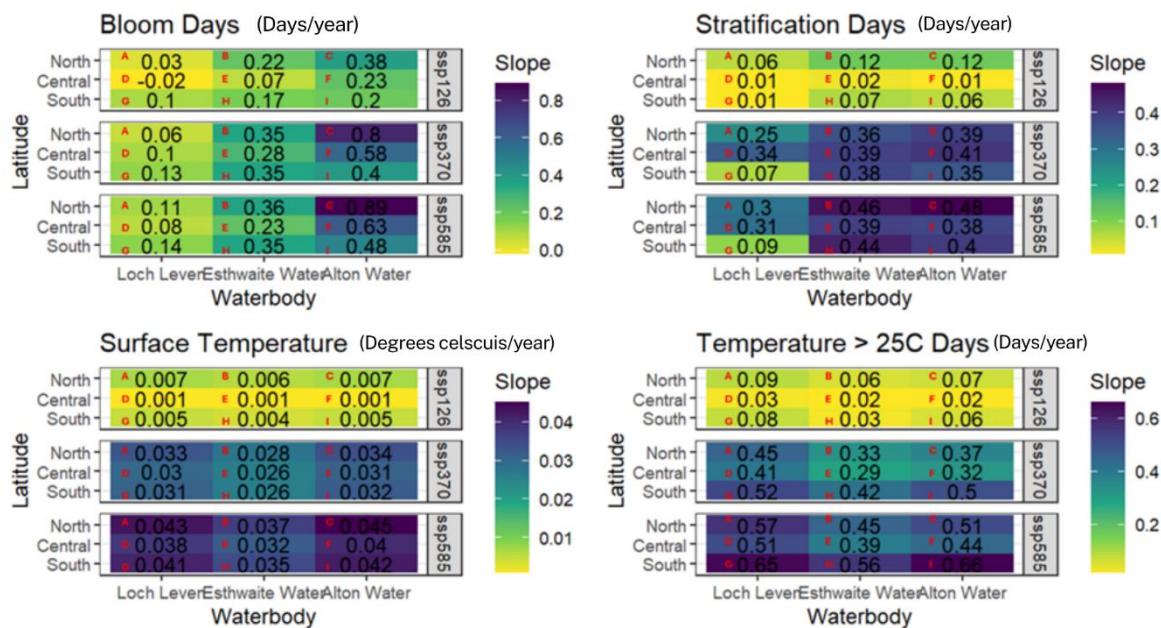


Figure 4.6 The slopes, change in variable from 2000 to 2100, of four waterbody characteristics across the latitudinal gradient, with red letters denoting distinct LWBCs. The darker colours indicate higher slopes, with the lighter colours indicating lower slopes. The plots are separated in the 3 climate scenarios and waterbodies.

An overall pattern emerged between the waterbody characteristics (Figure 4.6), showing the largest effect of SSPs on surface temperature. Across the LWBC gradient, surface temperature, bloom days, and stratification days showed the steepest slope in LWBC C (Alton Water in the north) in all SSPs except for stratification days in SSP3-7.0 (F), whereas temperature days above 25 °C reached their highest values under LWBC G (Loch Leven in the south).

Surface temperature consistently showed the highest slopes in the northern latitudes (LWBC: A, B, and C). Bloom days yielded the highest slope in the central latitude in Loch Leven (LWBC: D). Stratification days showed the highest slopes in the northern latitudes with SSP1-2.6 and SSP5-8.5, however the SSP3-7.0 resulted in the largest slope in the central-latitude scenarios (D, E, and F). Temperature threshold days resulted in the steepest slopes in southernmost scenarios (LWBC: G, H, and I) in the extreme SSPs, but showed the steepest slope in SSP1-2.6 to be the northern latitudes. This may be explained by the less severe temperature slope in SSP1-2.6 being more dominant in the northern latitudes where there were minimal days hitting that threshold. This may slightly increase for neighbouring days, however when the temperature slope went up in SSP3-7.0 and 5-8.5, the southern latitudes already had more days that crossed the threshold due to a higher initial temperature. As a waterbody, Alton Water showed the largest slope in bloom days, with temperature threshold days showing the largest slopes in Loch Leven. For stratification days both Alton Water and Esthwaite Water showed very similar slopes, where Loch Leven showed drastically lower slopes. The surface temperature slopes in Loch Leven and Alton Water were identical, whilst the slopes for Esthwaite Water were slightly lower for each of the SSPs and latitudes.

The least pronounced latitudinal slope differences were found in Loch Leven bloom days. Showing little to negative slopes. A reverse latitudinal effect, with the southern slopes being highest can be observed. Contradictory, in the other three variables (figure 4.6), Loch Leven does show the largest differences in slopes across latitudes. This shows that polymictic and large waterbodies like Loch Leven may be most impacted by the latitudinal gradient, whilst reservoirs like Alton Water were more impacted by the different SSP scenarios. Overall, the northern latitudes, independent of waterbody were most impacted in most of the water quality variables shown. With especially the reservoirs being heavily impacted by SSPs.

4.3.5 Algal blooms and chl-a concentrations

A closer examination of chl-a concentration across the latitudinal gradient revealed a larger chl-a increase in the northern latitudes ($1.8 - 8.6 \text{ mg m}^{-3}$) compared to the southern latitudes ($0.7 - 4.6 \text{ mg m}^{-3}$) (Figure 4.5).

The starting chl-a concentrations in the northern latitude water bodies (A = 26.6, B = 23.5, C = 18.0 mg m⁻³) were similar or lower than their southern counterparts (G = 30.8, H = 23.7, I = 18.0 mg m⁻³) especially prominent in Loch Leven (A,G) and Alton Water (C,I). Both the southern (G = 33.7, H = 27.3, I = 20.9 mg m⁻³), and northern (A = 34.3, B = 26.3, C = 15.8 mg m⁻³) latitudes were projected to reach similar or smaller difference in concentrations by 2100, resulting in a steeper slope. The lowest increase in chl-a (0.7 to 4.6 mg m⁻³) was observed in Esthwaite Water, followed by Alton Water (0.8 to 7.0 mg m⁻³) and Loch Leven (1.9 to 8.6 mg m⁻³).

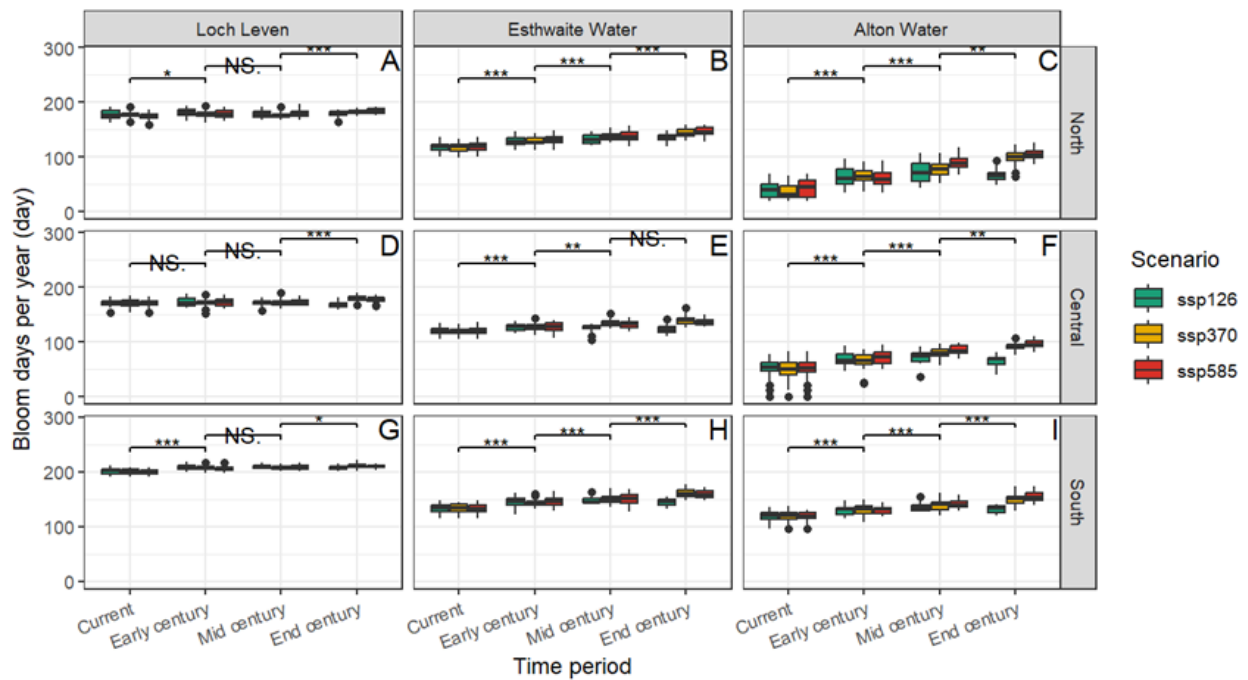


Figure 4.7 Projected changes in bloom days in Loch Leven (Shallow lake), Esthwaite Water (deep lake) and Alton Water (Deep reservoir) across the 21st century, shown for four time periods: Current (2000–2025), Early Century (2026–2050), Mid Century (2051–2075), and End Century (2076–2100). Values represent the average number of bloom days per year under each SSP, aggregated across all GCMs. (***) = 0.001, (**) = 0.01, (*) = 0.05, NS = Not significant)

In terms of algal bloom days (> 24 mg m⁻³ chl-a), the LWBCs B, C, F, H and I saw a constant significant increase in bloom days from Current to the End of the century (Figure 4.7). Loch Leven already has a starting chl-a concentration of 26 to 30.8 mg m⁻³, meaning that the bloom threshold was already reached.

4.3.6 The relative importance of latitude, GCM, waterbody and SSP

The relative importance of the four factors (Waterbody characteristics, Global Climate Models (GCMs), latitude and SSP scenarios) were subjected to an ANOVA to investigate which had the largest influences on the output. The variance in chl-a concentrations across

time periods was primarily explained (approximately 50%) by differences between the three water bodies.

However, when analysing each site separately (Figure 4.8), distinct temporal trends emerged, particularly in Alton Water and Loch Leven. In both waterbodies, the influence of latitude diminished over time, while the contribution of GCMs became increasingly significant. The SSP scenarios only explained variance from the mid-century onwards, in Loch Leven ultimately surpassing the influence of latitude by the end of the century.

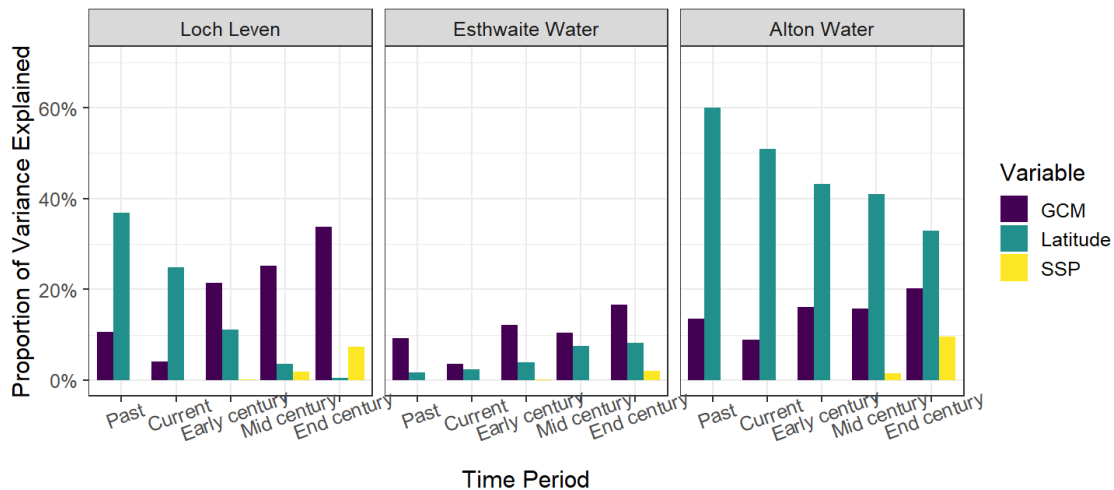


Figure 4.8 The variance explained for each of the important factors affecting chl-a concentrations in future time periods: Waterbody, latitude, GCM and SSP. The time zones considered (x-axis) are the Past (<2000), Current (2000- 2025), Early Century (2026 – 2050), Mid Century (2051 – 2075) and the End Century (2076 – 2100).

In contrast, Esthwaite Water shows a more complex pattern: both latitude and GCM influence increased modestly over time, but a large proportion of the variance remains unexplained and is attributed to residuals. The SSPs in Esthwaite Water play only a minor role throughout the entire time series.

4.4 Discussion

The model performance observed in this study, showed goodness of fit metric MAEs that are consistent with, or lower than those reported in the literature. For example, GLM-AED simulations in Western Lake Erie reported MAEs ranging from 19.08 to 41.66 mg m⁻³ (Q. Wang & Wang, 2021), which falls in line with our range of 10.7 to 18.3 mg m⁻³. While numerous studies have applied GLM-AED, they often focus on systems with lower chl-a concentrations, which typically yield lower MAEs. In contrast, the R² values achieved in this study, ranging from 0.12 to 0.47, were generally lower than those reported by Elliott and colleagues, who found R² values of approximately 0.51 for Loch Leven and up to 0.72 for Esthwaite Water (Alex Elliott & May, 2008; Elliott, 2010). However, (Ward et al., 2020)

reported R^2 values ranging from 0.12 to 0.19, indicating that the results for Loch Leven are consistent with those found in the existing literature. With the MAEs being better, R^2 being worse and the RMSE and MdSA being acceptable, we found this to be a good basis for investigation of latitudinal and SSP based effects on chl-a concentrations. The modelled SSP scenario output compared to the in situ chl-a resulted in similar goodness of fit metrics, further highlighting that the modelling output is acceptable (Appendix B).

In this work, we determined that waterbody type will be the most important factor in determining responses to climate change scenarios like SSPs. Next to that, latitude will be an important driver for a reservoir like Alton Water in the next 75 years. In contrast, Loch Leven is more strongly influenced by a combination of projected climate variables, such as temperature and wind speed, across different GCMs and SSPs. Lakes like Esthwaite Water showed to be least affected by the latitudes, GCMs or SSPs and may face more nutrient based threats. These findings highlight that while overarching patterns existed, the drivers of chl-a variability are highly Waterbody specific and evolve differently under future climate scenarios.

4.4.1 Climate change and algal blooms: a driver-focused perspective

Using simulations under multiple SSPs, we observed increases in bloom duration and chl-a concentrations of up to 8 more bloom days every 10 years. Whilst these findings are in line with previous literature (Carvalho et al., 2012; Gobler, 2020; Markelov et al., 2019; Moss et al., 2011; Paerl & Huisman, 2008; Wiley & McPherson, 2023), the scale and nature of these changes varied considerably, primarily driven by local waterbody characteristics, followed by geographic latitude, climate model dynamics, and the specific SSP scenario applied. Below, we unpack each of these key drivers.

Waterbody characteristics as the primary driver

The physical and hydrological characteristics of each waterbody shaped their response to climate forcing more than any other factor. Alton Water, a deep reservoir with fluctuating water levels, showed the most pronounced increases in chl-a and bloom duration across all scenarios (Bloom days: 0.2 to 0.89, chl-a concentration: 15.9 to 20.9 mg m⁻³ chl-a). Its strong and persistent stratification and changing volume likely amplify the impact of surface warming by enhancing nutrient retention and internal loading (Heaney et al., 1986).

In contrast, Loch Leven, a shallow, large lake with a polymictic nature, was moderately affected, most prominently in chl-a concentration (Bloom days: -0.02 to 0.14, chl-a concentration: 29.4 to 34.3 mg m⁻³ chl-a), while Esthwaite Water, despite experiencing a more stratification days, showed minimal change in chl-a and bloom days (Bloom days: 0.07 to 0.36, chl-a concentration: 26.2 to 27.3 m⁻³ chl-a). These results align with previous work using the PROTECH model, which found minimal chl-a response to warming alone in Esthwaite Water unless flow rates were also altered (Elliott, 2010). Similarly, Loch Leven only showed meaningful changes when nutrient inputs were included (Alex Elliott & May, 2008).

Latitude as a modulating factor

Despite the relatively narrow geographic range of the study sites, latitude emerged as a significant (up to 60% in Alton Water) secondary driver of change in chl-a concentrations, bloom days, and physical lake processes. Southern sites consistently exhibited higher baseline levels of algal bloom indicators such as chl-a and bloom duration. However, steeper slopes in these indicators were generally observed at more northern latitudes (Figure 4.6), suggesting that although current bloom risks are lower in northern regions, they could equal or even surpass those of southern sites if climate trends persist.

The main exception to the overall latitudinal trend was Loch Leven, which showed the steepest increase in bloom days at its southern-latitude position under SSP5-8.5 (slope: 0.14) and SSP3-7.0 (slope: 0.13). This may be explained due to the waterbody already having chl-a concentrations above the WHO threshold (24 mg m⁻³) in the current situation (26 -30 mg m⁻³), means most blooms already exceeded the threshold and were counted as bloom days. The southern climate may be slightly better for the current algal communities to thrive compared to the northern climate and push the lower chl-a concentrations over the threshold.

Additionally, its baseline characteristics as a natural lake located in a northern region, may buffer it against more pronounced climate-driven shifts. Despite this anomaly, the southernmost latitude consistently showed the smallest changes, reinforcing the pattern that latitude is a key gradient of climate sensitivity across the UK (Mayes, 2000).

The increased effect in northern latitudes aligns with findings by Woolway et al. (2021), who reported greater climate sensitivity in lakes at higher northern latitudes. In their study, Esthwaite Water experienced a 15-day increase in the stratification period. Our results show a

comparable 13.6-day increase under SSP1-2.6 at Esthwaite original (Central) latitude, with even larger increases in stratification days (slope North: 0.12 to 0.46, slope Central: 0.02 to 0.39) observed when the lake was placed at the more northerly latitude.

Similarly, surface water temperature projections followed this latitudinal pattern, with the steepest increases occurring in the northernmost positions (slope: 0.007 to 0.0045) across all three waterbodies. This indicates that latitude modulates not only ecological responses but also the underlying thermal regime. Overall, our findings confirm that latitude influences both the baseline state and the rate of projected change.

SSP scenarios: directionally consistent, magnitude-dependent

While differences between SSPs were clearly observable, they exerted a smaller influence on ecological change than latitude or local waterbody characteristics. Nonetheless, even under the lowest-emission scenario (SSP1-2.6), measurable increases in surface water temperature, chl-a concentrations, and bloom duration were projected. Under higher-emission scenarios, such as SSP5-8.5, these increases became more pronounced, but their magnitude was highly dependent on the specific waterbody and its location.

Our surface temperature projections for 2100 ranged from 0.75°C (SSP1-2.6) to 3.2°C (SSP5-8.5) increase at the end of the century, with corresponding bloom day increases of 10 to 50 days depending on the lake and latitude. These results are broadly in line with global findings from the ISIMIP lake model ensemble, which reported end-of-century surface water warming of 1.38°C and 3.85°C for RCP 2.6 and 8.5, respectively (Golub et al., 2022) as well as (Huang et al., 2024). The slightly lower warming observed in the colder central Esthwaite Water (0.48°C in SSP1-2.6, 2.46°C in SSP5-8.5), could indicate a more resilient lake structure.

Among the three study sites, Loch Leven exhibited the most pronounced warming response to SSP scenarios in its original latitude (e.g., 1.17°C in SSP1-2.6 and 3.67°C in SSP5-8.5), while Esthwaite Water remained the least responsive. These patterns were consistent across multiple water quality indicators and are supported by the variance and slope analyses, further emphasising that the impact of global climate scenarios is mediated by local lake features. In summary, while SSPs define the overall trajectory of climate forcing, their ecological consequences are filtered through local context.

Climate models and physical processes

While waterbody characteristics and latitude primarily shaped the scale of local responses, and SSPs established the directional trajectory of change, GCMs contributed notably to the variability in projected outcomes, particularly for chl-a concentrations. Although not explored in depth beyond their role in generating ranges in our analyses indicate that GCM selection explained up to 30% of the variation in certain scenarios (Figure 4.8).

This influence was highly waterbody-specific and became increasingly pronounced toward the end of the century, likely due to compounding uncertainties in long-term climate projections and the future becoming less predictable the further you get from the current situation. Additionally, as climate change reduces the latitudinal differences in light and temperature, enabling earlier blooms across all regions, the direct effects of climate forcing (as represented by the GCMs and SSPs) become more prominent. In other words, once light, due to more sunny days, and temperature are abundant and therefore growth promoting at higher latitudes, nutrient availability and other climate-driven processes begin to dominate bloom dynamics, amplifying the influence of the specific GCM and SSPs scenarios. Such findings underscore the importance of considering ensemble climate model outputs when interpreting future ecological dynamics, especially for management decisions that rely on precise estimations of change.

While GCMs did not determine the overall direction of change, they significantly shaped the range and uncertainty of outcomes, reinforcing their relevance in scenario-based planning, particularly in systems that are already near ecological thresholds.

4.4.2 Eutrophication considerations

With current plans like the Water Framework Directive and other active approaches to reduce or mitigate nutrient inputs (Grizzetti et al., 2021; Zamparas & Zacharias, 2014) our results are representative of the future under continued nutrient management. However, it is important to note that our approach isolates the direct effects of climate change on waterbodies and does not account for associated changes in catchment hydrology or nutrient inputs. Because we effectively “transplanted” waterbodies to new climatic zones without modifying their hydrological or nutrient input, indirect climate-driven processes, such as increased runoff, altered nutrient loading, or soil warming, are not included. Recent work by (Gai et al., 2025) suggests that warming within the catchment can amplify in-lake warming responses by

approximately 25%. This highlights that climate change impacts on water quality may be more severe than indicated by waterbody-only simulations, especially where catchment processes contribute significantly to nutrient delivery and thermal regimes. In a recent study by Tigli et al. (2025), increases in chl-a were primarily attributed to nutrient enrichment rather than climate warming alone, which was also shown for Loch Leven and Esthwaite (Alex Elliott & May, 2008; Elliott, 2010). Whilst Esthwaite Water in our study may be less affected now, an increase of the current nutrient load (Alex Elliott, 2012) or indirect effects (e.g. deforestation (Gai et al., 2025; Ghaffar et al., 2022), catchment warming) may pose a greater threat than temperature in the future. Integrated modelling of climate-nutrient interactions should be a priority for future work, whilst keeping latitudes and waterbody characteristics in mind.

4.4.3 Management implications

Even if extreme scenarios like SSP5-8.5 are seeming less likely (Scafetta, 2024), the results of this study demonstrate that even moderate warming scenarios still pose significant ecological risks. The model results show consistent increases in algal bloom risk across all UK waterbodies under future climate scenarios, indicating that proactive, lake-specific management will be essential to mitigate these impacts.

This study finds that all UK waterbodies are projected to experience increased algal bloom risk under future climate scenarios, although the magnitude and drivers of change differ by lake type and location. The results further indicate that sensitivity to warming, stratification, and nutrient dynamics varies across systems, highlighting the need for tailored, waterbody-specific strategies that reflect the dominant processes identified in each lake type.

Reservoirs (e.g., Alton Water)

Results indicate that reservoirs, particularly in northern latitudes, are projected to experience the largest relative increases in bloom severity, despite currently low baseline chl-a levels. This suggests that these systems are highly sensitive to future warming, likely due to their thermal structure and water level variability.

- Given this strong sensitivity to stratification under warming, aeration measures (Kortmann et al., 1994) may help maintain mixing and reduce surface warming effects.
- Because the model results highlight rapid increases in bloom risk in these systems, early monitoring is critical to detect initial shifts before thresholds are crossed.#

Polymictic lakes (e.g., Loch Leven)

The results indicate that shallow, polymictic lakes show strong sensitivity to climate forcing, with steeper projected increases in chl-a under warming, particularly in northern regions like Loch Leven. Although southern lakes currently exhibit higher chl-a levels, the model results suggest that northern shallow systems are likely to experience more rapid increases in bloom intensity in the future.

- Considering, the modelled sensitivity to warming, promoting cooling through increased wind-driven mixing and reduced light attenuation (Tanentzap et al., 2008) may help offset temperature-driven increases in bloom development.
- The results and expert knowledge indicate that nutrient-driven processes are likely to amplify these warming effects in shallow systems like Loch Leven. Therefore, prioritising nutrient control alongside temperature management (Alex Elliott, 2012), particularly in systems susceptible to internal loading (Ae & Van Nes, 2007; Scheffer et al., 1993), is essential to limit the combined drivers of bloom intensification.

Monomictic lakes (e.g., Esthwaite Water)

The results show that monomictic lakes such as Esthwaite Water exhibit relatively weak sensitivity to climate variables alone, with minimal changes in algal bloom intensity across scenarios. This suggests that current bloom dynamics in these systems may be more strongly controlled by nutrient availability than by temperature.

- Given that the model results indicate limited temperature-driven changes, early and site-specific nutrient monitoring and management (Maberly et al., 2020), are particularly important to prevent future increases in bloom risk driven by non-climatic factors.
- The lack of strong climate-driven signals in the results supports a precautionary approach, as even small increases in nutrient inputs could lead to disproportionate ecological responses over time in systems where blooms appear to be nutrient-limited.

4.5 Conclusion

This study shows that algal bloom risks will increase across all three of our case study UK waterbodies by 2100, with the strongest impacts in Northern latitudes, regardless of the emissions scenario. Reservoirs and shallow lakes are especially vulnerable. Northern latitudes are showing steeper increases in bloom days, surface temperatures, and stratification particularly under SSP5-8.5.

Waterbody characteristics were the most important drivers of change, followed by latitude, while SSP scenarios and climate model choice played smaller but still notable roles. These findings highlight the need for targeted, site-specific management that addresses both warming and nutrient pressures, especially in northern reservoirs and shallow systems, where risks are expected to rise fastest.

4.6 Acknowledgements

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Chapter 5: Discussion

Freshwater ecosystems are increasingly under threat from eutrophication and harmful algal blooms, which compromise ecological integrity and water security. Climate change is expected to intensify the frequency and severity of algal blooms due to warming temperatures and altered hydrological cycles. In situ monitoring is costly, time-consuming, and does not provide insights into the future state of waterbodies. In response, research has increasingly turned to modelling and earth observation as tools to support the monitoring and forecasting of bloom events and inform timely management actions. While modelling approaches can simulate chl-a concentrations and bloom dynamics, they often face limitations related to accuracy, transferability, and data requirements. Similarly, Earth observation offers valuable spatial and temporal insights but is constrained by data quality issues and lacks forecasting capabilities. Integrating these two approaches offers a promising pathway for improving the reliability and applicability of bloom forecasts. The thesis explored critical challenges in forecasting algal blooms in freshwater systems. As well as showed that the combined used of modelling and earth observation can enhance our ability to manage freshwater algal blooms. Through addressing technical and practical barriers in monitoring and forecasting, this work contributes to the development of tools that are not only useful in scientific context but also in real-world lake management under growing environmental stressors.

Three core research objectives structured the thesis. First, to evaluate the role of data frequency in driving and calibrating process-based models for algal bloom simulation.

Second, to quantify the uncertainty associated with satellite remote sensing products and assess their suitability for improving lake model calibration. Third, to explore how climate change may influence algal bloom dynamics across lakes in the UK, and to identify patterns of system-specific vulnerability.

5.1 Key findings and thematic insights

5.1.1 Data requirements for accurate bloom forecasting (Chapters 2)

Chapter 2 demonstrated the importance of high-frequency meteorological forcing data in accurately simulating bloom dynamics. Among all input variables, meteorological drivers were consistently the most influential in determining bloom onset and intensity. The frequency and quality of the chl-a calibration data was also critical, particularly for capturing the full range of chl-a concentrations. However, the available in situ data often failed to capture these peak events due to low sampling frequency, typically on a fortnightly basis. This limitation was evident even in Esthwaite Water, one of the most well-monitored lakes in the UK. In many other lakes, where monitoring is less frequent or entirely non-existent, the lack of high-resolution chl-a data presents an even greater challenge for accurate model calibration and validation.

This highlights a critical gap in current lake monitoring practices for aiding models and underscores the need for alternative data sources. In this context, remote sensing offers a valuable solution by providing broader spatial coverage and higher temporal resolution, which can complement sparse in situ data and enhance our ability to simulate and forecast bloom dynamics across a wider range of waterbodies.

5.1.2 Earth observation as a calibration tool for modelling (Chapter 3)

Chapter 3 builds on the findings of Chapter 2 by exploring whether remote sensing can serve as a viable complementary data source for modelling algal blooms. We demonstrate that chl-a concentrations can be successfully derived from Sentinel-2 imagery for our case study lakes, and that these satellite-derived observations can be used effectively to calibrate lake ecosystem models. This is a significant step forward, particularly for under-monitored lakes where in situ data are sparse or irregular, though the broader potential of Earth observation for model calibration has been previously recognised.

A key contribution of this chapter lies in the implementation of conformal prediction as a quality control method for Earth observation data. Satellite-derived chl-a data were still

subject to atmospheric interferences, sensor noise, and algorithmic uncertainty. We demonstrated that conformal prediction provides a powerful method to quantify and manage this uncertainty. This uncertainty filtering approach allowed us to retain only the most reliable observations which significantly improved model calibration, especially during high-bloom conditions. This approach led to substantial improvements in model calibration, especially during high-bloom events. These improvements were likely driven by a more complete representation of the full range of chl-a concentrations compared to in situ datasets, which, as highlighted in Chapter 2, often fail to capture peak bloom conditions due to limited sampling frequency.

Together, Chapters 2 and 3 highlight the critical role of chl-a data in model calibration and demonstrate that earth observation, when paired with robust uncertainty filtering, offers a scalable and practical solution, especially for under-monitored lakes where regular in situ data collection is limited by cost, accessibility, or seasonality.

5.1.3 Spatial and climatic variability in bloom responses (Chapter 4)

Following the improved models from Chapter 2 and 3, Chapter 4 explored the effects of climate change on algal bloom dynamics across UK waterbodies using multi-model climate projections. This chapter demonstrates the practical value of robust bloom forecasting tools, showing how they can be used not only for current monitoring and management, but also for anticipating future risks under a changing climate. By linking model improvements to real-world applications, Chapter 4 highlights the broader relevance of this research for long-term water resource planning and policy.

This work presented future projections of algal blooms across a latitudinal gradient by applying climate scenarios from three UK regions to three distinct waterbody types. This experimental design enabled the disentangling of the effects of climate, latitude, and waterbody characteristics on bloom dynamics. While all waterbodies exhibited an overall increase in bloom pressure over time, the magnitude and timing of responses varied considerably by location and waterbody type, highlighting pronounced spatial heterogeneity. Latitude emerged as the dominant driver, with northern waterbodies responding more sensitively due to their cooler baseline climates and higher rates of warming. By the late century, climate forcing scenarios became the primary determinant of bloom trajectories, indicating an intensification of global warming impacts over time.

The work also showed that reservoirs, which generally have highly regulated hydrology or large intra-annual water fluctuations, were disproportionately affected compared to more natural waterbodies. This likely results from synergistic interactions between hydrology and climate warming, for example through changes in retention time or the strengthening of stratification, which amplify bloom risk (Bănăduc et al., 2024; Richardson et al., 2018). These findings underscored the need for spatially targeted management strategies that incorporate regional climate projections, lake morphometry, and hydrological regime characteristics.

5.2 Overarching themes

While the key findings and thematic insights already highlight the connections between the chapters of this thesis, several overarching themes also emerge across the work as a whole. Firstly, decision making in modelling. Secondly, calibration data being critical for accurate simulation and forecasting. Third, earth observation will make models more transferable and lastly, complexity versus transferability.

5.2.4 **Black box modelling and hidden decision-making**

Despite being process-based, models such as GLM-AED often function as a “black box” in practice. While the main equations are well defined, the interaction between parameters, boundary conditions, and input data makes model behaviour difficult to fully interpret. This is particularly clear during calibration, where multiple parameter combinations can produce similar performance, obscuring the underlying system dynamics.

This thesis shows that part of this “black-box” perception arises not only from model complexity, but also from the decisions embedded within the modelling workflow.

Calibration was highly sensitive to the structure, frequency, and quality of input data, as discussed across all chapters. For example, in Alton Water, several chl-a data sources were available, including laboratory measurements, satellite-derived estimates, field sensors, and buoy-based observations. While all represent the same water body, they introduced different modelling challenges and outcomes. Showing the inherent impact that monitoring will have on your modelling outcomes and that picking the right monitoring strategy matters.

In addition, early calibration attempts and parameter choices often proved unsuccessful but informed later decisions. For instance, an initial attempt to model waterbody-specific phytoplankton species was abandoned after trial and error due to the difficulty of calibrating individual species. This led to the adoption of phytoplankton functional groups representing

dominant seasonal dynamics (diatoms and cyanobacteria). Similarly, while phytoplankton growth rates were optimised using a structured parameter sweep, defining chl-a thresholds at which blooms become problematic, and interpreting model performance in that context, required expert judgement from water managers.

Together, these elements show that model outcomes are shaped not only by process representation, but also by a series of implicit decisions made during setup and calibration. Improving transparency in these steps will be essential for enhancing reproducibility and confidence in model-based water quality assessments.

5.2.1 Calibration is critical

All three data chapters in this thesis underscore the importance of effective calibration for the GLM-AED model in achieving reliable simulations and forecasts of algal blooms. Chapter 2 illustrated that data frequency strongly influences model performance in capturing bloom dynamics. Chapter 3 showed how remote sensing can improve calibration through broader spatial coverage and by filtering uncertainties. Chapter 4 then applied these calibrated models for both retrospective simulation and forecasting, demonstrating their operational potential. While the general importance of high-quality input data is widely recognised in the modelling literature (He et al., 2017; Lindgren et al., 2022; Watson et al., 2021), this thesis places particular emphasis on the role of calibration data, not just its presence, but its structure, frequency, and uncertainty characteristics. Crucially, this work identifies where improvements in calibration data can yield disproportionate benefits across the modelling workflow.

This is especially relevant in a context where many water bodies lack sufficient in situ data. However, emerging data sources such as satellite Earth observation, low-cost sensors, and even citizen science initiatives are becoming increasingly accessible. These hold considerable promise for enhancing calibration, but also come with significant challenges, particularly related to data quality, uncertainty, and comparability. A key question for the field is how models can better incorporate these increasingly abundant imperfect datasets through robust quality control, uncertainty quantification, and data assimilation techniques.

Rather than relying solely on traditional high-frequency monitoring, this thesis suggests that water managers could adopt more flexible and hybrid data strategies for model calibration for example Earth observation or other data sources in combination with conformal prediction.

By doing so, they could expand coverage while maintaining sufficient data quality to support reliable bloom forecasting and scenario analysis.

5.2.2 Transferability through Earth observation

The spatial coverage and repeatability of satellite-derived data make it a powerful tool for extending bloom forecasting beyond intensively monitored lakes. While not a substitute for in situ data, Earth observation enhances both the consistency and generalisability of model calibration. Chapter 2 highlighted the need for complementary data sources, showing the limitations of relying solely on sparse in situ measurements. Chapter 3 demonstrated that Earth observation data, when filtered using conformal prediction, can not only supplement but also improve model calibration and performance. Building on this, Chapter 4 demonstrated that the calibrated models performed well when validated against current in situ data, increasing confidence in their use for projecting climate change impacts and for identifying waterbodies at greatest risk across the UK.

Therefore, the key advantage of using Earth observation is its ability to provide chl-a data consistently across many waterbodies. In addition to broad spatial coverage, the methods are repeatable and can be standardised across different waterbodies and regions, making EO a scalable solution for long-term monitoring and comparison.

This is especially valuable given the importance of calibration data demonstrated throughout this thesis. Earth observation makes it feasible to calibrate models for waterbodies that were previously excluded from modelling efforts due to lack of data. As a result, the use of Earth observation improves not only the monitoring coverage but also expands the potential for model application. Thus, transferability refers not just to the broader use of Earth observation data, but also to the increased ability to apply calibrated models across many different lakes, both within the UK and beyond.

5.2.3 Complexity and transferability

As modelling approaches become increasingly transferable using Earth observation, the main constraint shifts from data availability to model complexity. While data can now be generated consistently across many locations, the practical challenge lies in scaling up bloom forecasting, as building and maintaining complex models for each individual waterbody remains time-consuming and resource intensive. Although not the central focus of this thesis,

the issue of model complexity is a critical theme that underpins the broader challenge of applying forecasting tools across diverse freshwater systems.

In modelling, greater complexity is often assumed to improve realism by capturing more of the system's processes. However, increased complexity comes with a cost: more parameters to define, more data requirements, and more expert knowledge needed for setup and calibration. This can limit the ease with which models like GLM-AED can be applied to new systems, even when data availability improves. In this thesis, Earth observation helped to overcome data limitations and expand the transferability of model calibration, but parameterisation still required careful consideration. Parameters were often derived from site-specific knowledge, literature, or default values, all of which become increasingly time-consuming to justify and apply as the number of modelled waterbodies grows.

This highlights a fundamental trade-off. As we push for broader application of models, we may need to constrain complexity to maintain feasibility. Future work could explore ways to reduce model complexity, such as minimising the number of variable parameters, without sacrificing too much accuracy. Striking the right balance between complexity and transferability will be essential for developing scalable and practical tools for freshwater management.

5.3 Management implications and recommendations

One of the main goals in this thesis was to demonstrate that models can provide valuable insights for water management based on our findings. The results across all three data chapters converge on a set of practical recommendations for future monitoring and management:

- **Integrated monitoring and modelling using remote sensing:**

Monitoring programmes should be co-designed with modelling objectives in mind, particularly for algal bloom management. This includes prioritising high-quality flow and chl-a datasets that capture a wide range of bloom conditions. Remote sensing offers a scalable, spatially extensive, and temporally rich data source that can complement in situ measurements, especially in remote or data-scarce regions. When combined with uncertainty filtering techniques such as conformal prediction (as demonstrated in Chapter 3), satellite-derived data become a reliable input for model calibration and validation. Investment in a remote sensing processing pipeline, strategically integrated with targeted in situ data collection, can significantly enhance

modelling efforts while reducing long-term monitoring costs. Water managers should therefore actively explore and adopt remote sensing tools as part of their catchment-scale management strategies.

- **Prioritisation based on risk:** Findings in Chapter 4, point to disproportionate impacts in northern and hydrologically managed waterbodies. These areas should be prioritised for both advanced modelling efforts through higher quality data and calibration, and proactive management interventions, such as adaptive reservoir operations or early-warning systems. Whilst data may be scarce in more northern regions due to more remote landscapes, modelling should not be disregarded approach as shown in Chapter 2 and 3 where it was shown that data scarcity can be accepted or limited using remote sensing data.
- **Investment in regional climate modelling:** The high influence of latitude of UK waterbodies to climate drivers highlights the importance of regionally downscaled climate projections. Meaning more complexity captured by the models whilst still being transferable. These more detailed models like GLM-AED can inform more accurate and lake-specific adaptation strategies, not only in the UK, but across the globe. Remote sensing data can help validate and supplement these projections as satellites get increasingly better at small spatial resolutions.
- **Interdisciplinary work:** The findings across all chapters underscore the critical importance of interdisciplinary collaboration in effective water management, particularly for improving the forecasting of algal blooms. Ongoing dialogue between researchers, water managers, and stakeholders is essential to ensure that forecasts are both scientifically robust and practically relevant. While collaboration between scientists and water managers can yield accurate predictions of bloom dynamics, stakeholders may prioritise different concerns, such as whether it is safe to swim, rather than focusing more complex algal community dynamics. Addressing diverse needs requires integrated communication strategies that bridge disciplinary and institutional boundaries.

5.4 Limitations and future research

While this thesis presents several advances in the use of remote sensing and process-based models for forecasting algal blooms, future developments remain, particularly when

considering the future of operational water quality forecasting and emerging technologies in environmental modelling.

One major area of development is the growing focus on digital twins for lakes and catchments (Qiu et al., 2023). These virtual representations integrate real-time data with 3D model data to support continuous environmental monitoring and decision-making (Chen et al., 2023; Qiu et al., 2022). The modelling approaches demonstrated in this thesis, particularly the integration of remote sensing with process-based modelling and uncertainty filtering, align closely with the foundational components of digital twins. However, fully operational digital twins for lakes require seamless data ingestion, high temporal resolution observations, and automated forecasting capabilities. Future work should explore how frameworks such as GLM-AED and/or EO can be adapted or scaled into digital twin platforms, especially in combination with remote sensing pipelines and real-time sensor networks.

Closely linked to this is the challenge of operational forecasting. This thesis focused primarily on hindcasting and long-term scenario simulations; however, real-time bloom forecasting remains a crucial application. Tools such as the FLARE system (Carey et al., 2022; Paíz et al., 2024; Thomas et al., 2020) illustrate how process-based models can be coupled with real-time data for short-term forecasting. Yet several barriers remain, most notably, limited access to high-frequency data or other water variables, challenges in automating data processing workflows (particularly for biological variables such as chl-a), and the absence of robust data assimilation methods that can dynamically update forecasts as new observations become available. Integrating remote sensing into operational modelling workflows is a promising yet underdeveloped avenue, especially when satellite-derived data are subject to uncertainty and variability. However, the uncertainty filtering framework established in Chapter 3 provides a critical foundation for this next step. By reliably identifying high-quality observations, this approach enables future research to explore the assimilation of satellite-derived chl-a into forecasting models with greater confidence and scientific rigour, as well as possible other data sources.

Another future direction lies in the spatial dimensionality of modelling. This thesis used a 1D modelling approach (GLM-AED), which is appropriate for many applications and

computationally efficient. However, the use of remote sensing inherently provides spatially distributed observations, particularly surface chl-a fields. Next to that, digital twins also operate on a 3D dimensional plane. This raises the question of whether more spatially explicit modelling approaches, such as 2D or 3D models, might be necessary to utilise the full capabilities of EO data and forecast algal blooms. Whilst for this work, the 1D model was sufficient, expanding to higher-dimensional models may be warranted in more complex or morphologically heterogeneous lakes, especially where spatial variability in blooms is of management concern. Advancing toward data assimilation and more operational modelling frameworks comes with increased demands, both in terms of computational resources and error propagation. This includes more intensive parameterisation, greater data requirements, and ultimately, reduced spatial transferability. In essence, we return to the long-standing trade-off between complexity and transferability: is it more valuable to develop highly accurate models for a few well-studied systems, or to prioritise broader scalability by accepting lower precision in data-limited contexts? Addressing this tension will be central to the future of lake ecosystem modelling, particularly as the field moves toward real-time forecasting and large-scale environmental monitoring.

This trade-off was already visible in GLM-AED, where model structural limitations also persist. As with all process-based models, GLM-AED relies on simplifications that may constrain its applicability in highly dynamic systems. Overfitting remains a risk when calibration lacks structure, and generalisation may reduce accuracy at site-specific applications. The development of standardised calibration protocols, specifically focused on the most sensitive and impactful parameters, could improve both the reliability and transferability of models like GLM-AED.

Finally, it is important to emphasise the broader modelling capacity of GLM-AED beyond chl-a. The framework simulates a wide array of physical and biogeochemical variables, such as thermal stratification, dissolved oxygen, and nutrient concentrations, which are valuable for ecosystem health assessments and management. These outputs position the model well for integration into multi-sectoral decision-support systems, particularly under climate and land-use change pressures. The integration of remote sensing, lake modelling, and climate projections offers a powerful, scalable toolkit for managing freshwater ecosystems. As environmental monitoring evolves toward real-time, adaptive frameworks, future research

should focus on bridging gaps between data acquisition, assimilation, model generalisability, and operational deployment.

5.5 Concluding remarks

Algal blooms are an increasingly global problem, likely to worsen under future climate scenarios. While both modelling and remote sensing have long been recognised as promising tools, barriers such as data scarcity and uncertainty have limited their operational uptake. This thesis shows that, even under imperfect data conditions, robust bloom forecasting is achievable. Calibration remains the most important factor for model accuracy, and we demonstrate that satellite-derived chl-a, when properly filtered, can fill critical data gaps. These calibrated models, when coupled with climate projections, reveal that bloom risk is greatest in northern UK lakes and reservoirs, where climate and hydrological pressures converge.

The findings highlight the potential of remote sensing and open-access climate data to advance lake management across the UK. Finally, this thesis calls for greater interdisciplinarity in freshwater research: by bridging remote sensing, process-based modelling, and climate science, we can build forecasting systems that are more robust, cost-efficient, and relevant to management under future change.

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X;TECHMETA=119,123,134;SUBJMETA=158,2459,286,4112,47,704;KWRD=ELEMENT+CYCLES,FRESHWATER+ECOLOGY,LIMNOLOGY

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Appendices

Appendix A

Process-based models in literature considered for this work

PCLake is a model that focuses on the competition between phytoplankton (three species) and macrophytes. It includes interactions with zooplankton, fish, benthic organisms, and biophysicochemical exchanges between water and sediment. One of its key outputs is a hysteresis graph that illustrates the shift between turbid and clear water states, making it useful for assessing food web dynamics and nutrient cycling. It is primarily implemented in Excel, which makes it relatively accessible, though it can also be used in other platforms. However, it is only applicable to shallow, non-stratifying lakes, which limits its scope. Additionally, it requires a large amount of input data and can be quite complex to use.

PCLake+ is an extended version of PCLake that includes lake stratification and additional oxygen dynamics. It is designed for theoretical studies, global assessments, and case studies of specific lakes. While it offers more advanced modelling capabilities, it is still under development and not yet widely adopted. It remains a complex and data-intensive model, requiring significant expertise to use effectively. Moreover, it has not been historically used for forecasting, which could limit its practical applications in predictive studies.

MyLake is a multi-year lake simulation model designed for seasonal simulations. It is particularly suited for modelling ice and snow cover, as well as the daily distribution of heat, light, phosphorus, and total phytoplankton chlorophyll-a within the water column. The model is well adapted for Monte Carlo simulations, which allow for sensitivity and uncertainty analyses. Because it takes a relatively simple approach, it is easier to use compared to more complex models. However, this simplicity means it only represents the most significant physical, chemical, and biological processes, resulting in some finer ecological details may be missing. Another potential drawback is that it is implemented in MATLAB, which may require additional learning for users who are not familiar with the platform.

DYRESM-CAEDYM is widely used for limnological studies and consists of two components: DYRESM, which handles the physical aspects of the lake, and CAEDYM,

which models biological and chemical interactions. The model can also be expanded into 3D simulations by replacing DYRESM with the ELCOM model. It can simulate up to seven phytoplankton groups or five zooplankton species, making it a powerful tool for studying lake ecosystems. However, a major limitation is that it can only simulate predefined species groups, meaning it does not account for species immigration or succession in response to external changes such as nutrient loading or climate shifts. Additionally, the biological model requires many parameters, which increases uncertainty and makes it difficult to determine cause-and-effect relationships within the system.

PROTECH is designed to simulate the dynamic response of up to 10 phytoplankton groups in relation to seasonal or annual changes throughout the water column. It provides daily biomass updates for each taxon, allowing for detailed tracking of phytoplankton dynamics. However, a challenge with this model is that the physical thermal profile must either be calculated using meter data and inflow water temperature or imported from observations or another model, adding an extra layer of complexity. Another issue is that the model is not generally publicly available, making access more difficult for researchers who do not already have a connection to it.

FABM (Framework for Aquatic Biogeochemical Models) provides a flexible framework for coupling hydrodynamic models with various biogeochemical sub-models. It acts as an intermediary layer, facilitating communication and data exchange between different models through an extensive set of application programming interfaces (APIs). While it offers a structured and efficient way to integrate different models, one downside is that it is Fortran-based, which could be a barrier for users unfamiliar with the language. Additionally, it is primarily designed for integrating complex models rather than serving as a standalone tool, meaning it requires a separate hydrodynamic model to function effectively.

Appendix B

This section presents the model validation for Chapter 3, which is currently under review for publication in *Water Research X*. Due to the condensed format required by the journal, the manuscript does not include a detailed model validation. However, to ensure the completeness of this thesis, the full model validation is provided in the appendix.

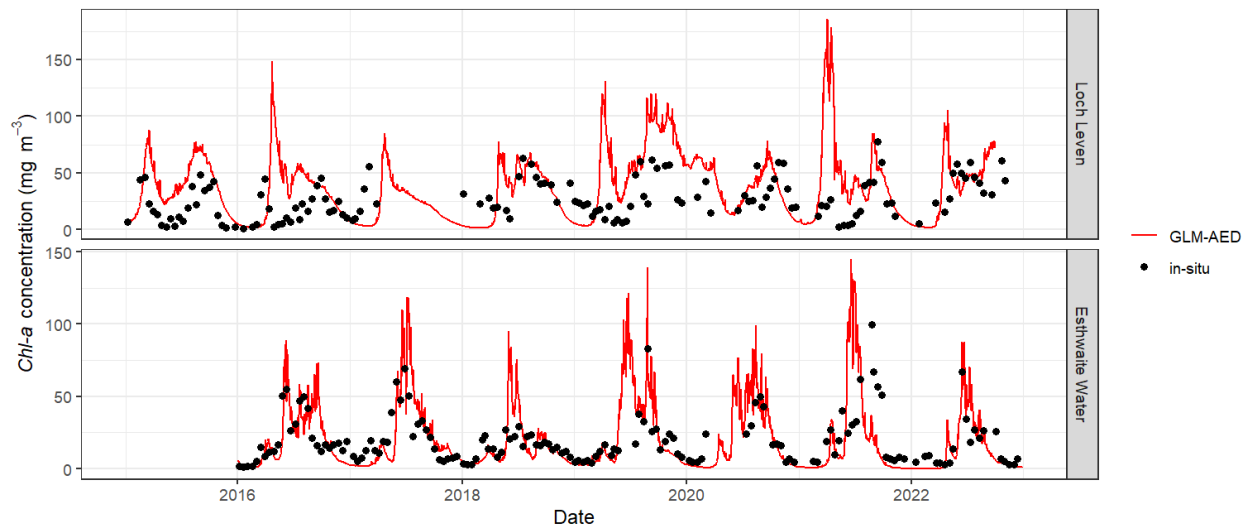


Figure 0.1 Chl-a concentrations of the modelled (red) versus in situ (black) of the original model.

Table 0.1 Validation error metrics for the two lakes. The RMSE, MAE and MdSA.

Lake	RMSE	MAE	MdSA
Loch Leven	33.3	24.8	124.2
Esthwaite Water	18.8	11.7	83.4

Model performance of the full temporal range varied considerably between the two lakes. For Loch Leven, the RMSE and MAE were relatively high at 33.3 mg m⁻³ and 24.8 mg m⁻³, respectively. The MdSA was also high (124.2%), suggesting large relative errors and limited model reliability at this site. In contrast, model performance at Esthwaite Water was notably better, with lower RMSE (18.8 mg m⁻³) and MAE (11.7 mg m⁻³), reflecting moderate agreement. The MdSA at Esthwaite (83.4%) was also lower, indicating improved predictive accuracy. These differences may reflect contrasting lake characteristics (e.g., size, depth, or trophic status), local hydrometeorological conditions, or the sensitivity of model parameters to site-specific processes. Overall, while the model captured general patterns more effectively

at Esthwaite Water, performance at Loch Leven suggests the need for further calibration or the inclusion of additional drivers to improve accuracy.

Appendix C

The original locations (LWBC A,E and I) of the water bodies (Loch Leven (North), Esthwaite Water (Central) and Alton Water (South) and their respective climate forcings resulted in a median MAE of 11.7 mg m⁻³ chl-a, and median of 69.59 %. With the MdSA of the pre-industrial control climate forcing being on the higher side for all water bodies. The yearly patterns of all climate forcings per lake show high similarity in the period of 2016 to 2023, with the pre-industrial control showing the largest differences. The models in the historical period or current period in this century are therefore deemed to be representative and can be used for future projections.

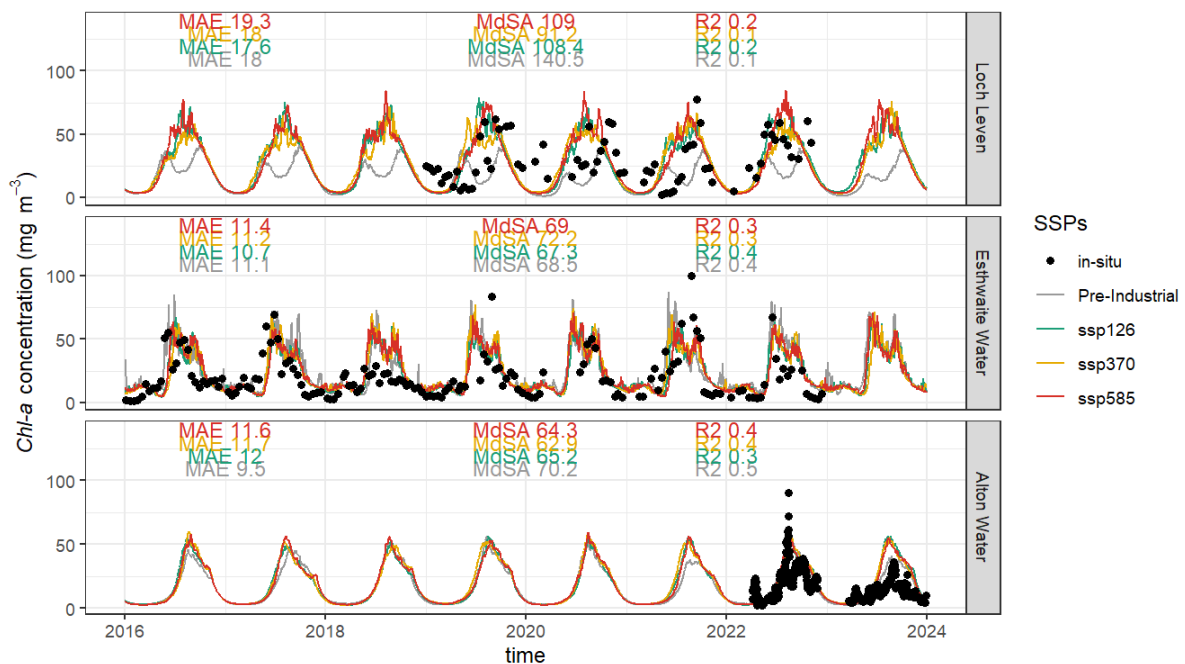


Figure 0.2 The four climate forcings (pre-industrial, ssp126, ssp370, ssp585) compared to the in-situ chl-a concentrations in each waterbody. The mean absolute error (MAE) and the median symmetric accuracy (MdSA) and R per scenario per lake.