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Coupling MODFLOW and GLM-AED for integrated simulation of lake–aquifer interactions

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Abstract: Lakes and aquifers are often studied separately, a practice that overlooks the critical feedback mechanisms between these dynamically interconnected systems. Hydrogeologists frequently treat lakes as simple recharge or discharge zones, while limnologists often consider groundwater inflows and outflows as static, external drivers, particularly when considering water quality. This leads to significant deficiencies in our ability to predict the behaviour of coupled lake-aquifer systems under environmental and human-driven change. To address this, we aimed to develop a comprehensive modelling tool that dynamically integrates groundwater flow and transport, lake eco-hydrodynamics, and geochemical reactions. Specifically, this tool was designed to couple MODFLOW, GLM-AED, and PHREEQC (Figure 1). This paper presents the initial stage of this effort, focusing on the successful dynamic coupling of MODFLOW and GLM-AED, with the integration of PHREEQC still under development.

The presented framework's utility is demonstrated through synthetic case studies, which revealed that a lake's internal dynamics, such as thermal and density stratification, can drive complex groundwater circulation patterns that traditional, single-domain models do not capture. Furthermore, our results highlight the lake's role as an active biogeochemical reactor, capable of transforming contaminants before they are transported into the surrounding aquifer. This integrated approach provides a more robust and holistic tool for predicting contaminant fate and transport. We conclude that this work is a foundational step, and the full coupling of all three codes will ultimately provide an unprecedented level of detail and predictive power for complex applications where geochemical reactions are the dominant processes.

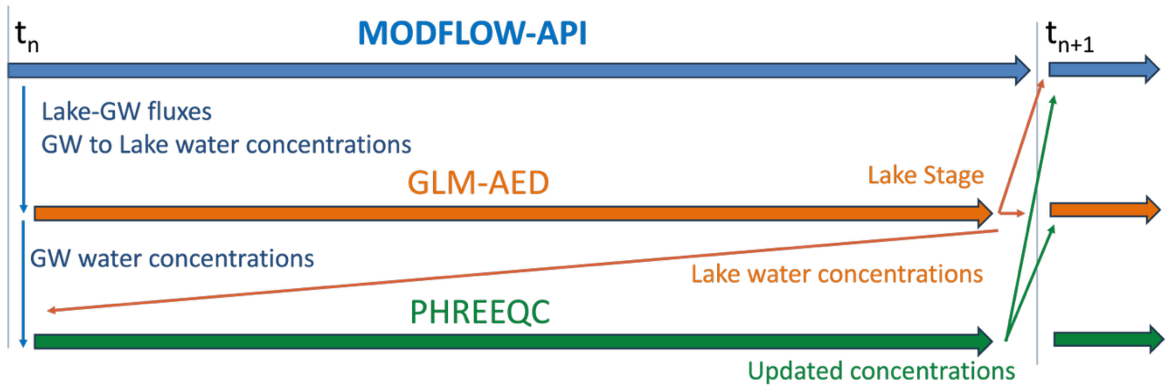

Figure 1 Conceptual summary of the coupling between MODFLOW, GLM-AED, and PHREEQC within a MODFLOW time step using the MODFLOW API.

Keywords: *Coupled lake-aquifer modelling, eco-hydrodynamics, integrated assessment framework*

1. INTRODUCTION

Lakes and aquifers are often interconnected components of the hydrological cycle, exchanging water, solutes, and energy across their boundaries. These interactions can influence water quantity and quality in both domains, with implications for ecosystem health, water resource management, and the fate and transport of contaminants. Understanding such coupled processes is therefore critical for predicting system behaviour under natural variability and anthropogenic pressures. Although feedback between lakes and aquifer domains may be critical, traditional approaches often focus on one domain while treating the other as a boundary condition. For example, when studying groundwater systems, hydrogeologists frequently treat lakes simply as recharge or discharge zones, overlooking the fact that a lake's internal evolution (such as seasonal stratification) could both depend on and influence the changes occurring in the connected aquifer. On the other hand, when studying lakes, limnologists often account for groundwater inflows and outflows independently of the lake's dynamics, rather than as variables that may respond to and interact with the lake's behaviour over time. This reflects a common one-way influence assumption used in both hydrogeology and surface hydrology, which is often the result of the limited understanding of the complexity of the lake-aquifer interactions.

These practices are often the rule of thumb when running process-based numerical simulations of both lakes and groundwater systems. For instance, lake eco-hydrodynamic models, such as GLM-AED (Hipsey et al. 2019) can simulate seasonal mixing regimes and nutrient evolution; however, they cannot dynamically resolve water exchanges between the lake and aquifer domains, and these models require groundwater to be resolved coarsely as input parameters. On the other hand, while groundwater flow and transport models like MODFLOW (Langevin et al. 2017) are suitable for simulating the overall evolution of both the groundwater system and lakes within the model domain, they are unable to simulate lake stratification or internal reactive processes within the lake. Furthermore, many lakes affected by geochemical reactions, such as acidic post-mining pit lakes, are often simulated using only geochemical simulators like PHREEQC (Parkhurst and Appelo 2013), disregarding lake hydrodynamics and aquatic biogeochemical processes and the potential feedbacks with the surrounding aquifers. A few exceptions exist in the literature where biogeochemical models have been integrated into groundwater flow and transport models (e.g., Davis et al. 2006) and eco-hydrodynamics models (e.g., Salmon et al. 2017). The lack of an integrated package capable of linking groundwater dynamics, lake eco-hydrodynamics, and the associated biogeochemical reactions between them highlights a significant research gap and is a deficiency in our ability to predict environmental outcomes where lake-aquifer interactions are considered to be important (Figure 2).

In response to these challenges, we have sought to develop a lake–aquifer modelling tool that integrates lake hydrodynamics with groundwater flow and solute transport by coupling MODFLOW, GLM-AED, and PHREEQC. As the PHREEQC coupling is still under development, this paper focuses on the first aspect, which is the integration of MODFLOW and GLM-AED. To demonstrate the utility of the coupled model, synthetic case studies are presented that capture processes and connections between both the groundwater and lake domains, and we highlight the risk of overlooking key outcomes when only one domain is considered.

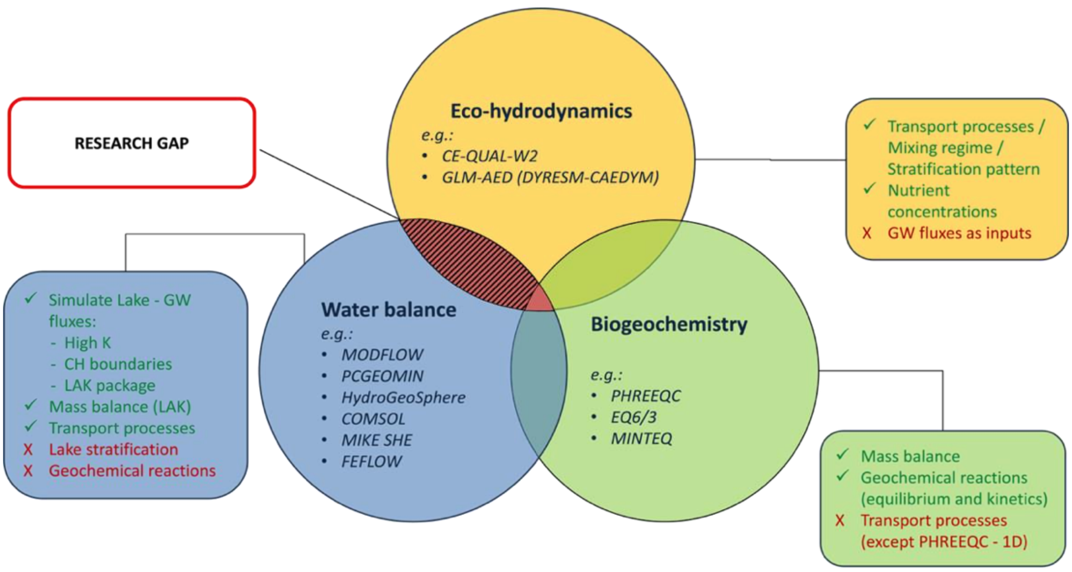

Figure 2. Codes used to simulate lakes and groundwater, highlighting research gaps in the coupled simulation of lakes and aquifers (red hatched area) and integration with biogeochemical models (central red area).

2. MODELLING APPROACH

The coupling of MODFLOW and GLM-AED was conducted within a Python wrapper, where the MODFLOW Application Programming Interface (MODFLOW API, Hughes et al. 2022) served as the primary host for the coupling, as it facilitates the sequential linking of the codes within the time loop of MODFLOW. A brief description of MODFLOW, the MODFLOW API, and GLM-AED is provided for context.

2.1. MODFLOW

MODFLOW is a USGS-developed numerical model for simulating three-dimensional groundwater flow, and it is a global standard in hydrogeology due to its flexibility, modularity, and high level of validation for diverse use cases. Its importance stems from enabling the reliable prediction of groundwater behaviour under natural and human-induced changes, supporting water management, environmental impact assessments, and research on groundwater–surface water interactions. Specialized packages, such as the Lake Package (LAK), allow for the explicit simulation of lakes within the groundwater system. The LAK package was preferred for use in the coupled model over other MODFLOW boundary conditions because of its intrinsic definition of LAK connection cells, which represent the spatial links between the lake and the groundwater system, thereby facilitating the mapping of the lake within the MODFLOW spatial domain and having the ability to define lake properties, such as bed leakage and to differentiate between horizontal and vertical lake-aquifer connections.

In addition to flow simulation, the latest core version of MODFLOW (MODFLOW 6) incorporates a modular Groundwater Transport (GWT) model for simulating the transport of solutes and contaminants in groundwater. Additionally, this MODFLOW version is the only one that supports the use of the MODFLOW API. Accordingly, MODFLOW 6 was used in the coupled model. The GWT model can handle advection, dispersion, sorption, and decay processes, and it can be tightly coupled with flow simulations to track the transport of species through the aquifer. The simulation of the lake within the groundwater system as a source or sink of solute mass was conducted using the SSM package and auxiliary (AUX) variables associated with the LAK package. Additionally, the Buoyancy (BUY) Package is incorporated in MODFLOW 6 to simulate variable-density groundwater flow by accounting for changes in fluid density due to solute concentrations, such as salinity or temperature variations.

Currently, the coupled model only allows the use of MODFLOW’s structured grids.

2.2. MODFLOW API

The MODFLOW API is an interface that allows the integration of external codes with MODFLOW during its simulation. The API was developed using a Basic Model Interface (BMI) standard, which consists of three primary stages to control a time loop: initialise, update, and finalize. During the initialization stage, the model properties are defined from a set of MODFLOW input files. During this stage, instantiation of objects is also handled, as well as calculation of initial properties, and allocation of memory to store state and auxiliary variables. During the update stages, the model is advanced by a single time step, while during the finalize stage any open files are closed and the memory used to store state and auxiliary variables is released after the simulation time is reached.

The BMI standard also provides “getter” and “setter” methods that allow the interface to retrieve variables stored in memory (getter methods) and overwrite others (setter methods) when needed. Handling these getter and setter methods is the core of coupling functionality, as they allow us to retrieve variables from a model and provide them to the coupled model during the MODFLOW’s time loop *on the fly.*

2.3. GLM-AED

The General Lake Model (GLM) is a one-dimensional hydrodynamic model that simulates thermal structure and mixing regimes in lakes and reservoirs (Hipsey et al. 2019). The model adopts a Lagrangian (moving) layer structure to resolve lake density profiles, with the layer structure adapting to the prevailing stratification. When coupled with the Aquatic EcoDynamics (AED) ecological modelling framework, it is also able to account for water quality and ecosystem interactions. Its importance lies in integrating environmental and limnological processes, allowing for a robust evaluation of how lakes respond to climate and inflow variability, management actions, and engineering interventions.

2.4. Python packages

A Python wrapper was developed to control the MODFLOW API “getter” and “setter” methods to integrate MODFLOW and GLM-AED. This utilised the FloPy Python package (Bakker et al. 2016) to modify MODFLOW input files, and the GLMpy Python package to control and adjust the GLM-AED simulations.

3. COUPLING SEQUENCE

The coupling of GLM-AED into MODFLOW is implemented by modifying the state variables of the LAK package within the groundwater domain through the MODFLOW API. To prevent the LAK package from calculating the internal mass balances through MODFLOW, its status is set to "CONSTANT". Additionally, the memory-stored variable "NOAUXUPDATE" is set to True for the LAK package. In this way, the coupled model leaves all the lake's internal mass balance calculations to GLM-AED. Meteorological information, including precipitation, evaporation, and aquifer recharge, is provided to both GLM and MODFLOW to drive water balance processes. Solar radiation and wind speed are supplied specifically to GLM, where they influence the lake's thermal structure and mixing regime, but do not directly affect groundwater processes (Figure 3).

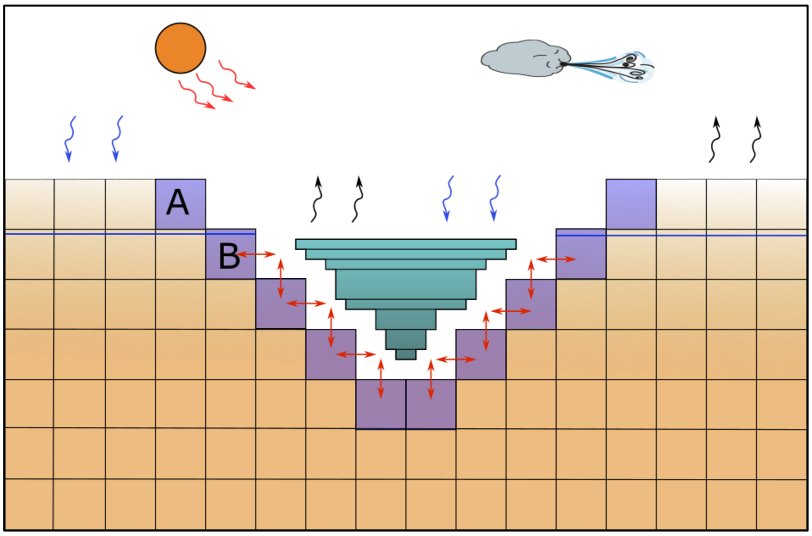

Figure 3. Conceptual spatial discretization of the coupling between MODFLOW and GLM-AED. Water fluxes across the lake and aquifer are calculated for each LAK connection cell within MODFLOW (purple cells).

Specific considerations are required for the spatial and temporal coupling of both models. The spatial coupling necessitates interpolation due to differences in vertical discretization: GLM employs a Lagrangian approach to generate layers of variable thickness, which cannot be directly matched by the fixed layers of MODFLOW (Figure 3). Fortunately, GLM inflows and outflows only require a single elevation value corresponding to the midpoint of each LAK connection cell. Meanwhile, the Python wrapper interpolates the vertical distribution of salinity and species in the lake to the MODFLOW grid before transferring the values back, ensuring that spatially resolved properties are communicated between the domains. On the other hand, since GLM requires daily inflow and outflow data, the coupled simulation must use a daily time discretization. If, during a daily time step, the lake stage calculated by GLM drops below a MODFLOW lake connection cell bottom, that cell will not account for lake-aquifer fluxes (cell A in Figure 3). However, if the lake stage falls between a lake connection cell, this connection will only account for horizontal fluxes, while vertical fluxes will be set to zero (cell B in Figure 3). This approach comes from the LAK package implementation of drying and rewetting sections in a lake (Langevin et al. 2017).

The coupled simulation begins with a single initialization phase, followed by multiple update phases at each time step. During initialization, MODFLOW defines the groundwater system grid and boundary conditions, including the location and properties of lakes within the three-dimensional model. Simultaneously, the Python wrapper prepares GLM input files for inflows and outflows, creating one set of files for each LAK connection cell. For the update phase (first time step), MODFLOW computes lake–aquifer fluxes at the LAK connection cells from initial conditions, updating heads, salinity, and species concentrations in the groundwater system. Salinity and species concentrations at LAK connection cells are retrieved from memory via getter methods and written to the corresponding GLM inflow or outflow files. GLM is then run for one day, updating the lake stage and the vertical distribution of salinity and species. The resulting lake stage, salinity, and species concentrations are retrieved from GLM outputs and used to overwrite the corresponding state variables for each LAK connection cell in the MODFLOW LAK package using setter methods. The updated values serve as initial conditions for the next time step during the following update phases. This approach ensures that the vertical differentiation of species within the lake is reflected in the groundwater simulation, thereby maintaining consistency between spatial and temporal dynamics.

To accurately represent lake stratification and salinity transport, the coupled model incorporates a density-dependent formulation for groundwater fluxes and head distribution by activating MODFLOW's BUY package. Users can choose whether density is calculated using salinities from GLM with the linear approximation in the BUY package or by applying the TEOS-10 equation, which accounts for both temperature and salinity, consistent with GLM calculations.

4. SYNTHETIC CASE STUDIES

Two synthetic case studies were designed to test the capabilities of the coupled model and to demonstrate the significance of including dynamic interactions between the lake and groundwater domains.

4.1. MODFLOW-LAK VS MODFLOW-GLM

A cross-sectional model was created to simulate a flow-through, meromictic lake. The model domain was defined as 200 m in the vertical direction and 3000 m in the horizontal extension. Two Constant Head (CHD) boundary conditions were defined for the left and right borders of the model to reproduce a hydraulic gradient of 0.3% and a flow to the right. A lake of 80 m depth was defined using the LAK package within the MODFLOW model, as illustrated in Figure 4. A total mass of 18 tonnes of "salt" was added to the lake, contrasting with the aquifer background salinity of 1 mg/L. This setup was used to compare the saline plume evolution when considering the stratification of a lake relative to vertically-averaged concentrations. Both simulations were run for 10,000 days.

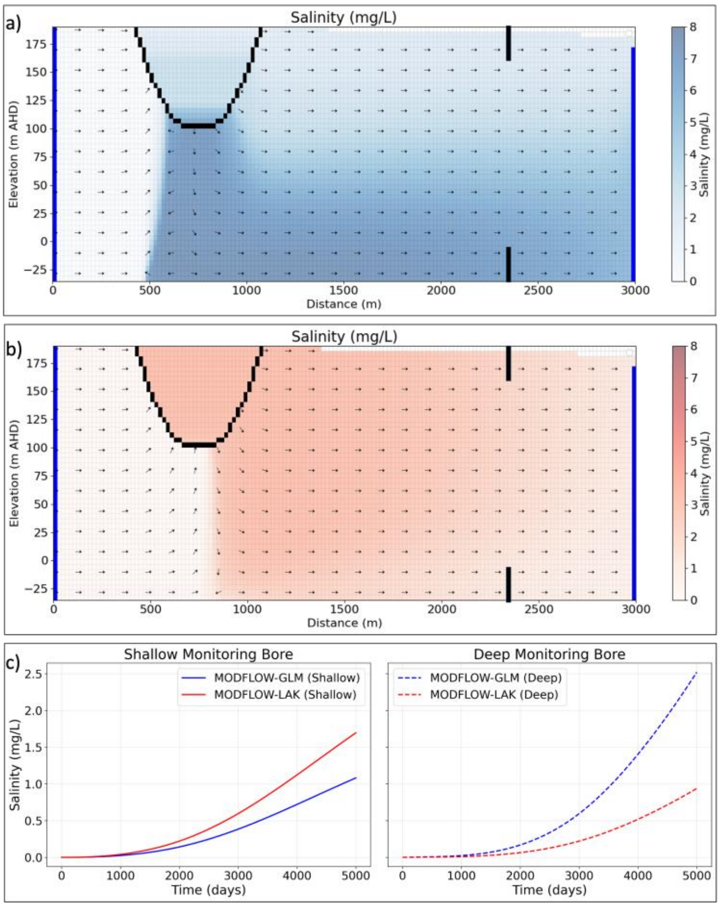

Figure 4. a) Cross-section of a coupled simulation using MODFLOW and GLM-AED. Note how the lake's long-term stratification is reflected in the saline plume. b) Cross-section of a MODFLOW simulation using LAK package. c) Breakthrough curves of salinity at a distant observation point.

The MODFLOW-LAK model distributed the total mass of "salt" as a constant concentration (~3 mg/L) in the entire lake volume (initial volume of 5.8 GL). The simulation results showed that despite the significant difference between lake and aquifer salinities, the simulation results showed that advection driven by the hydraulic gradient is a key factor in groundwater flow dynamics. On the other hand, the total mass of salt in the MODFLOW-GLM simulation was distributed to reproduce a meromictic lake, with lower salinities at the surface (~2 mg/L) and higher salinities at the lake bottom (reaching 8 mg/L). The results of this simulation showed that a density-driven flow creates a more complex circulation between the lake and aquifer, with notable differences under the lake. In particular, the simulated salinity concentrations at two downgradient observation wells reveal the importance of considering the lake's vertical profiles. In the shallow well, the vertically averaged simulation showed higher concentrations, whereas the simulation that included lake stratification produced significantly higher concentrations in the deeper well.

4.2. SEASONAL AND REACTIVE CHANGES

The next example builds upon the pre-existing framework described above, but with a key modification which is the introduction of a reactive contaminant plume. Specifically, an ammonium (NH_4) plume, originating from a source to the west of the lake, was simulated to represent a common form of point source pollution, such as the leakage from septic systems. This modification was designed to demonstrate the fate, transport and transformation of this contaminant as it moves through the lake-aquifer system. The core lake model itself was configured with an idealised temperate monomictic lake with a natural, seasonal cycle of thermal and oxygen stratification during summer months due to surface heating and subsequent evaporation.

To simulate the key biogeochemical processes, the Aquatic Ecosystem Dynamics (AED) model was included into the GLM simulation. AED was specifically employed to model the process of nitrification using the aed_nitrogen module, which involves the microbially-mediated transformation of ammonium into nitrate (NO_3). This reaction is a crucial component of the nitrogen cycle and is dependent on several factors: it is temperature-dependent (occurring more rapidly in warmer conditions) and is limited by the availability of both oxygen (O_2) and ammonium. This setup allows for an analysis of how the seasonal physical dynamics of the lake influence the rate and location of nitrification, thereby controlling the overall distribution of nitrogen species in the downgradient plume. No reactive transport in the groundwater was simulated in this example.

The model results are illustrated in **Error! Reference source not found.** with the upper panels (**Error! Reference source not found.**a and **Error! Reference source not found.**b) showing a cross-sectional view of the coupled aquifer-lake system at simulation day 650. This view clearly shows the simulated ammonium plume entering the lake from the left (**Error! Reference source not found.**a). As the ammonium enters the lake and undergoes nitrification, a subsequent nitrate plume is generated (**Error! Reference source not found.**b). This new plume then exits the lake and travels through the aquifer to the right, driven by the regional hydraulic gradient and associated advective flow. The lower panels (**Error! Reference source not found.**c, d, e, and f) present two-dimensional plots showing the vertical distribution of ammonium, nitrate, oxygen, and temperature within the lake over time, respectively.

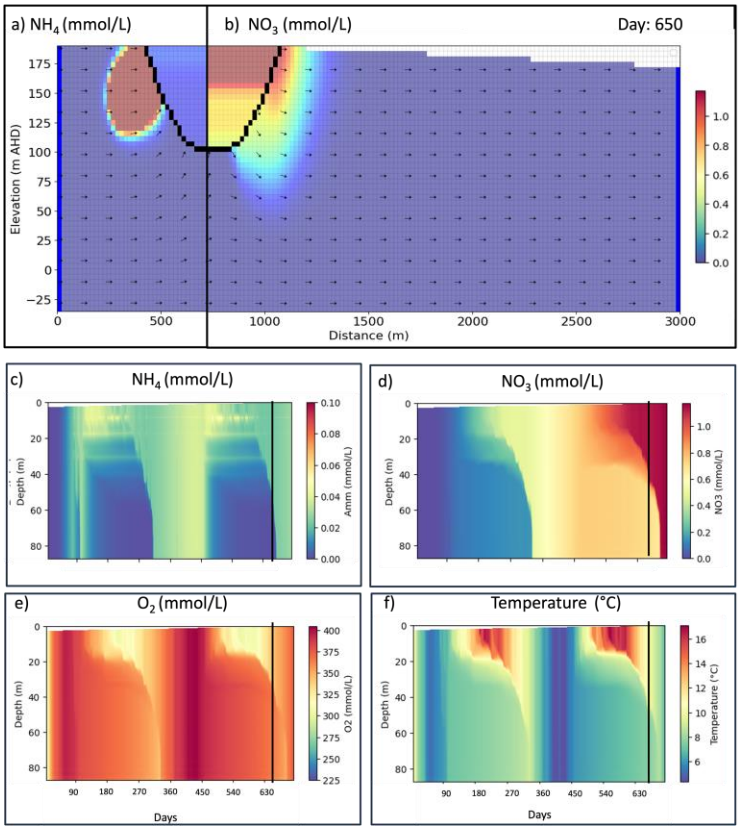

Figure 5. a) Cross-section of a coupled simulation using MODFLOW and GLM-AED to simulate the inflow of an NH_4 plume. b) Cross-section of a coupled simulation using MODFLOW and GLM-AED to simulate the outflow of an NO_3 plume. c) vertical distribution of NH_4 over time in the lake. d) vertical distribution of NO_3 over time in the lake. e) vertical distribution of O_2 over time in the lake. f) vertical distribution of temperature over time in the lake. Vertical black line indicates the time that is shown in panels a and b.

The results reveal a clear interplay between physical mixing, temperature, and biogeochemical cycling. The simulation shows that the ammonium plume first reaches the lake at approximately day 60, as depicted in panel (c). The seasonal mixing patterns, driven by meteorological conditions, create ideal conditions for nitrification to occur, particularly in the warmer, oxygenated upper layers of the lake during summer. A notable result is the abrupt decrease in ammonium concentration after day 450, even though the plume continues to provide a constant source of ammonium to the lake. This drop in ammonium is directly linked to the high concentrations of dissolved oxygen, which, coupled with favourable temperatures, significantly enhances the rate of nitrification. Consequently, this leads to a pronounced increase in nitrate concentrations, which then becomes the dominant nitrogen species leaving the lake. The simulation effectively demonstrates how seasonal changes in lake dynamics can directly control the transformation and export of contaminants.

5. CONCLUSION AND ENVIRONMENTAL IMPLICATIONS

The integrated MODFLOW-GLM-AED framework marks a crucial step toward more robust modelling of lake-aquifer systems. Traditionally, the isolated study of groundwater and surface water systems has led to a fundamental weakness in our ability to predict the behaviour of coupled systems. Our approach overcomes this limitation by enabling a dynamic simulation that accounts for the mutual dependency of processes within a lake and its surrounding aquifer. This holistic modelling approach reveals complex feedback mechanisms that are missed by traditional single-domain models, which treat the other domain as a static boundary condition.

This integrated capability has notable implications for predicting system behaviour under significant environmental stressors, such as climate change and mine closure. For climate change, the model can simulate how altered temperatures and precipitation patterns influence lake thermal stratification and mixing regimes. In turn, it shows how these changes in lake dynamics would alter the hydraulic gradient and groundwater-lake exchange fluxes, which are crucial for predicting changes in regional water balances and the distribution of dissolved substances. Our modelling framework has also been coupled with the recent Groundwater Energy Transport Model (GME, Morway et al. 2025) within MODFLOW 6 to reproduce heat transport from solar radiation and seasonal changes in shallow groundwater systems. This additional linkage, coupled with GLM-AED to include seasonal ice layer formation over lakes, is sought to unravel other levels of feedback mechanisms between lakes and aquifers with direct implications on lake management in the face of a warming climate. For mine closure, the model is invaluable for assessing the long-term stability and water quality of pit lakes. It can simulate density-driven flows from mineralized lake water into the surrounding aquifer and capture the influence of seasonal stratification on contaminant transport and transformation. This enables a more accurate prediction of environmental risks, informing more effective long-term management strategies.

While this study presents a working coupled model for simulating the dynamics of lake-aquifer interactions, it is also just an initial step in a broader vision for a truly comprehensive platform. Acknowledging the current limitation of not having a direct coupling with reactive geochemical models, our current work is focused on integrating PHREEQC into the Python wrapper. This will enable the simulation of complex mineral dissolution, precipitation, and speciation reactions in both the lake and aquifer. We anticipate that a future MODFLOW-GLM-AED-PHREEQC tool could provide a significantly enhanced level of detail and predictive power, which would be highly beneficial for applications where geochemical reactions, such as those driving the formation of acidic pit lakes, are the dominant processes affecting long-term environmental outcomes.

ACKNOWLEDGMENTS

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