Integrating Geochemical and Hydro(geo)logical Modelling to Predict Long-Term Water Quality in Pit Lakes

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Abstract

Developing reliable predictions of water quality in post-mining pit lakes supports long-term environmental protection and helps determine whether water reuse schemes are feasible. Integrating hydro(geo)logical and geochemical modelling provides robust predictions of future water quality and helps identify treatment options that support closure objectives. By coupling two industry-leading modelling software packages, GoldSim and PHREEQC, a comprehensive framework has been developed to assess long-term water quality and guide effective, sustainable solutions, that protect water resources during the transition to post-mining land use.

Introduction

SLR Consulting Ltd (SLR) was appointed to provide geotechnical and hydro(geo)logical support to a client redeveloping a site within a mining-legacy area in Europe. The site includes a pit lake, which will be pumped out and enlarged to support a hydroelectric power plant (HEP). This project is subject to non-disclosure agreements, therefore no mention of the site is made herein, and diagrams do not represent the actual site. This modelling study used data gathered as part of the Environmental Impact Assessment (EIA) and historic data collected during operation and closure.

This paper discusses geochemical and hydro(geo)logical modelling to predict the fill rate and water quality of the new pit lake referred to as the 'Lower Reservoir'. This long-term prediction enables assessment of the scaling and corrosion risk to HEP impellers and discharge water quality to maintain the operational water balance. The modelling required the integration of individual technical components (surface water, groundwater, climate and geochemistry) using a GoldSim model, which was adapted to include the geochemical modelling software, PHREEQC. The approach and dependencies of each technical element are presented in Figure 1. This approach can be adapted to specific site or project requirements.

Methodology

A desk-based review of previous historic site studies and environmental impact assessments supported development of a conceptual model for the site (Figure 2), from which source terms (inputs) for the hydro(geo)logical and geochemical model were defined. Data used in the model included primary sources collected during SLR's field work (environmental monitoring) and historic data from previous studies. A strong conceptualization of the site hydrodynamics (above and below ground) is fundamental for accurate predictive modelling.

GoldSim is an industry-leading Monte Carlo simulation software for dynamically modelling complex systems for mining projects and other hydrochemical systems (GoldSim Technology Group, 2026) (GoldSim Technology Group, 2026). GoldSim supports decision-making and risk analysis by simulating future performance while quantitatively representing the uncertainty and risks inherent in all complex systems associated with pit lake closure situations.

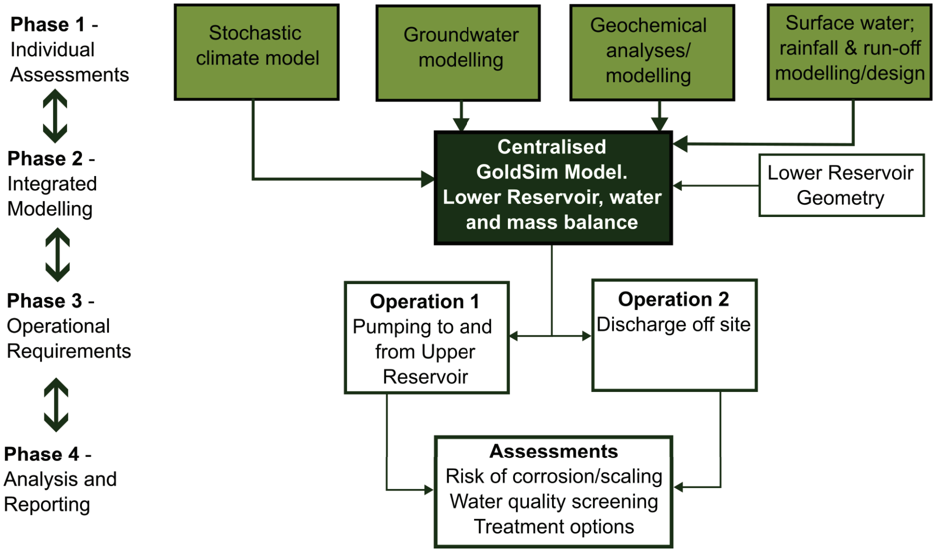

Figure 1 Integrated modelling approach, adapted from (Robinson, Klimczak and Smyth, 2023).

Monte Carlo methods are especially useful for simulating systems with many coupled degrees of freedom, such as water. To model the complex chemical processes of equilibration, speciation and sorption, GoldSim’s external element with dynamic link library (DLL) was used to communicate with a PHREEQC script and extension (Eary, 2007) and more recent updates in 2018 (Johnson, Rohal and Eary, 2018). PHREEQC stands for ‘pH-redox-equilibrium’, developed by the US Geological Society to simulate chemical reactions and transport processes (Parkhurst and Appelo, 2013). It has been widely used to predict chemical species, mineral solubility, redox equilibrium and reactive transport. PHREEQC can be linked to a variety of thermodynamic databases, which inform the chemical processes undertaken in PHREEQC. In this exercise, the Wateq4F.dat database was used as it is a comprehensive database for low-temperature geochemical processes.

An iterative approach for both models was adopted, to calibrate and check for errors in the model’s function and dynamically link between them. The model was developed with built in flexibility to system changes, as data is collected with subsequent site investigations. The DLL was written using C++ coding language and compiled with Microsoft Visual C++ Studio. This approach has the advantage of providing a generalized procedure to model complex chemical processes at each time step.

Conceptual Site Model

The site lies within a limestone formation in which barite was extracted by open-cast mining. Sulfide deposits were also mined underground for zinc, lead and nickel ore, and these are hosted in a dolomitised zone beneath the limestone formation. The current pit geometry sits within the limestone bedrock (Lithology 1, Figure 2). Historic maps of the area showed several surface water channels draining towards the pit prior to mining. The understanding at the beginning of the project was that upstream drainage had been culverted and channelled around the open pit. However, SLR’s site investigation proved one surface water input had formed, which helped determine accurate hydrological catchments alongside topographical data from LiDAR surveys. The groundwater is understood to follow the topography within the site, going from south to north. No groundwater studies have been conducted in recent history post-2000. SLR has plans to conduct a detailed ground investigation in which groundwater assumptions can be tested. Groundwater flows into the pit and is either discharged through a surface water point or as seepage.

Historic mine waste dumps are located upstream, within which massive sulfide has been observed (Figure 2). Further assessment of these dumps is needed to understand the longevity of any potential source material. Current monitoring includes runoff from the mine waste dumps. The proposed geometry for the HEP reservoirs is shown in Figure 2. The lower reservoir will be developed further underground from the existing pit lake and will expose the dolomitised, sulfide ore body (Lithology 2). There has been limited geochemical characterisation of the lithologies and waste dumps exposed on site, and it has been recommended that more detailed geochemical analysis be undertaken to test the surface water inputs used in the current model.

Source Definition and Hydro(geo)logy Modelling Results

The current conceptual site model and data available has been used to populate the GoldSim and PHREEQC models. There are planned site and ground investigations to test the assumptions made in this initial modelling.

Water Inputs/Outputs

Rainfall and Evaporation

Direct rainfall to the water surface is a small but important part of assessing the long-term water quality. In addition, the gaseous exchange between the water level surface and the atmosphere will influence the long-term water chemistry. Rainwater chemistry was ascertained by sampling the rain gauge on site and analysing for a range of parameters. Local climate data has been used for the evapotranspiration from the water surface.

Surface Water (including contact water)

As part of the EIA, monthly surface water samples were collected, including water levels of the existing pit lake. Observed site rainfall runoff behaviour was used to inform surface water inputs to the pit lake. The upstream water quality in catchments discharging to the pit lake have been averaged for input chemistry at this stage, it is assumed these represent long-term water quality from contact with mine waste dumps. As the model progresses, the monthly water quality measurements will allow GoldSim to select monthly surface water chemistry through each timestep to account for variability in surface water quality.

Groundwater

At the time of writing, SLR has not collected groundwater data or geochemical data of Lithology 1 and Lithology 2. The geochemical characterisation of the host lithologies are scheduled in future works using static and kinetic testing to understand and predict the long-term groundwater quality from them. Therefore, groundwater flow and chemistry from historical studies between

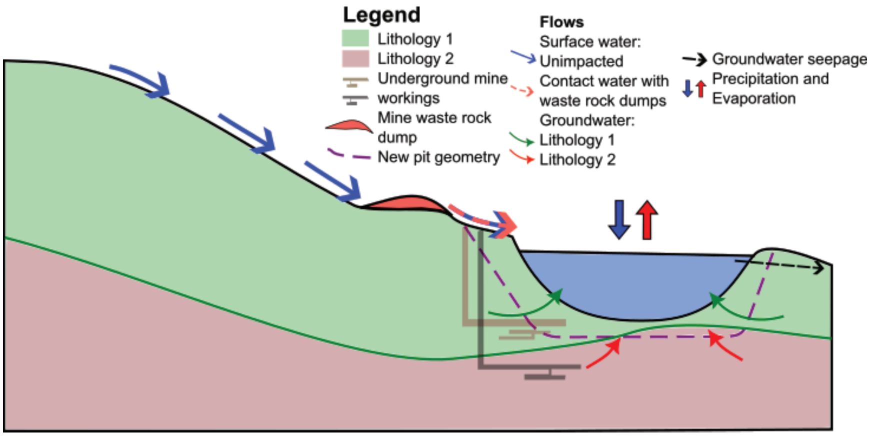

Figure 2 *Conceptual site model, dashed line represents Lower Reservoir geometry.*

1997 and 2001 have been used to develop the model. The new reservoir geometry has been imposed onto the geological model for the site, which will expose Lithology 2 (Figure 2). SLR's planned ground investigation will validate and update the assumptions made in the modelling process so far.

Results

To model the dynamic hydro(geo)chemical processes, a calibration model for the water level using the hydro(geo)logical inputs discussed above was developed, versus the measured pit lake water levels. This provides an opportunity to update inputs that support observed water levels whilst awaiting more site-specific data. Further, a static geochemical model was created to understand the hydro(geochemical) processes within the pit lake currently occurring. These findings helped inform the initial set up of the working GoldSim-PHREEQC model.

Calibration Model

Using the groundwater inflow rates from the historic groundwater studies, results of the calibration showed a large overestimate in pit water level, leading to a rapid water level rise relative to the rate observed on site. As a result, the groundwater inflows were reduced by between 30% and 45% for summer groundwater inflows and 80% to 85% for winter groundwater inflows. In addition, runoff rates within the upstream catchment were lowered. These new groundwater inflows resulted in a better fit for modelled water levels compared to measured water levels between July 2024 and March 2025 (Figure 3). This highlights the importance of obtaining hydrodynamic data for the site which is ongoing at the time of writing.

Static Geochemical Model

The water quality inputs were mixed and equilibrated in PHREEQC using a mixing ratio determined from the calibration model. The resultant chemistry was compared with SLR's measured chemistry of the pit lake. This indicated several modelled metals/metalloids elevated above their baseline concentrations and exceeding general acceptance criteria (GAC) for the site. The GAC at this stage, uses local regulatory water quality standards. Review of the saturation indices showed iron hydroxide minerals were super-saturated. Iron hydroxide was allowed to precipitate, and the mass of precipitate formed was calculated using the change in iron (II) and stoichiometric principles. This mass of precipitated iron hydroxide was used in PHREEQC's sorption command. The water chemistry after precipitation of, and sorption with, iron hydroxides was akin to the measured pit lake chemistry. To test this modelling step, SLR plan to sample sediments in the pit lake to validate the step further. An additional consideration is the stratification

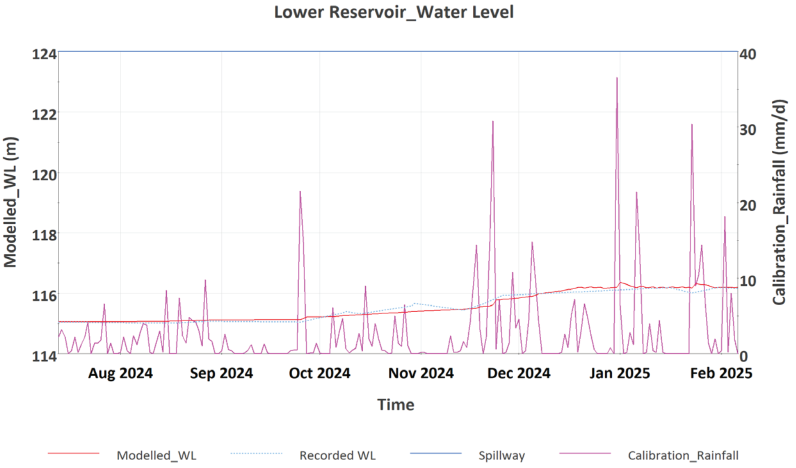

Figure 3 Calibrated Lower Reservoir Water Level.

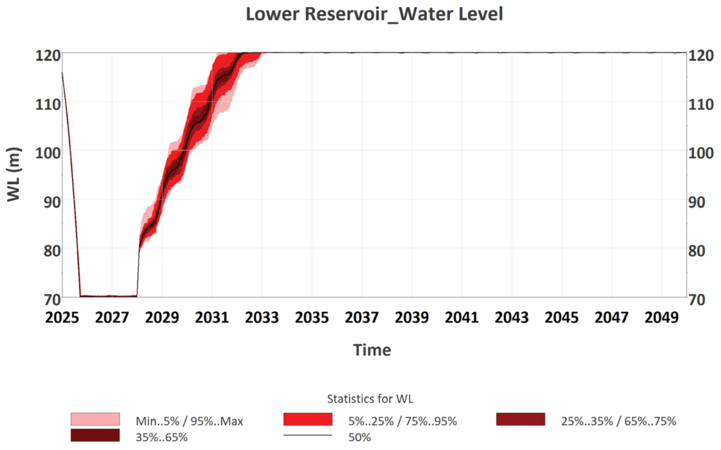

***Figure 4** Lower Reservoir Filling Rate, WL = Water Level.*

of the pit lake. SLR conducted conductivity, depth, temperature surveys on three locations within the pit lake. This showed no stratification within the pit lake and has not been considered further at this stage.

Water Balance

The water levels in the Lower Reservoir were modelled based on the stage-storage curve provided by the client, local rainfall data and calibrated groundwater/runoff flows, modelled on a daily time step (allowing unscheduled sub-daily timesteps in GoldSim where needed). A number of operational phases were modelled in the lower reservoir to simulate HEP operations. The new reprofiled and lined pit comes online in 2028, with groundwater outflows and seepage removed. The pit rebounds over a period of 4-5 years and reaches the new spillway depth, intermittently spilling and lowering below the spillway level. The water level and rebound rate was used to inform geochemistry concentrations and operational pumping rates. The spillway volumes were calculated by the model and would be used to inform the viability of passive wetland systems downstream of the reservoir.

Water Quality

At each timestep of the water balance model the mass balanced chemistry was exported from GoldSim into the PHREEQC model, to equilibrate, precipitate and sorb. It was found that pumping between the Lower and Upper Reservoirs by-passed areas of the PHREEQC export, leading to chemical concentration build up within the water balance, which was not realistic. As a result, the water balance between the Lower and Upper Reservoirs was considered a single cell to communicate with PHREEQC. The chemical equilibrium for major ions is reached by 2035. The pH at equilibration is roughly 7.1 in the sorbed model, compared to 6.1 from the GoldSim model and 8.5 after equilibration. Alkalinity stabilises at roughly 85 mg $CaCO_3$/L after sorption. Chloride was also modelled as a hydrochemical check on the model due to its conservative nature and showed no changes in any modelling step.

The lead concentrations across all three outputs are presented in Figure 5. The lead concentration does not change between the GoldSim output and the equilibrated chemistry and exceeds the GAC. After the precipitation of iron hydroxides and sorption, the lead concentration is several orders of magnitude lower and now below the GAC as observed in the static model. In comparison, zinc (Figure 5) decrease slightly after sorption, but not enough to fall below the GAC. This indicates there is a risk zinc will exceed the GAC in discharge from the site, highlighting that more detailed risk assessment is required. Further, it allows for a suitable treatment options study to be defined. This also provides evidence for local

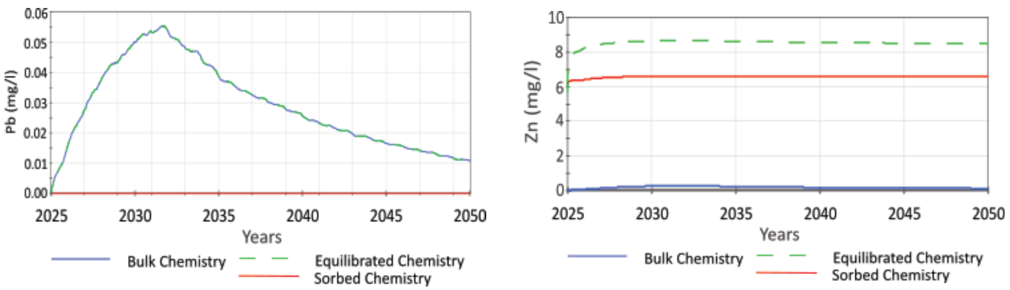

Figure 5 *Modelled chemistry trends for the HEP Water Balance.*

permitting requirements which provides rationale to exclude lead or other metals/metalloids in permitting requirements, as they have been shown to be removed by geochemical processes in the pit lake.

Scaling and Corrosion Assessment

As part of the phase 3 assessment of the model outputs, a preliminary assessment of the risk of corrosion and scaling to the HEP impellers was conducted. This used the long-term average of the modelled water quality of the HEP water balance. This is widely used across materials assessments and risks based on environmental conditions (Singley, 1981; Roberge, 2007) and will help identify whether corrosion or scaling is a long-term risk.

These indexes assess the likelihood of carbonate scaling or dissolution (Langelier-Saturation Index (LSI, (Langelier, 1936)), Ryznar Stability Index (RSI, (Ryznar, 1944)), Puckorius Scaling Index (PSI, (Puckorius and Brooke, 1991))) and corrosion (Riddick Index (RI, (Riddick, 1941)) and Larson-Skold Index (LSI, (Larson and Skold, 1958))). These indices are founded on either laboratory experiments or site-specific studies such as the Larson-Skold Index, which has been developed using the corrosion potential of waters from the Great Lakes (Roberge, 2007). Results show the modelled water quality will dissolve carbonate scaling i.e. the LSI (-1.37), RSI (9.85) and PSI (9.62). The risk of corrosion based on the model outputs to date indicates the potential for corrosion is unlikely.

Conclusion

A robust modelling approach has enabled prediction of the long-term water balance and water quality for a planned redevelopment of a legacy mining site. The outcomes will help define operational limits for the HEP operators. The dynamic chemical modelling results show that several parameters exceed the GAC when a mass balancing approach was used. The field observations informed the modelling approach, indicating sorption of chemical species was needed within the model. This step reduces the list of potential contaminants based on the mining legacy alone. This can be used to inform the development of passive treatment options.

The modelling approach has assisted in developing the conceptual understanding of the site without detailed site investigations at the prefeasibility stage of the project. This helps inform the site and ground investigations needed to validate and test the assumptions made in the model. An iterative modelling approach allows new data to be input to the model structure to improve the outputs.

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