Linking fundamental geochemistry and empirical observations for water quality predictions using GoldSim

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Abstract Prediction of water quality across different components of a mine site is often a challenging proposition, due to both the technical challenges of water quality modelling and the variability of available data. A methodology of integrating site-specific mine waste characterization results and mine-water balances through the use of fundamental considerations and empirically-derived constraints to predict water quality from mine waste sources has been developed. The adoption of GoldSim as visual interface software with capacity for matrix calculations has facilitated the development of linked water quality sub-models for different mine facilities. Fundamental and observed geochemical responses from on-site monitoring, field kinetic tests and laboratory data have been incorporated with PHREEQC and Geochemists Workbench modelling to identify the most important geochemical processes across the mine site. Based on the static geochemical data to populate the models, the determined geochemical generation rates, the site specific geochemical properties and the mine-site water balance, the GoldSim platform has been used to realise the conceptual understanding of each aspect and construct a framework to provide mine scale water quality projections. In this way, models have been built to assist in a range of situations from a large operating poly-metallic open cut mine to assess mine waste and mine water management alternatives to determination of likely water quality at a proposed large mine in a tropical environment.

Key Words Water quality, predictions, integrated mine water management, GoldSim

Introduction

At the scale of an entire mine, comprising several waste sources and complex water management requirements, the determination of future water qualities is a challenging undertaking. The assessment of the potential water quality is achieved through characterisation of the geochemical properties and a firm understanding of the conceptual model of each component within the environment. For many mine sites, a variety of hydrogeochemical models are used to assess the range of potential water qualities associated with each waste facility and the most important drivers on these water qualities.

These hydrogeochemical models are used to characterise and interpret the geochemical drivers on expected contaminant loads, predict contaminant concentrations and loads and assess treatment needs. Hydrogeochemical models are most useful when coded into an appropriate computer model describing the different interactions. These can provide, if not a direct quantitative description, at least a far better qualitative understanding of the geochemical and physical processes under investigation than might otherwise be possible (Lichtner, 1996).

Methodology of model development

As an initial step, mines are conceptually partitioned into individual reacting components. For each of these components an initial conceptual model of the interactions and subsequent hydrogeochemical behaviour is constructed. These conceptual models allow the different contributing factors in each component to be included and appropriately scaled to obtain a set of likely hydrogeochemical responses. The most important step is to construct the correct conceptual model. To do this, a number of factors must be considered, including; a consideration of reactive surface areas, the contribution of different layers, the expected mass of reacting material, inhibitors or accelerators of reaction rates, and the influence of water added or removed from the system. Younger and Sapsford (2006) provide guidance in terms of the requirements for developing an initial conceptual hydrogeological model for upscaling of field or laboratory experiments.

A generalised model development approach includes the following steps:

- Simplifying the water balance of each mine component and the mine site as a whole so that the most important aspects to be linked to the geochemical reactions and transport of these reaction products is taken into account.
- Model the geochemistry of each component separately. This step entails the conversion of the conceptual model into the equivalent geochemical system with the reactions and flows taken into account. For the mines under consideration in this paper, use was made of PHREEQC (Parkhurst and Appelo, 1999) and Geochemists Workbench (Bethke, 2008).
- Using mine infrastructure plans, waste schedules and static geochemical test results to define mass of reactants for each component and field kinetic cells data to define expected reaction sequences and kinetic loading rates. Site monitoring records are used to define expected behaviour and provide reasons for deviations from expected flows or concentrations.
- Develop the appropriate algorithms to describe the geochemical and hydrologic interactions and code these in a robust modelling platform. In the case described here, GoldSim was selected and used to very good effect (Fig 1).
- Use the field observations to refine scaling factors and refine when necessary.

For each mine component, the loading water quality contribution is based on empirically derived experimental laboratory test data coupled with primary geochemical observations and constraints. The laboratory leaching rates and leachate contributions cannot be used directly for most mine components unless conditions are directly analogous to the field. Scaling factors such as water contact, oxidative reactants and surface areas are included to adapt laboratory test data to field scale loading rates.

Mine Site Applications

This approach has been used successfully at several mine sites, with the largest scale operation case included here being the Antamina mine which is situated in the rugged Central Andes, approximately 4,200 m above sea level and 280 km northeast of Lima. Ore is extracted from the Antamina mine using open pit mining techniques. Waste material generated by the mining process is deposited in a number of waste rock dumps (WRD) and a tailings storage facility (TSF). Several communities reside downstream of the project site.

Working with Antamina, Klohn Crippen Berger Ltd (KCB) first developed a predictive closure water quality model; incorporating the open pit, two WRDs and a tailings storage facility (Figure 1). This model was developed based on the available site data and, most importantly, based on fundamental geochemical principles. The main function of the model is to allow the user to simulate scenarios where water management is modified, causing a change to either flow volumes or water quality. These modifications include waste rock cover systems, treating discharge water, discharging without treatment and various pump-back options. The model can incorporate stochastic rainfall and uncertainties to allow for extreme weather conditions.

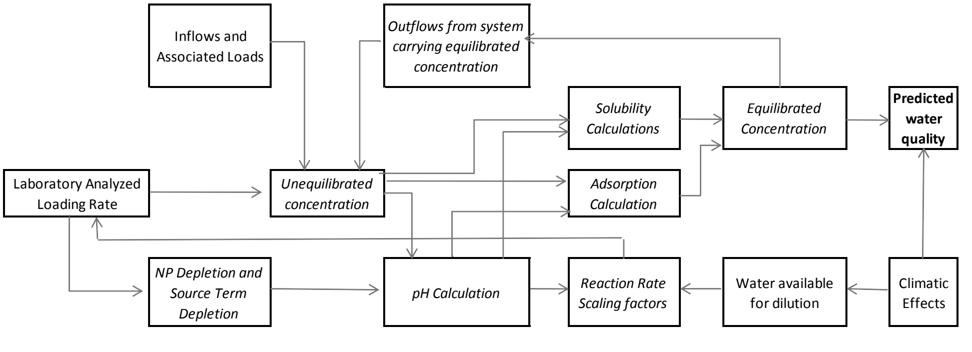

Figure 1 *Overview of water quality algorithm included in the model*

Once the closure model was shown to have the capacity to simulate different post-closure water qualities, a life-of-mine water balance and water quality model encompassing various waste and waste management plans was developed for Antamina. This life-of-mine model includes a variety of different flow configurations, different options for additional mine waste facilities, preset scenarios encompassing potential systems failures and comparison to different sets of compliance criteria (both flow and water quality) at different points within the system.

An integrated water balance and water quality sub-model approach has been applied for cases ranging from feasibility level water quality predictions where the geochemistry was directly linked to a complex water-balance model developed in GoldSim for a proposed large open pit, polymetallic mine in a high rainfall tropical environment through to closure assessment of pit rebound rates, expected water qualities and environmental controls in a dry environment.

Deriving the fundamental geochemistry

The models built for Antamina are based on a comprehensive on-site geochemical testing regime. Fundamental reactions which were included in the model and the conceptual geochemistry model were derived by detailed interpretation of the site monitoring data, determining kinetic loading rates for different waste types from the on-site kinetic cells and the supporting mineralogy and static test data (Aranda, 2009). Through the use of this data and PHREEQC and GWB the expected geochemical reactions were identified. These reactions were considered in the model development.

In many of the mine components the major mineral assemblage are dominated by calcium containing carbonates. This mineralogy results in pH levels being largely controlled by the presence of carbonates, the carbonate mineral composition (e.g. the range of calcitic to dolomitic carbonate present), the threshold concentrations of these carbonates below which they can no longer buffer acidity and the factors that control carbonate solubility and equilibrium. These factors include the fugacity of CO_2, (confirmed by on-site research by Bay, 2009) the overall salinity of the water, temperature and the effect of other processes which consume alkalinity or impact concentrations.

Key process for water quality variation appears to be the oxidation of sulphide minerals. Sulphide oxidation drives increases in salinity, sulphate and acidity. Neutralisation of acidity may occur through the water's natural alkalinity, but principally through the dissolution of Ca-containing carbonates.

Sulphide oxidation with concurrent buffering increases salinity and releases the associated metal in the sulphide (e.g. Fe, Cu, Zn or Pb). Increased sulphate and calcium results in gypsum ($CaSO_4$) precipitation, while the continued presence of carbonates maintains neutral to alkaline conditions which limits mobilization of many of the metals, apart from neutral drainage species such As and Mo.

Sulphate generation is used as an estimate of the amount of generated acidity; from this, the amount of carbonate needed to buffer this acidity is subsequently calculated (i.e. depletion of calcite/dolomite as a result of sulphide oxidation). The resultant salinity and water quality evolution (including pH) is used as the basis for the calculation of subsequent reactions.

The site observations confirm that the concentrations of the majority of metals are a function of the pH conditions, overall salinity and mineral solubility constraints. Required geochemical mechanisms including pH determination, acid generation and neutralisation, salinity calculations and solubility constraints which are all included in the model based on site observations.

Model development platform

GoldSim was used as modelling platform as it allowed integration of multiple data streams (matrix calculations as opposed to linear calculations) and the integration of water quality and water balance. GoldSim allows a hierarchical approach to model development which meant that the required algorithms for both water flows and the geochemical reactions for different mining components could be written into individual components or containers as they are called in GoldSim. Common data such as rainfall and geochemical mechanisms and constants can be globally linked to the different components.

All of the required equations describing water flow and all geochemical and mass transfer interactions were compiled and written into the GoldSim model (Fig 1). As a final product, the mine is provided with a GoldSim player file which is interactive and allows selection of different scenarios and input parameters. This allows the post-closure impact of different water and waste management options to be easily evaluated by mine staff.

Functionality of the developed tools

The functionality of the model to be used by the mine personnel included the following components:

- Include the waste inventory/footprint of each mining component and have an integrated water balance within the model,
- Combine acid generation with neutralisation consumption in each facility,
- Constrain water quality by applicable processes such as kinetic rates or loading rate limits as observed from the onsite kinetic testing and mass transport controls such as solubility limits and processes such as adsorption. These processes needed to be linked to the overall water quality evolution of each system,
- Simplified operability of the model for end users who may not be geochemical experts, requiring a high level of error checking and automated calculation definition,
- Flexibility which would include the ability to change model as options are evaluated,
- Providing easy to understand outputs to guide and assess water management options.

Conclusions

A great deal of geochemical characterisation data is required for detailed water quality predictions on site-wide scale. In these projects, it has been shown that where high quality data is combined with feasible conceptual geochemical models, selection of the appropriate defining geochemical reactions and a versatile platform such as that provided by GoldSim, it is possible to develop water quality prediction tools that can simulate a variety of geochemical and hydrologic situations. These tools can be used to aid mines in aspects ranging from integrated site-wide water management plans during operation through to closure.

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