Model-based Investigations of Acidity Sources and Sinks of a Pit Lake in Western Australia

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Abstract Lake Kepwari is a rehabilitated lake in the Collie Basin lignite mining area in Western Australia. The water quality of Lake Kepwari was modeled with the pit lake hydrodynamic and water quality model PITLAKQ. Based on a hydrodynamically validated model, water quality scenarios were used to quantify the sensitivity of different acidity sources including groundwater exchange, surface runoff and erosion, providing new insights into the system. The technique of monthly aggregation of all sources and sinks of acidity, based on detailed model output, provided the basis for useful conclusions. Model results suggest a new focus of field investigations to improve modeling certainty and a follow-up, improved phase of modeling.

Key Words water quality modeling, pit lake, PITLAKQ, acidity, acid mine drainage

Introduction

Mining pit lakes can form in open cut mining pits that extend below the groundwater table. Final lake surface levels generally represent the greatest risk of pit lake closure to stakeholders due to potential overflow and discharge to regional surface water bodies and groundwater resources. An essential prerequisite for managing this risk is a good understanding of the lake's water budget.

Pit lakes in the Collie Coal Basin (Western Australia) form a lake district currently consisting of 13 lakes exceeding a total volume of 200 GL of acid and metalliferous contaminated water (McCullough *et al.*, 2010). Lake Kepwari is a new rehabilitated lake that was partially filled with water from the Collie River from 1999 to 2005 during winter periods. The lake has a maximum depth of about 67 m, a volume of about 25 GL, an area of over 1 km^2 and is characterized by steep slopes.

Lake Kepwari's water quality depends on a variety of factors such as groundwater exchange, river water flooding, surface water runoff, pit wall erosion and solute release from submerged sediments. Determinants of water quality are complex and little is known about the interactions among these processes. Pervious studies looked at climatic conditions at the site (Huber *et al.*, 2008) and lake water quality (Salmon *et al.*, 2008). Data from these studies were used to parameterize the model.

Given long-term risks for off-site contamination, regulatory agencies often rely on geochemical predictions of future pit lake water quality to evaluate closure strategies that protect the sur-

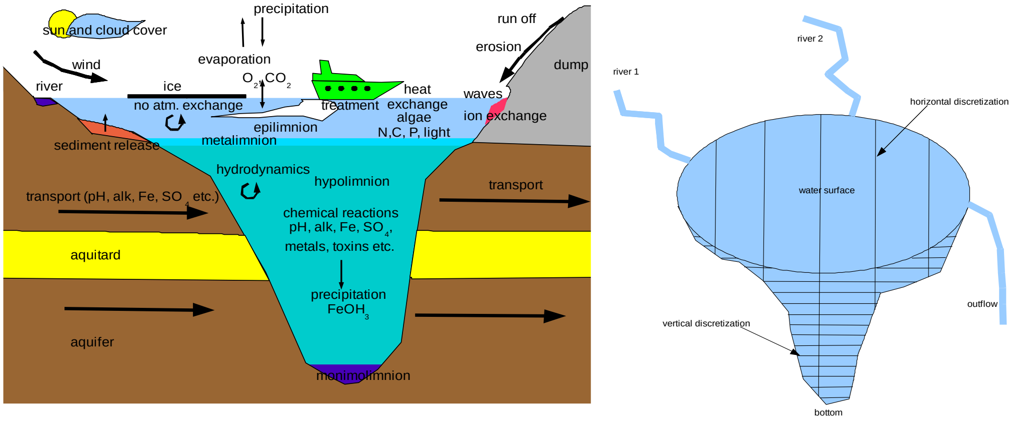

Figure 1 *a) Schematic of processes in PITLAKQ and b) principle of spatial discretization.*

rounding environment (McCullough *et al.*, 2009). This report focuses on one important aspect of water quality of Lake Kepwari, the sources and sinks of acidity. Other aspects were also investigated but are only briefly mentioned here due to space constrains.

Methods

A pit lake model, based on the hydrodynamic and water quality model PITLAKQ (Müller 2011), was established for Lake Kepwari. The PITLAKQ (Müller, 2011) numerical modeling software is based on MODGLUE (Müller, 2004), which had been applied to several lakes (Müller & Werner, 2004; Müller, *et al.* 2008, Werner *et al.*, 2008). PITLAKQ accounts for the determining physical, chemical, and biological processes of acidic mining pit lakes. Figure 1a gives a schematic overview of important processes in acidic pit lakes that are implemented in the model. The principle of spatial discretization is shown in Figure 1b.

PITLAKQ couples CE-QUAL-W2 (Cole & Buchak, 1995) and PHREEQC (Parkhurst & Appelo, 1999) and adds new functionality to account for the pit lake requirements. For example, several sources of acidity such as erosion or release from submerged sediments and spatially distributed groundwater inflow help to better represent pit lake conditions. Furthermore, PITLAKQ can account for the effects of water treatment on water quality. The two-dimensional model setup with one vertical and one horizontal dimension allows

Table 1 *Processes in PITLAKQ.*

Processes	Description
hydrodynamics	Solution of the Navier-Stokes-Equation in two dimensions with density-dependent flow. Calculations of velocities, water temperature distribution and hence stratification.
transport	Transport of dissolved substance in the lake with about 40 species.
heat exchange	Budgeting of heat terms at water surface.
wind impact	Wind energy effects water velocity of upper most lake layer.
ice cover	Formation and melting of ice. No atmospheric exchange during ice-covered periods.
tributary inflow	Inflow from an unlimited number of sources (flow, concentrations, and temperature).
atm. O_2 exchange	Oxygen can enter and leave at water surface layer.
atm. CO_2 exchange	Carbon dioxide can enter and leave at water surface layer. Solubility depends on pH.
precipitation	Precipitation enters surface layer with amount, temperature and concentrations.
evaporation	Water evaporates from surface layer.
groundwater exchange	Groundwater characterized by flow, temperature and concentrations can enter and leave lake at any given cell.
groundwater flow and transport	The groundwater inflows and outflows can be given as inputs (off-line coupling) or can be supplied by a coupled groundwater model (on-line coupling) to model feedback.
erosion mass input	Precipitation and wind waves move material into the lake.
erosion water quality impact	Eroded material effects lake water quality by adding dissolved substances and cation exchanger loadings that release substances.
algae and nutrients	Algae grow depending on temperature, available light and nutrients including carbon.
chemical lake reactions	Equilibrium and kinetic reactions in all model cells. Organic matter from biological process is used as electron donators (linking chemical and biological reactions).
mineral precip.	Forming minerals can be allowed to precipitate.
sediment release	Sediment at lake bottom can release substances. Release rates can be given as function of time or can depend on current lake water composition.
treatment	Substances can be added to the lake at any location with a time-variable scheme.
alkalinity of sinks and sources	In a post-processing step the alkalinity contributions of sinks and sources can be determined with a monthly time step.
coupling of all processes	All processes can use information generated by other processes. For example, lake water temperature is used in chemical reactions.
process additions / modifications	The model implementation is modular and allows for addition or modification of processes according to site specific needs.

sources and sinks with defined spatial locations. Table 1 gives an overview of the process that can be modeled with PITLAKQ.

The bathymetry of the lake was constructed from a digital elevation map (DEM) and was used as the basis for the two-dimensional discretization (compare Figure 1b for principle of discretization). The water level-volume relationship of the discretized model has less than 1% difference compared to calculating the volumes with a vertical step size of 0.1 m for each point in the DEM, and can therefore be regarded as adequately representing the lake volume.

The lake receives water from inflowing groundwater, precipitation, surface water runoff and the Collie River inflow. Evaporation and groundwater outflow constitute lake water sinks. All sources carry heat, i.e. have a temperature and dissolved constituents influencing lake water quality. The out flowing groundwater leaves the lake removing heat and constituents. Erosion adds constituents to the lake water through two pathways, (1) dissolved constituents as found in the pore water of eroded material and (2) cation exchange capacity providing loaded exchangers that release cations to the lake water depending on the chemical composition of the lake water.

Groundwater exchange data stem from a regional groundwater model. Values for surface runoff and erosion were varied within reasonable limits due to lack of measured data.

Based on the hydrodynamic representation of the lake in the model, water quality investigations over different scenarios were performed. Focusing on acidity, simulation runs were carried out with varying strengths of sources and sinks of acidity. These cover the variations in groundwater exchange rates as well as effects of lake wall erosion and surface runoff.

A total of eight modeling scenarios were run with different combinations of acidity sinks and sources:

- groundwater exchange (minimal, likely and large flux scenarios)
- surface runoff (no runoff, high and low acidity scenarios)
- lake wall erosions (no erosion, low, medium and high acidity scenarios)

Sediment release was not modeled because no suitable data were available. Furthermore, since surface runoff and erosion were already varied, adding another process with variation of its parameters within estimated limits would not yield new insight. Once measured values for sediment and lake wall composition are available, the process of sediment release should be reconsidered.

Results

Hydrodynamic properties such as lake stratification, lake volume development over time and the lake surface evaporation could all be reproduced with good accuracy. A comparison of modeled and measured values for these parameters suggests that the model adequately represents the hydrodynamic system. A detailed presentation of these comparisons is out of the scope of this paper.

The results of the eight water quality scenario runs provided comprehensive output of all modeled constituents in space and time. This report focuses on time series of acidity sinks and sources, because analysis of these results helped develop an understanding of how Lake Kepwari's water quality is influenced by different environmental factors. The timing of the river water flooding events combined with seasonal variations in surface runoff and groundwater exchange resulted in large water quality differences over time. However, we found that the same source might have different impacts on lake water quality. For example, erosion adds materials with cation exchangers to the lake and can therefore release or take up substance from the lake water depending on its composition.

Figure 2 shows the different sources and sinks for acidity to the lake for four different water quality scenarios. Acidity was calculated by titration simulation against pH 6.0. This titration was done in monthly time steps for each single source or sink by adding only this one source/sink to the lake from the previous time step. This way the isolated effects of each source/sink could be quantified.

The scenarios in Figure 2a-c use likely groundwater inflow. Due to the filling with water from the Collie River until mid 2004 (with a small volume in 2005), there was likely little or no groundwater inflow into the lake until mid-2004. From then on, after a short period of increased inflow, inflow and outflow of groundwater were quasi-constant with only small seasonal variations. Therefore, two phases (1) up until mid 2004 and (2) later can be distinguished.

Figure 2a shows the results for the scenario with neither surface runoff nor erosion. It can be clearly seen that there are essentially now acidity sources in phase 1. The filling water from the Collie River is the major source of alkalinity in this phase. In phase 2, both groundwater inflow and outflow constitute acidity sources. This is due to the fact that groundwater inflow adds more acidic water to the lake and groundwater outflow removes water with pH above 6.0 (the pH titration was simulated against) and therefore lowers alkalinity. This is expressed as acidity source in the Figure 2a. In general, this scenario quickly reaches

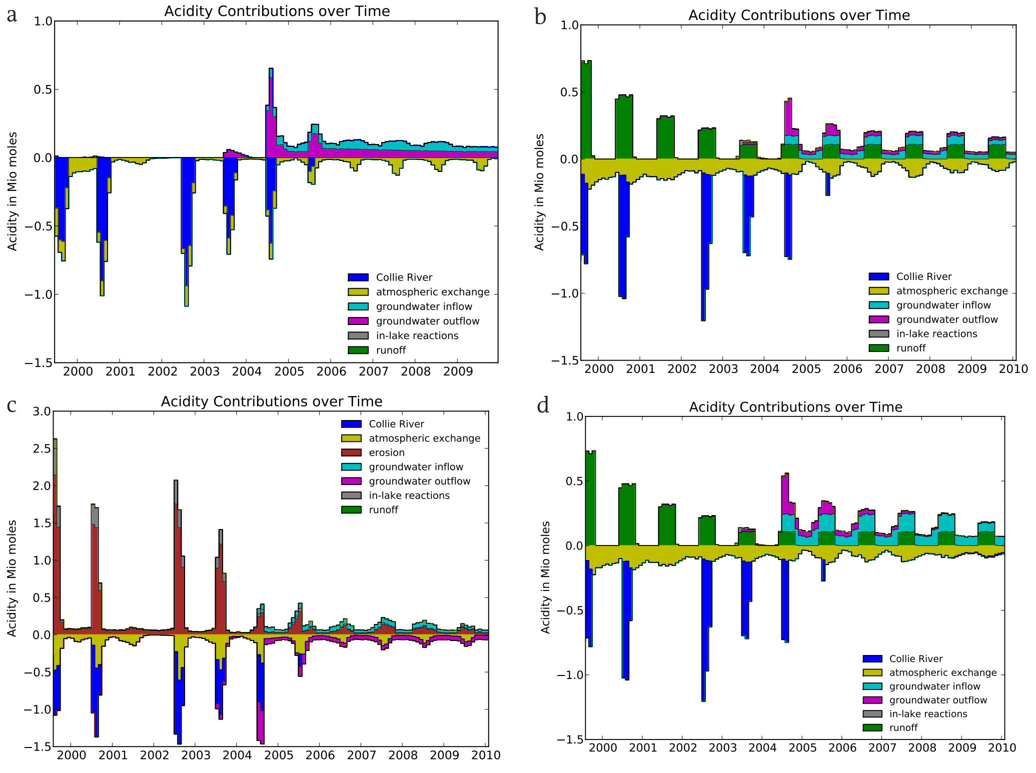

Figure 2 *Sources and sinks of acidity a) no surface run off, no erosion b); high-acidity run off, no erosion; c) low-acidity runoff, high-acidity-erosion; d) high-acidity runoff, no erosion, high groundwater exchange (a through c have likely groundwater exchange, acidity is positive, alkalinity negative on y-axis). Note: The scale for acidity in c) is different from these in the other sub figures.*

lake-pH values around 7 where observed values are between 4 and 5.

Figure 2b shows the results for the scenario with high-acidity surface runoff but no erosion. Again, the same two time phases can be distinguished. During phase 1, the filling water from the Collie River contributes most of the alkalinity followed by atmospheric exchange. The effect of atmospheric exchange can be contributed to CO_2 leaving the lake at its surface at low pH values where its solubility is low. During the first phase, surface runoff is the main source of acidity. The seasonal peaks can be clearly seen as well as the decreasing amount due to smaller areas that form runoff after the water covered lake area increases every year. The second phase looks similar to the second phase in Figure 2a but with a superimposed surface runoff and a therefore larger atmospheric exchange effect. Modeled lake-pH values range from 4.5—7, where observed values are between 4 and 5.

Figure 2c shows the results for the scenario with low-acidity surface runoff and high-acidity erosion. The model represents erosion as being caused by two effects, (1) mass eroded by precipitation from the not water-covered lake area, and (2) lake wall erosion triggered by the extending lake surface. Therefore, erosion effects are large in the beginning when the not water-covered areas are large and during expansion periods of the lake when large portions of the lake walls are eroded. Consequently, erosion constitutes the major source of acidity during the first phase. Note that the amount of acidity is much larger than for the other two scenarios (Figures 2a and 2b) described so far. Erosion peaks at the same time when filling water from the Collie River is added. This is due to the fact that the second type of erosion (lake wall erosion) is much stronger than the first type (precipitation-driven erosion). It may be argued that surface runoff and precipitation-driven erosion overlap in terms of processes. Therefore, the parameterization of this type of erosion was chosen to have only slight effects as acidity source. Modeled lake-pH values range from 3.5 to 4.5, where observed values are between 4 and 5.

Figure 2d shows the results for the scenario with high-acidity surface runoff and no erosion. In contrast to the other scenarios that work with the most likely groundwater exchange, the groundwater exchange rates are doubled. These exchange rates result in exactly the same water level and volume development in the lake over time. This non-uniqueness of groundwater exchange can be contributed to existing groundwater modeling results. The groundwater model is targeted towards large-scale regional investigations making the lakes relatively small features in the model. Furthermore, lakes are implemented as general head boundary conditions that need the lake water levels as inputs. Since lake water levels were kept constant for the groundwater modeling, inflow rates have a high uncertainty. Comparing Figure 2d with Figure 2b, there is no difference in phase 1 because during this time addition of river water prevents any groundwater inflow. During phase 2, a significantly higher acidity contribution of groundwater inflow can be seen. Modeled lake-pH values range from 4.5 to 6, whereas observed values were between 4 and 5.

In addition to the development of sources and sinks of acidity over time, other model results were evaluated. These include (1) spatial and temporal distributions of single constituents such as sulfate, iron, total dissolved solids or pH, (2) whole-lake budgets of acidity sources and sinks over the whole model period as pie charts and (3) development of in-lake acidity of the epilimnion and hypolimnion over time. These results including movies showing spatial and temporal distributions can be found at Müller (2011).

Conclusions

Even though available data describing lake water quality process were limited, modeling could help to provided quantitative insight into the system. There must be additional sources of acidity besides groundwater inflow to create the measured lake water quality. Surface water runoff alone is unlikely to be the only additional source. Modeling results suggest that erosion may be a significant acidity source. Further investigations of lake wall material and sediments are needed to determine their acidity potential. These data can than be used to narrow the range of erosion parameters leading to more certain modeling. In addition, sediment release of acidity might need to be modeled if field investigations suggest a significant water quality influence.

Overall modeling improved the understanding of the system and could quantify the relative importance of different processes such as groundwater exchange, surface runoff and erosion. The next iteration consisting of field and laboratory investigation will improve the water quality model parameters that can be used in a subsequent modeling step. This can lead to a much better understanding of what determines lake water quality and can provide a basis for targeted, effective monitoring and long-term predictions of water quality development.

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