TECHNICALPAPERS

Probabilistic quantification of uncertainty in predicting mine pit-lake water quality

Introduction

Decision makers evaluating open-pit mines need estimates of future pit-lake water quality that are more accurate than current analytical modeling can provide. Analogous problems exist in other industrial sectors, such as nuclear waste disposal or fossil fuel consumption. Economic interests drive activities that produce short-term gains, and public policy requires disclosure of potential impacts; yet un-

certainty in key parameters limits the ability to even bracket the probability of incurring environmental damage.

Critics have argued that, when uncertainty is incompletely quantified, computational models are not appropriate or that error bars imply a misleading confidence in the level of accuracy portrayed. However, current policy requirements can be supported only through predictive science, and the development of modeling techniques to more reliably estimate uncertainty depends on detailed reporting of error propagation in progressively more sophisticated modeling investigations.

This paper summarizes the current understanding of the components that limit accuracy in predicting pit-lake water quality. This information is intended to support modelers in adequately qualifying their predictions and to assist mine operators and regulators in making decisions that rely on such predictions.

Economic implications

Pit lakes represent a substantial potential liability, both because of the sheer number of mines (17 pit lakes have formed or are forming in Nevada alone and some 23 more are predicted to form in that state under current permits) and because of the potential costs associated with remediating them if necessary A pit

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with unacceptable metal concentrations would cost ~\$60 million to backfill (100 Mt at 60 cents/t) or ~\$13 million to treat for removal of trace metals (i.e., \$0.00026/L for ferric sulfate flocculation). The magnitude of financial risk clearly warrants development of accurate water-quality predictions.

Development of a modeling approach

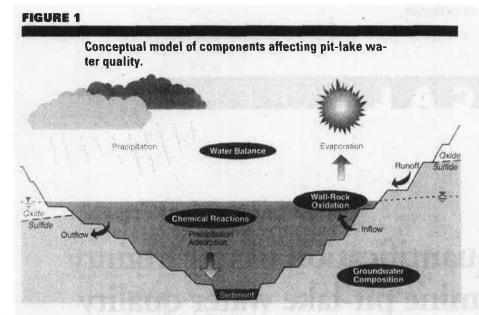
Ideally, predictive modeling would begin with broad confidence intervals on results, and those intervals would narrow as the parameter estimates are refined. Instead, estimated uncertainty has tended to increase as models have become more sophisticated and ranges of values for key parameters have expanded as models are compared to empirical data.

Developments in pit lake models have focused largely on improving the treatment uncertainty. In the authors' modeling group, uncertainty was initially evaluated using sensitivity analysis and deterministic simulations (US Bureau of Land Management, 1993). For the

next five lakes, the group treated bulk solute loading probabilistically, and, for the last 11 studies, the group used probabilistic techniques to propagate uncertainty through bulk loading and chemical reactions (e.g., Kempton et al., 1997). Based on a recent comparison of model results to measured limnology (Atkins et al., 1997) and water quality (Locke et al., 1997) in existing lakes, the authors believe that the computational tools are now adequate to bracket uncertainty in pit-lake water-quality predictions (although all models have room for improvement). However, the ability to bracket true uncertainty remains limited by incomplete estimates of parameter uncertainty. Thus, the authors believe the effort to improve

Abstract

The scrutiny given to model predictions of pit-lake water quality has focused attention on the uncertainty associated with long-term predictions. Although comparison of probabilistic predictive modeling of water quality in existing pit lakes suggest that short-term predictions can bracket most parameters, uncertainties in wall-rock reactions and the stability of groundwater composition and climate remain unquantified. This overview of the uncertainties associated with longer-term predictions is presented as support for those considering policy decisions that must be made in the nheonro of rolinhlo octimatos of fu-



on establishing accurate probability distributions for key model parameters.

Conceptual model of pit-lake evolution

Conceptual models of pit-lake evolution have identified sulfide oxidation in wall rock, groundwater composition, overall water balance and chemical reactions as the critical components affecting water quality evolution (Fig. 1; Ross, 1992; Kempton et al., 1997).

Dewatering and excavation exposes wall rocks to atmospheric oxygen, and solutes released by oxidation of sulfide minerals are flushed into the lake by runoff or groundwater. Solutes in groundwater load to the lake in proportion to their concentration in groundwater and the rate at which the groundwater flows into the pit. Longer-term solute loading from groundwater depends on the water balance, which is a particularly important component in semiarid or arid climates where evaporation continuously increases solute concentrations. During lake evolution, solutes are removed by chemical reactions, primarily precipitation of minerals, and, where significant dissolved-iron loading occurs, by adsorption to hydrous ferric oxide (HFO).

Estimating uncertainty for key model parameters

Quantitative modeling is most useful when accurate probability distributions are available for each component in the conceptual model. Below is an assessment of uncertainty estimates for each of the four key components of pit-lake water quality.

Groundwater quality. By definition, ore bodies are areas with anomalous metals concentrations, and this fact is often reflected by elevated metals concentrations in surrounding groundwaters. A probability distribution for average groundwater composition can be generated from the variability observed among multiple representative chemical analyses (Fig. 2, Kempton et al., 1997), where accuracy is limited by the number of samples and their spatial representation of the source area. However, groundwater composition can change temporally, particularly in response to increased flow rates induced by mine dewatering.

Figure 3 shows temporal arsenic trends measured in three lithochemical zones during dewatering. A constant concentration (assumed in most modeling studies) occurs if aqueous concentrations are limited by low partitioning from solid to water (e.g., in the presence of a sparingly soluble mineral or strongly adsorbing aquifer matrix).

Solute concentrations could decrease with increased groundwater flow if aqueous concentrations are limited by dissolution kinetics. And solute concentrations could increase where pumping-induced changes in water quality increase dissolution, such as from introduction of oxygenated water to sulfide minerals.

While such hypothesized explanations for observed temporal water-quality trends are useful, quanti-

fying this effect for probabilistic water-quality predictions remains tenuous. A reasonable approach is to assume constant concentrations in initial water-quality modeling and then to continue to monitor groundwater composition as mining proceeds, refining the model later by incorporating the new data. Solute concentrations should generally return to premining levels as the groundwater flow regime returns to premining conditions. But estimates of groundwater composition far beyond the end of mining are necessarily speculative, particularly where dewatering-induced water quality changes were observed.

Water balance. The overall water balance — inflow, outflow and evaporation — controls the loading and removal of solutes from a pit lake and is, thus, a critical control on water quality. The groundwater inflow rate is always directly proportional to the loading of solutes dissolved in the groundwater, but the actual effect of the water balance is more complex because it also affects solute removal by outflow and the duration of wall-rock oxidation.

The initial infilling rate affects the duration of wall-rock exposure to oxygen and, thus, the loading rate of wall-rock oxidation products. In the longer term, the steady-state water balance typically dominates water quality. If there is some outflow from the pit lake, solutes introduced by groundwater will approach a theoretical maximum concentration, assuming that wall-rock loading is negligible after the lake is full (Fig. 4).

However, in a terminal lake (a condition predicted for many pit lakes in semi-arid climates where potential evaporation greatly exceeds precipitation), there is no physical limit on solute concentrations. Rather, solute levels increase until they become limited by chemical mechanisms such as precipitation, coprecipitation or adsorption.

Uncertainty in water balance is likely to increase with increasing time as the limit on inflow rate shifts from aquifer hydraulics to climate. As the lake fills, groundwater inflow is determined by the hydraulic conductivity and storage capacity of the aquifer, so the modeled initial infilling rate should be about as accurate as

the predicted dewatering rate, often about $\pm 30\%$ in the opinion of groundwater modelers (Fig. 5). At later times, long-term water balance is determined more by net evaporation, particularly in terminal lakes where groundwater inflow exactly balances evaporation and predicted water quality becomes very sensitive to climate.

Climate-driven effects are highly uncertain because the magnitude and even the general direction of climate change remains unclear. The Intergovernmental Panel on Climate Change (IPCC) "projects an increase in global mean surface temperature of about 1° to 3.5°C by 2100." Yet, while the IPCC notes that semi-arid lands, such as the mining districts of the southwestern United States. are "particularly vulnerable to climate change," the text is highly qualified (e.g., "Regional scale climate change predictions are uncertain; our current understanding of the critical processes is limited; and systems are subject to multiple climatic and nonclimatic stresses, the interactions of which are not always linear or additive" (United Nations, 1995).

A separate review of climate experts (Morgan and Kieth. 1995) indicates disparate views among climate modelers, including reasonable forecasts that precipitation in these areas could either increase or decrease. Two points are clear: "there is a reasonable probability that the climate will be significantly different by ~2100 when atmospheric CO₂ is expected to have doubled from preindustrial levels" and "dramatic increases in the accuracy of long-term climate forecasts are unlikely for the next 10 to 15 years" (Morgan and Kieth, 1995). Thus, any forecasts of pit-lake water quality beyond ~100 years will necessarily contain unquantified uncertainty.

Solute loading from wall rock. Solute loading from wall rock derives mainly from the oxidation of sulfide minerals exposed to atmospheric oxygen by mining. The following three components affect wall-rock solute loading:

- the amount of oxidation that occurs before the lake is full.
- the associated release of solutes by oxidation and
- rock/water interactions as solutes move from wall rock to the lake.

Oxidation: The successful calibration of diffusion-limited shrinking core models of sulfide mineral oxidation (Davis and Ritchie, 1987) to measured oxidation rates in pit benches (Atkins et al., 1997) suggests that such models are reasonable tools for at least short-term predictions. Reaction rates are controlled by sulfide content, exposure duration, fragment size, interfragment diffusivity and intrafragment diffusivity (Davis and Ritchie, 1987; Wunderly et al., 1995). Oxidation is unlikely to be moisture limited, even in semiarid climates, because the zone in which evaporation from typically unvegetated rock dries the pores enough to slow oxidation extends only a few centimeters from the surface into the rock (Cook et al., 1997).

Uncertainty in the key parameters needed to model the effects of wall-rock oxidation (sulfide sulfur, exposure duration and initial oxidation rate) can be quantified accurately with direct measurements, providing accurate confidence intervals for early times (e.g., ~10



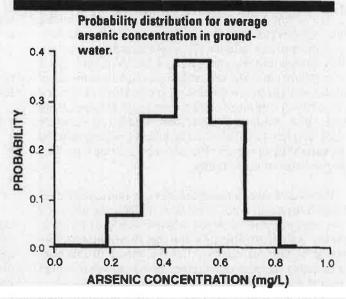
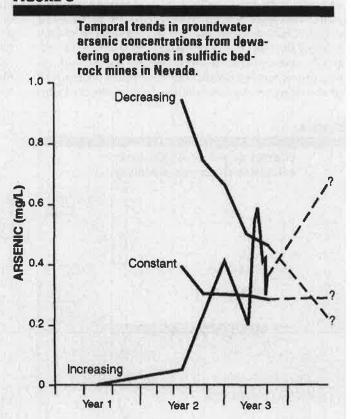


FIGURE 3



years or less). At longer times, however, wall-rock oxidation rates may slow relative to model predictions as more oxidation occurs in larger, poorly defined fragments. Alternatively, rates may increase due to wall failures that expose new materials at the surface or advection of air drawn through sulfidic pit walls to replace extracted groundwater (Larsen and Postma, 1997). Thus, uncertainty in predicted waste-rock oxidation rates at longer times (e.g., ~20 years or more) remains poorly quantified.

Solute release: Sulfate release from wall rock is a direct product of oxidation. But metals releases are related to total concentration as well as metals speciation among

sulfide, oxides and adsorbed phases. The authors believe this complexity is best addressed using empirical oxidative weathering tests, such as humidity cells, to measure solute releases (relative to sulfate) during oxidation. Several of the authors' studies show significantly more variability among metals releases from different rock types at a constant amount of oxidation than in individual samples at variable oxidation degrees. Thus, estimated probability distributions based on metals releases from single-point oxidation experiments (e.g., cumulative metals release from a 20-week humidity cell) capture the most variability in metals releases, representing a reasonable predictor of uncertainty.

Water/rock interactions: Solutes can undergo chemical reactions as they are carried to the lake by meteoric water, making wall-rock loads particularly difficult to quantify. Acid neutralization and metals attenuation depend on water/rock contact, but the nature of this contact depends strongly on whether meteoric water moves as runoff over the pit walls or as subsurface flow.

At the hillslope scale (100 to 10,000 m²) in natural drainages, the bedrock surface is the dominant control on water flow (McDonnell et al., 1996). In pit walls, an analogous "bedrock contact" for preferential flow may exist along the base of the horizontal blast rubble or vertical blast-induced fracture zone around the pit wall. Ignoring runoff reactions with wall-rock probably leads to overestimating total solute loading, but the effect of run-

Effect of long-term pit-lake water balance on solute concentrations.

Net Evaporation

Net Evaporation

Net Evaporation

Time

Inflow

Inflow

Inflow

Inflow

Inflow

Inflow

Inflow

Inflow

TERMINAL LAKE

off on overall water quality is difficult to predict because of the nonlinearity in chemical reactions. Reducing this uncertainty in water/rock reactions is probably best accomplished using empirical studies at existing pit lakes.

Chemical reactions in the lake. The following three types of chemical reactions within a pit lake strongly affect water quality:

- mineral precipitation and adsorption in the water column.
- sediment reactions that affect metals adsorbed to HFO and
- reactions between lake water and the pit walls.

Precipitation of major minerals, such as calcite, during evaporative concentration can be simulated accurately with an equilibrium chemical model, and tests have shown that significant coprecipitation of trace metals (e.g., arsenic) is possible (Kempton et al., 1997). Also, uncertainty in trace-metal adsorption to HFO is well bracketed at pH levels above 5 using probabilistic equilibrium adsorption modeling and probabilistic treatment of thermodynamic data (Kempton et al., 1997; Martin et al., 1997). Overall, uncertainty in aqueous reactions can be quantified with available information, although coprecipitation reactions that are not predicted by the model may occur, resulting in overestimates of some trace-metal concentrations at longer forecast intervals.

Adsorption to HFO is often an important mechanism for removing metals from pit-lake waters. Therefore, the stability of HFO in the sediment is a critical component of long-term water quality. A study of three saline western United States lakes (Domagalski et al., 1989) showed that algal detritus reduced iron and manganese oxides in either the bottom brine (Great Salt Lake) or the top few centimeters of the sediment (Mono and Walter Lakes), and the study showed that iron is reprecipitated as FeS near the sediment/water interface.

Presumably, many metal cations released by HFO dissolution would be reprecipitated as metal sulfides in a sulfate-reducing environment. Field evidence, however, indicates that arsenic stabilization in sediments may be problematic. Under reducing conditions, including sulfate reduction, HFO-bound arsenic can be released from lake sediments (Ahmann et al., 1997), although much of the arsenic can be readsorbed by HFO precipitated from the oxic zone (Sohrin et al., 1997). Given the large range in iron and nutrient loading rates to mine pit lakes and the complexity of metal cycling, sediment stability is probably best evaluated using studies of existing natural and manmade lakes.

Finally, reactions between lake water and pit walls, particularly acid neutralization, remain poorly quantified. Classic studies of calcite dissolution by Berner and Morse (1974) found that the reaction rate was diffusion limited only at pH <4, with rates at higher pH levels reflecting surface reaction rates and extreme sensitivity to trace amounts of phosphate. A rigorous estimate for a particular pit lake thus would need to account for calcite dissolution kinetics, surface area and the effect of armoring minerals by precipitates. Although groundwater is often at equilibrium with calcite, the ratio of water to surface area in a lake is many orders of magnitude lower than in a porous medium, and an assumption of

calcite equilibrium in a pit lake requires site-specific justification. As with sediment stability, it is probably best estimated by empirical studies of reactions in existing lakes.

Policy guidance for pit-lake modeling

The central problem caused by predictions of delayed and long-term environmental impacts in mining that decision makers need a level of accuracy for waterquality predictions that exceeds the capability of current analytical modeling—will remain for the near future. In response to similar dilemmas surrounding nuclear waste disposal and climate change, policy guidance has been developed for conducting environmental analysis based on incomplete information. Key recommendations pertinent to modeling studies of mine pit lakes include:

- make the analysis as simple as possible, but not simpler (Morgan and Henrion, 1990);
- provide documentation sufficient to allow reproduction of general findings (Morgan and Henrion, 1990);
- identify all significant assumptions (Morgan and Henrion, 1990) (in addition to disclosing these for reviewers, key assumptions form the basis for a discussion of uncertainty);
- clearly articulate uncertainties (Morgan and Henrion, 1990; Pielke et al, 1999);
- provide a quantitative analysis of uncertainty (Morgan and Henrion, 1990);
- generate predictions primarily with the needs of the user in mind (Pielke et al., 1999).
- recognize that predictions themselves are events that cause impacts on society (Pielke et al., 1990) (overstated model accuracy could prematurely divert limited resources toward ineffective mitigation); and
- consider alternatives to modeling predictions (Pielke et al., 1999) (the most effective method for reducing vulnerability may be flexibility — e.g., plan for long-term but infrequent monitoring, then fund targeted remediation only when required).

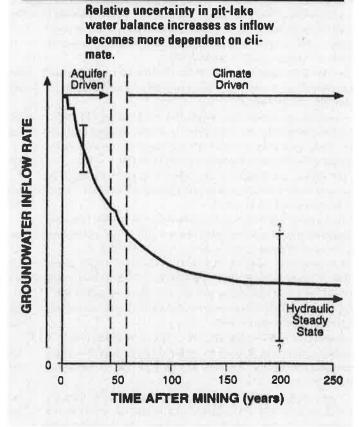
Modeling studies that include these components should address most public and private stakeholder concerns, leading more quickly to selection and permitting of acceptable operating and closure plans.

Conclusions and recommendations

For the near future, policy decisions that rely on predictions of pit-lake water quality will have to acknowledge an incomplete understanding of uncertainty. Uncertainty in groundwater quality, long-term wall-rock oxidation rates, water/wall-rock interaction, and metal stability in sediments is inadequately quantified. Also, estimates of long-term, climate-influenced water balance are unlikely to be bracketed accurately for at least the next ten years.

Although current models can provide useful quantitative estimates of pit-lake water quality during the initial infilling period, the uncertainty range in these predictions is probably underestimated. Beyond the infilling period, one can still identify general trends in water quality, but the accuracy of these predictions is limited by unquantified uncertainty in wall-rock oxida-





tion, water/wall-rock reaction, groundwater composition, and climate stability.

In response to parameter uncertainty, near-term research on pit-lake modeling should focus on improving estimates of wall-rock oxidation rates, solute loading by runoff over sulfide rock, and temporal trends in ground-water quality. In parallel, a standard pit-lake test case should be established for comparing different models. Initially, this test case should be based on available data from existing studies, then it should be extended as soon as possible to include characterizations of existing pit lakes as they begin to form. Such an intermodel comparison would establish a standard for evaluating consistency among various research teams, and eventual comparisons of model predictions to existing lakes would provide a much-needed degree of accountability. Both should be of keen interest to operators and regulators

Finally, uncertainty in environmental modeling is not unique to mining, and accepting that predictions of future water quality in mine pit lakes may not be reliably bound identifies an established policy approach.

Including the pillars of established environmental policy analysis — simple models, clear reporting, explicit assessment of uncertainty and consideration of alternative models — makes mine pit-lake studies more defensible by putting them on par with other potential long-term environmental issues. The results should be faster selection and permitting of acceptable operating and closure plans.

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