Bureau of Mining Regulation and Reclamation

GUIDANCE FOR GEOCHEMICAL MODELING AT MINE SITES

1. Introduction

Mining operations in the state of Nevada commonly interact with local and regional groundwater systems. Interactions between the mining environment and the groundwater environment can be complex, both hydrologically and geochemically. Due to the complexity of these interactions, modeling approaches may be applied in order to predict future water quality, or to understand the geochemical processes that have led to current water quality. These types of models may be required by the Nevada Division of Environmental Protection, Bureau of Mining Regulation and Reclamation (the Division) during permitting actions. Additionally, modeling studies may be required by other State or Federal agencies during the permitting process. This guidance document summarizes the background and Division requirements for geochemical modeling submittals. This guidance may not be comprehensive and may require updates as scientific understanding and geochemical modeling methods evolve. The purpose of this guidance document is to state Division requirements for submitted geochemical models, and to provide a reference for Division employees, mining operators, and other users/reviewers of geochemical models. By clearly stating requirements it is also hoped that this guidance document will decrease the number of technical comments required during Division review of geochemical models, thereby increasing permitting efficiency and decreasing permitting timeframes. While this guidance describes industry standard procedures, the Division or other agencies may have additional requirements due to site-specific issues.

1.1 Usage and Scope

A determination as to when geochemical modeling is required in the permitting process relates directly to the proposed mining operation and site-specific conditions determined through baseline hydrologic data collection (i.e., surface water and groundwater quantity and quality) and groundwater flow modeling. This document should be used in conjunction with the Division's *Guidance for Hydrogeologic Groundwater Flow Modeling,* found on the Division's website NDEP Regulation Branch Guidance Documents. Because water quality is directly dependent on water quantity, all geochemical models submitted to the Division must be built upon a groundwater flow model or other understanding of fluxes and flow paths in the project vicinity, and when applicable, one that the Division has previously approved. This requirement is not to state that a complex, three-dimensional groundwater flow model must be used. In many cases, a simplified analysis of groundwater flow or a site conceptual model is reasonable, and in fact encouraged. The modeler is directed to the groundwater flow modeling guidance for additional information. Because the majority of geochemical models submitted to the Division are predictive models of pit-lake water quality, these types of models are emphasized in this guidance. However, geochemical models may also be applied to the evaluation of many processes at mine sites, including among others, waste rock drainage (Lapakko, 2015), understanding the evolution of groundwater geochemistry along a flow path (Glynn and Brown, 2012), and comparing pit backfill with pit lake scenarios. For processes and project alternatives such as these to be considered explicitly they would need to be included in modeling efforts.

In its most general definition, a model is a simplification of reality (Bredehoeft, 2003; Nordstrom and Campbell, 2014), and in the case of a geochemical model, the model represents the modeler's perception of the geochemical system of interest (Nordstrom, 2012). For the purposes of the Division, geochemical models are tools that can be used to assess possible impacts to the waters of the State, in accordance with Nevada Administrative Code (NAC) 445A.121 (surface water), 445A.424 (surface waters of higher quality and groundwater), and 445A.429 (pit lakes and associated groundwater). For a mine pit lake, the applicability of these regulations and associated water quality standards depends on whether the lake is a terminal hydrologic sink or a flow-through pit lake that discharges to groundwater. A terminal hydrologic sink pit lake is not subject to the groundwater quality provisions in NAC 445A.424/445A.429 (because of the lack of a discharge to groundwater), but is subject to the surface-water quality provisions in NAC 445A.121/445A.429 (comparison with Division Profile 3 reference values and possible ecological risk assessment). A flow-through pit lake is subject to both the groundwater provisions in NAC 445A.424/445A.429 (comparison with Division Profile 1 reference values and natural background groundwater concentrations) and the surface water quality provisions in NAC 445A.121/445A.429 (Division Profile 3 and possible ecological risk assessment).

In some instances, the Division requires geochemical modeling studies in site-specific water pollution control permits (WPCP). Whether required by the applicable WPCP or separate correspondence, all geochemical models submitted to the Division must adhere to general requirements set forth herein. This guidance is not intended to be overly prescriptive, however, as to the exact layout and design of geochemical model reporting. Not every process discussed in this document will be applicable at every site, and additional processes may warrant investigation at specific sites.

The end goal of geochemical modeling is to inform permitting decisions made by the Division, and the results of these models may play a significant role in the future of proposed mine sites (i.e., determining permitting conditions). The specific use of geochemical modeling in permitting decisions is to provide future water–quality predictions at mine projects. Because of the importance of these models and their inherent uncertainty, individuals preparing geochemical models have a duty to evaluate and communicate the objectives and uncertainties of the model, as well as possible alternative actions to reduce environmental impacts, in appropriate correspondence and reports (Bredehoeft, 2005; Oreskes et al., 1994). Reviewers of geochemical models also have a duty to provide fair and reasonable reviews based on accepted scientific principles and practices.

2. Principles of Aqueous Geochemistry

Aqueous geochemistry is generally the study of the chemical composition of water, processes governing composition, and any phases interacting with water (e.g., minerals, gases, etc.). In general, the principles of low-temperature (0-100 ℃) aqueous geochemistry are applicable to Nevada mine sites. There are a number of processes that control the composition of water, including speciation, complexation, mineral precipitation and dissolution, gas dissolution and exsolution, oxidation-reduction (redox), sorption, and biogeochemical processes. The modeler must also consider whether equilibrium thermodynamics or kinetics are most applicable to the system of interest. Principles of thermodynamics are most usefully applied to systems for which an assumption of equilibrium has been justified. While thermodynamics also apply in non-equilibrium conditions, thermodynamic calculations have limited use in these systems. In contrast, principles of kinetics are applicable in systems where reactions do not reach equilibrium or take an extended period of time to do so (Appelo and Postma, 2005). In mining-related systems, assumptions of equilibrium may not always be reasonable (Nordstrom, 2009b). Modelers should carefully evaluate equilibrium assumptions in

geochemical model reports submitted to the Division, consider kinetics as applicable, and evaluate whether enough kinetic data are available to simulate the system of interest.

2.1 Geochemical Applications to Mining-Related Systems

Several geochemical processes listed above are of particular importance in the simulation of mine-related waters – specifically, metal sulfide oxidation, aqueous ferrous iron (Fe^{2+}) oxidation, carbonate dissolution, hydrous metal oxide precipitation, and sorption. The primary mineral that produces acid mine drainage (AMD) is pyrite, although pyrrhotite and marcasite are also important in some ore deposits. These key geochemical processes govern the partitioning of components between solid and aqueous phases, and ultimately determine the mobility of constituents of interest in mine-related waters. Several of these processes are intimately related to the measurement and simulation of acidity and alkalinity in mine waters, which are commonly misunderstood (e.g., Kirby and Cravotta, 2005a; 2005b). For example, the generation of acidity from hydrolysis reactions has been treated in a variety of manners in models submitted to the Division. The inclusion of these processes is not always consistent with modern scientific understanding. Modelers should pay particular attention to how these quantities are incorporated into geochemical models.

The applicable theory for each of these processes and details of modeling is beyond the scope of this document. For additional information see Appelo and Postma (2005), Alpers and Nordstrom (1999), Castendyk et al. (2015), Glynn and Brown (2012), Nordstrom (2011), Nordstrom and Alpers (1999), Nordstrom and Campbell (2014), and Smith (1999). Models submitted to the Division must appropriately address the applicability of each of these processes to the issue at hand, based on the purpose of the model.

It is also important in modeling geochemical systems to incorporate the different characteristics of groundwater and surface water. The major differences between groundwater and surface water systems include residence time and the possibility for exchange of gases with the atmosphere, primarily oxygen (O_2) and carbon dioxide (CO_2). In reference to gas partial pressures, surface water systems will likely be closer to equilibrium with gases in the atmosphere. In contrast, groundwater commonly contains greater CO_2 concentrations than the atmosphere (depending on aquifer composition), and lesser O_2 concentrations (Appelo and Postma, 2005). Pit lakes are a special case, representing a mixture of groundwater and surface water. Pit-lake gas equilibria are further complicated by stratification and mixing, which may result in distinct layers with differing gas partial pressures. Additionally, it should be noted that aqueous nitrate (NO_3) and ferric iron (Fe^{3+}) are strong pyrite oxidants in the absence of oxygen (Appelo and Postma, 2005; Gammons, 2009; Weber et al., 2006). Blasting at mining operations may result in elevated concentrations of NO_3 in mine waters, and presence of either nitrate or ferric iron in deeper waters of pit lakes could promote the oxidation of pyrite under anoxic conditions. Modelers must carefully examine these and other geochemical characteristics of the water body of interest during the creation of geochemical models.

3. Conceptual Geochemical Models

The first step in site-specific geochemical modeling is the development of a conceptual model. Conceptual models represent the modeler's interpretation of the prevalent geochemical processes that occur on the site or are expected to occur in the future. The conceptual model should be based on abundant and representative geologic, climatologic, geochemical, and hydrologic data. Additionally, conceptual models should ascribe to the principle of parsimony (also known as Occam's Razor): that is, the conceptual model should be the simplest description of the system possible that includes all significant processes while still containing enough complexity to represent important system behavior. It is imperative that site-specific geochemical conceptual models include all geochemical

and hydrologic processes that may potentially occur at the site that could alter future water quality for constituents of interest. A conceptual model need not include unnecessary detail but must include all processes that are reasonably expected to occur and may result in significant water-quality impacts. Examples of potential processes for inclusion in a pit-lake geochemical conceptual model include: groundwater inflow and outflow; limnology and potential for turnover or permanent stratification of the water column; surface runoff on highwalls from meteoric precipitation; interaction with water in underground mine voids and pore-waters in highwall fractures impacted by blasting; mineral equilibria (e.g., precipitation and dissolution); adsorption of aqueous species to mineral phases; gas equilibrium; biogeochemical reactions; and redox reactions. See Castendyk (2009a) for additional information on conceptual models for pit lakes. A geochemical conceptual model for a groundwater system would be substantially different, as many equilibrium constraints (for gases and minerals) and other processes applicable to a pit lake would not apply to a groundwater system, and vice versa.

It is important that conceptual models be reviewed against observed conditions and revised as additional data are collected or the mine plan changes. There should be an iterative process whereby the conceptual model improves over time by incorporating new data and any mine plan revisions. Conceptualization, modeling, and data collection are intimately linked because the collection can and should be guided by modeling efforts (Bredehoeft, 2005). The need for a realistic conceptual model cannot be overstated, as numerical modeling based on unreasonable conceptual models are of little use in evaluating future conditions (Nordstrom, 2012).

One aspect of pit-lake conceptual models that should receive additional attention is the common assumption that Nevada pit lakes undergo full turnover annually (i.e., that all Nevada pit lakes will be holomictic). Although the majority of existing Nevada pit lakes appear to be holomictic, some deeper pit lakes in Nevada may be meromictic (i.e., never undergo full turnover of the water column). Management and modeling of meromictic pit lakes requires special attention and different assumptions (i.e., a different conceptual model) than for holomictic pit lakes (Schultze et al., 2016). There are a variety of manners in which a screening-level assessment of the physical limnology of pit lakes can be completed (Castendyk, 2009b; Jewell, 2009). These methods do not always show good predictive abilities however (Schultze and Boehrer, 2009). Additional discussion of appropriate methods for evaluating limnology are discussed in Section 6.3 below. Highwall stability may also impact pit-lake limnology (e.g., if highwall collapse were to cause mixing). However, geochemical models are likely not able to simulate this process realistically.

4. Data Collection and Model Integration

In the experience of the Division, it is common for geochemical modeling exercises to reach advanced stages without adequate representative characterization data, which are required per NAC 445A.396 for overburden, waste rock and ore, and NAC 445A.395 for groundwater and surface water resources. Adequate characterization would include abundant data on the characteristics and spatial distribution of all potential sources for constituents of concern on the site (typically Division Profile 1 plus or minus Profile 3, depending on the application). For a pit lake model, these sources would include all distinct groundwater aquifers and a thorough sampling of the spatial distribution of all lithologic, alteration, and mineralization units that will remain in the immediate vicinity of the ultimate pit walls. The geochemical characteristics of interest for these distinct potential solute sources could include mineralogy, leachable quantities of constituents (e.g., determined using the meteoric water mobility procedure [MWMP] and humidity cell tests [HCTs]), and acid-base accounting (ABA).

Data gaps that commonly appear in submittals to the Division include hydraulic parameters, subsurface lithologic relationships, climatic conditions, and information on geochemical attributes such as mineralogy and reactivity. When modeling proceeds with these critical data gaps unaccounted

for, the resulting model predictions may not be representative of the project and may require revision. This issue is a common cause of Division requirements to revise submitted models, which leads to delays in permitting decisions. A geochemical model is only as useful as the field data that constrain it (Nordstrom, 2012).

In addition to geochemical characterization data, geochemical models also commonly incorporate the predictions of other numerical models, specifically hydrogeologic groundwater flow models, in their calculations. The dependence of geochemical models on groundwater models arises from the fact that water quality is directly influenced by water quantity, but the reverse is not true. Groundwater flow model results are commonly incorporated as if they were data rather than predictions; therefore the resultant uncertainty introduced into the geochemical model should be evaluated (see section 7 Sub-Models below). Geochemical models therefore can be greatly impacted by the inputs derived from groundwater model predictions. Because of this dependence, all geochemical models should be based on Division-approved groundwater flow models of the same or greater spatial dimensions. For example, pit-lake and solute-transport geochemical models should use as inputs the predicted water budget for the region of interest derived from a groundwater flow model for the project. It is common for both groundwater flow modeling and geochemical modeling reports to be submitted to the Division concurrently. While this practice is acceptable, it risks additional delays if required revisions to the groundwater flow model necessitate revisions to the geochemical model.

4.1 Parameter Variability

One of the main aspects of data collection that should be considered during construction of conceptual and numerical models is spatial and temporal variability. It is common for environmental variables such as concentrations of geochemical constituents to vary through time, across a site, and from one lithologic unit or alteration zone to another. As noted above, one of the major issues observed in some rock characterization documents is the lack of adequate sampling, both spatially and in terms of how well sample variability replicates variability observed in the field. The extent to which geochemical attributes are realistically and representatively captured in testing procedures is also a concern (Parbhakar-Fox and Lottermoser, 2015). Additionally, temporal variability should be considered where possible (e.g., for climatic or geochemical variations; Nordstrom, 2009a). There are a variety of methods useful for statistical analysis of spatial and temporal variability (Helsel and Hirsch, 2002; ITRC, 2013). The geochemical model report and supporting documentation must include appropriate characterization data and must demonstrate that these data are inclusive of the variability that is observed on the site or reasonably expected to occur in the subsurface or through time. For example, trace-element geochemistry typically varies between different lithologies and may also display significant variation spatially within a given lithology. At mine sites, such lithology-based variations are commonly overprinted by variations in major-element and trace-element geochemistry related to hydrothermal alteration and mineralization zones, and to different depths and intensities of weathering. The distribution of trace elements is of critical importance to the geochemical model of the site because many trace elements are toxic and are regulated by the Division according to Profile 1 or Profile 3 reference values. A model that assumes geochemical homogeneity among lithologic units, or zones of alteration, mineralization, or weathering rather than documenting the actual range of variation, is unacceptable because it fails to demonstrate that the characterization is representative as required in NAC 445A.396. In the case of geochemical modeling, adequate characterization data are required to illustrate the full range in geochemical characteristics representative of each major lithologic, alteration, and mineralization unit and zone across the site that is identifiable and discrete.

The determination of adequacy of characterization data will be made by the Division based on best scientific and engineering judgment. The required amount of characterization data is not consistent

across all sites, and sites that are more geologically and geochemically complex or that have a greater potential to degrade waters of the State will require more thorough characterization. For pit lake studies, it is important to include all necessary geochemical parameters in characterization procedures. The list of parameters that must be included is essentially a combination of Profile 1 and Profile 3 reference values. Additional information specific to characterization for pit-lake studies may be found on the Division's website NDEP Regulation Branch Guidance Documents. Details and considerations applicable to many characterization studies are also summarized in McLemore et al. (2014).

5. Geochemical Modeling Codes

The differences between models and computer codes is an important concept that is commonly misunderstood. As previously stated, a model is a simplified representation of reality that allows the modeler to test assumptions and, in some cases, predict future conditions. A code on the other hand is an algorithm that allows for the calculation of complex mathematical formulas. In the practice of geochemical modeling, a conceptual model is generally converted in some way into a geochemical modeling code, which is used to evaluate speciation and sorption, allow mixing and possibly other processes, and predict future conditions. The underlying theory and mathematics of geochemical modeling is beyond the scope of this document. For additional information the modeler is referred to Alpers and Nordstrom (1999) and Nordstrom and Campbell (2014).

There are numerous modeling codes that could be used to predict the geochemical conditions on mine sites (see Table 4 of Maest et al. [2005] or the review in Steefel et al. [2015]). In the experience of the Division, the United States Geological Survey (USGS) code PHREEQC (Parkhurst and Appelo, 2013) is the most widely applied. This code is open-source, well documented, and has been utilized in numerous peer-reviewed publications. Additional codes that have wide applicability include EQ3/6 (Wolery and Jarek, 2003) and MINTEQA2 (and subsequent updates; Allison et al., 1992). There are also specialized codes for simulating the coupled hydrodynamics and geochemistry of pit lakes, see Section 6.3 for a review of these.

As also stated in the Division guidance on groundwater modeling, proprietary codes are not accepted for geochemical modeling, due to issues with transparency and public accountability (Drever, 2011; Nordstrom, 2012), unless specifically approved by the Division. If the modeler wishes to use a proprietary code, the reliability of the code must be demonstrated using benchmark geochemical problems, such as those described by Dwivedi et al. (2016), or Meyer et al. (2015), with the results of code testing being reported to the Division. Codes can also be tested using relevant examples provided in the code manual, especially those related to AMD, as described in Nordstrom and Nicholson (2017). Once a specific code has been tested, and the testing has been approved by the Division, that code need not be tested again by future users, unless the code has subsequently been modified or the field conditions warrant additional analysis. The Division maintains a listing of tested codes on its website NDEP Regulation Branch Guidance Documents. Also, an operational copy and instruction manual of any proprietary code must be supplied to the Division for use in model review.

It is useful to discriminate between geochemical modeling codes that require approval, and other software programs that do not. Geochemical modeling studies commonly utilize a number of "background" programs such as Microsoft Excel or geographic information systems (GIS). These types of programs are not required to be approved by the Division. Approval is only required for codes that explicitly simulate geochemical reactions or groundwater processes. If a simple spreadsheet model is the methodology, however, then the spreadsheet must be included with the final model report.

Regardless of the code utilized in simulations, the resulting predictions are heavily dependent upon the database(s) used. In terms of geochemical modeling codes, applicable databases would include thermodynamic (e.g., Pitzer, WATEQ4F, MINTEQ Version 4, etc.), kinetic (Palandri and Kharaka, 2004), and databases related to mineral-surface chemistry for sorption (Dzombak and Morel, 1990; Tonkin et al., 2004). These databases contain the thermodynamic and kinetic parameters needed to complete the model computations. The Division does not prescribe which database(s) should be used in geochemical modeling, although the decision must be fully documented and justified in the model report. No specific databases have been determined to be preferred or unacceptable. The most commonly used thermodynamic database in the experience of the Division is MINTEQ, Version 4. A useful description of various databases (as well as modeling codes) is found in Nordstrom (2017). Additionally, modelers should be aware of potential internal inconsistencies in some databases (Nordstrom and Archer, 2003) as well as the potential for some constituents to be controlled by species not included in common thermodynamic databases (Eary and Schafer, 2009; Tempel et al., 2000).

6. Incorporation of Conceptual Processes in Code Implementation and Execution

Following the completion of a robust and defensible site conceptual model, the inputs for geochemical modeling codes are assembled and the code is executed. Simple execution of the code however does not guarantee applicable or useful simulation results. The modeler must consider the myriad of processes that could influence geochemical conditions on the mine site of interest, and how these processes are incorporated into the numerical modeling. All processes identified in the conceptual model must be included in the numerical modeling and subsequent calculations. As noted above, the conceptual model must be reviewed carefully as additional data are collected or the mine plan changes to ensure that all significant processes have been incorporated. The modeler should be familiar with the basic concepts of mass balance, speciation, mass transfer, phases and components. A summary of these concepts can be found in Nordstrom and Nicholson (2017). It is imperative that major assumptions or controls (those that could significantly affect results) be explicitly described, for example, whether a constituent of concern is being precipitated or adsorbed, or whether mineral precipitation is allowed or suppressed. Several of these processes require special attention, as detailed below.

6.1 Equilibrium Assumptions and Calculations

The concept of thermodynamic equilibrium versus kinetics described in section 2 above is one that is commonly misapplied in geochemical models submitted to the Division, generally in reference to mineral precipitation or dissolution. The principles of thermodynamics are used to calculate mineral saturation indices (which indicate whether the mineral in question has a driving force to precipitate or dissolve). Results of thermodynamic calculations however do not incorporate other processes that have the potential to retard precipitation or dissolution, such as kinetic barriers, residence time of water in the reservoir of interest, and various other factors (Nordstrom, 2009b). Ongoing research indicates that biogeochemical pathways can have a significant impact on reaction kinetics (Nordstrom and Campbell, 2014). These factors may mean that although mineral precipitation is thermodynamically favored, precipitation may not necessarily occur. It is important to note that different geochemical modeling codes have varying abilities to handle kinetic constraints. Modelers should remain cognizant of recent advances in modeling codes when instituting kinetic processes.

Beyond the concepts of equilibrium and kinetics, any simulation that predicts mineral saturation or solubility must take into account several site-specific considerations. The first consideration is if the mineral in question has been observed at the site or in other similar environments. Because of the

prevalence of mining in Nevada, other sites may be used as potential analogs for the site in question. Although mineralogic determinations may be difficult on mine sites (due to crystallinity or other concerns), it is imperative to establish how likely it is for a given mineral to exist at a particular mine site, especially if it has not been widely reported in similar environments. Otherwise, the predicted presence of the mineral at the site of interest could be questionable. For example, alunite is generally formed only under acidic conditions or through catalysis (Nordstrom, 2009b); therefore, alunite would be a questionable mineral phase to be predicted in a circumneutral pit lake. Additionally, the environment of formation for the mineral species must be evaluated (e.g., does the mineral generally form through hypogene or supergene processes, or in acidic, basic, oxidizing or reducing conditions?). Finally, a mass balance must be conducted for all mineral equilibrium calculations to ensure that the predictions are physically feasible. For example, does the predicted mass of a particular element precipitated in a pit lake exceed the estimated total supply available in the surrounding country rock and brought in by groundwater? If so, the calculations may contain an error. An additional method to perform mass-balance checks is to include inverse modeling (e.g., Plummer et al., 1983).

Nordstrom (2009b) supplies a robust review of the considerations discussed above and lists common phases likely to occur at mine sites (see Figure 1 of Nordstrom [2009b]). Eary (1999) provides a similar review specifically in reference to thermodynamically probable minerals in pit-lake environments, and Bowell and Parshley (2005) provide a summary of mineralogical analyses from an existing Nevada pit lake. Of utmost importance, as discussed by both Nordstrom (2009b) and Eary (1999), is that mineral equilibrium assumptions be rooted in reality. Eary (1999) specifically notes that further site-specific research is required as to which mineral phases are actually present in pit lakes, as opposed to those simply thermodynamically predicted. This critical consideration is commonly lacking in studies submitted to the Division – even in those that cite Eary (1999) as the source for minerals included in modeling. Modelers must carefully consider many aspects related to mineral equilibrium, as opposed to blindly applying only thermodynamic calculations. Additionally, many models assume that all precipitated mineral phases are removed from the overall system and unavailable for remobilization. Research indicates however that this is commonly not the case and that benthic fluxes may contribute mass to mining-impacted lakes, specifically in the hypolimnion (Martin and Pedersen, 2002). While quantitatively assessing benthic fluxes remains difficult, it may be adequate to provide a screening-level evaluation of these processes. An example screening-level analysis to evaluate benthic fluxes in an existing pit lake could involve coupling an analysis of the concentrations redox sensitive elements throughout the water column with simple diffusion calculations.

Currently there are surprisingly few published observations of minerals precipitated in pit lakes. The following provides a summary of some investigations detailing mineral equilibrium in pit lakes. Fennemore et al. (2000) describe mineralogical analyses of precipitates found in a mature pit lake, where calcite ($CaCO_3$) was noted with some substitution of manganese (Mn), lead (Pb) and strontium (Sr) into the mineral structure. Although the location of the samples was not originally reported by Fennemore et al. (2000), the observations may be useful for Nevada pit lakes. Also in reference to Nevada-specific investigations, Davis (2017) described calcite, barite ($BaSO_4$), gypsum, and aluminum (Al) hydroxides in pit-lake samples collected from Nevada pit lakes. Schafer et al. (2006) conducted batch testing of a synthetic pit-lake solution applicable to a Nevada mine, followed by mineral analysis by XRD and scanning electron microscopy (SEM) of the precipitates. Schafer et al. (2006) found aragonite ($CaCO_3$), calcite, amorphous iron-oxyhydroxides, and minor barite. Although the analyses of Schafer et al. (2006) were applicable to Nevada, it is important to note that the precipitates were not collected from an existing pit lake but from laboratory testing.

The following studies have reported observations of pit-lake mineral precipitates outside of Nevada. Twidwell et al. (2006) report an x-ray diffraction (XRD) analysis of precipitates in the Berkeley pit lake and equilibrium calculations of co-existing water (pH<3). These results indicated the coprecipitation of jarosite, $KFe^{3+}_3(SO_4)_2(OH)_6$, and gypsum, $CaSO_4 \cdot 2H_2O$, in pit-lake waters. Santofimia et al. (2015) provide a detailed analysis of the mineralogy of precipitates collected from an acidic pit lake in Spain, and report evidence of schwertmannite precipitation. Carabaello et al. (2013) (although not specifically focused on pit lakes) found that schwertmannite is a common precipitate in acid mine waters and likely the dominant mineral whenever dissolved iron oxidizes; however this mineral is commonly difficult to characterize and has a variable composition.

While the conclusions of Santofimia et al. (2015) and Twidwell et al. (2006) may not be directly applicable to Nevada pit lakes due to the variations in geologic, hydrologic, and geochemical characteristics of the site, the overall methodologies should be applied to more Nevada pit lakes to determine reasonable phases for use in geochemical models. Santofimia et al. (2015) and Schafer et al. (2006) also provide examples of a thorough review of thermodynamic data, which should be common practice for geochemical modeling.

6.2 Empirical Testing and Scaling Factors

Geochemical models commonly use empirical testing to evaluate the release of constituents from waste rock and open pit highwalls. These tests may include HCTs (Maest and Nordstrom, 2017; Parbhakar-Fox and Lottermoser, 2015) or field-scale testing (Plante et al., 2014). There are a variety of factors that may make solute release rates derived in the testing different from the field rates. Empirical release rates are therefore commonly scaled using a simple scaling factor. A summary of scaling factors provided by Kempton (2012) provides a range of factors for a variety of processes including moisture content, fragment size, temperature, water contact, and oxygen concentration. Kempton (2012) notes that several of these processes (and therefore scaling factors) are linked to one another. In addition to the overview provided by Kempton (2012), a number of site-specific studies have evaluated scaling factors for a wide variety of constituents and environments.

Kirchner and Mattson (2015) calculated bulk scaling factors based on field and lab testing from two sites. These indicated the range of bulk scaling factors (i.e., with scaling from the aforementioned processes all included) that could be applied to different geochemical species. In a study of an ore stockpile that had been subjected to weathering for 52 years, Bornhorst and Logsdon (2016) concluded that field-scale weathering may be difficult to scale to HCTs without long-term tests, and that HCTs may not reach steady-state as rapidly as is commonly assumed. Bornhorst and Logsdon (2016) showed that solute concentrations draining from the field-scale ore pile were less than would be predicted using analytical models, However, the investigation was unable to quantify the amount of leaching that the exposed ore stockpile had undergone over the weathering period. Therefore, the mass of solutes removed from the system prior to the start of observation cannot be known and the temporal evolution of solute release rates cannot be quantified. In mechanistic studies of solute release in the field and the laboratory Evans and Banwart (2006) and Evans et al. (2006) found that field and laboratory release rates could differ by orders of magnitude, and that the type of laboratory method used (i.e., column or batch tests) was important. Evans et al. (2006) went on to recommend that a coupled and multi-disciplinary approach including mineralogical and hydrologic analyses should be used for mine-waste characterization. These suggestions are similar to those of Parbhakar-Fox and Lottermoser (2015).

These studies all suggest that geochemical models should carefully consider the scaling factors utilized, given the wide range in reported bulk scaling factors. Also, Division experience at a number of sites has shown seepage from waste rock facilities or other repositories may in some cases be

extremely concentrated when compared to HCTs of similar material. For these reasons it is important to consider site-specific factors such as grain size, mineralogy, mineral morphology, paragenesis, climate, hydrology (flow paths and residence times), and others in establishing scaling factors and solute-release rates used in modeling. At this time the Division is not requiring the use of any specific scaling factors in modeling, however, the model report must discuss any scaling factors utilized and how they influence the study.

6.3 Limnological Character

Another important consideration when implementing numerical modeling of pit lakes is limnology, as briefly discussed above in reference to gas equilibria. Pit lakes may be complex environments with several distinct hydrogeochemical layers. These layers may or may not participate in seasonal mixing. There are several modeling codes that incorporate the various limnologic, geochemical, and hydrologic processes likely to occur in pit lakes, specifically CE-QUAL-W2 (Wells and Berger, 2010) and DYRESM. Castendyk et al. (2015) provides a review of these codes as well as limnologic characteristics of pit lakes in general. In addition to these hydrodynamic codes, PITLAKQ (Pit Lake Q documentation page) is a Python package specifically designed for simulating the coupled hydrodynamics and geochemistry of pit lakes. The aforementioned codes generally require significant data inputs and parameterization, however, and have not been widely used in Division permitting actions in the past. Because of the potential geochemical significance of limnology, the Division may require specific limnologic modeling based on scientific and engineering judgment. Regardless of whether specific limnologic modeling is required, each pit-lake modeling report must address potential stratification and turnover of the pit lake in question, through reasonable qualitative or quantitative means to evaluate the range of possible geochemical outcomes.

6.4 Model Period and Discretization

Two critical components in model execution are the total period of time considered in the model and the temporal and spatial (in the case of transport simulations) discretization. In determining the period of prediction for pit-lake models a number of aspects should be considered including the predicted water balance, the geochemistry of inputs to the pit lake, and the predicted hydrologic character. Differing inputs to these key parameters may necessitate differing prediction interval lengths (see discussion in Schafer and Eary [2009]). The Division makes no specific requirements as to the prediction interval, except that a model must be run until the pit lake, or groundwater as applicable, is hydrogeochemically stabilized, or nearly so (or is repetitively cycling through similar hydrogeochemical states). Overall, the period of prediction must be long enough to adequately inform the permanent closure of the pit lake and/or groundwater system. The reasoning behind the period of prediction must be justified in the modeling report.

The temporal discretization utilized in modeling is important both for geochemical models of pit lakes and groundwater systems. For pit-lake models, the Division has noted a tendency for submitted reports to utilize very large time steps (the length of time between geochemical calculations), on the order of many years in some cases. Large time steps such as these ignore the rapid geochemical changes that have been observed in existing pit lakes. Division experience indicates that concentrations of some constituents of interest, including arsenic (As), copper (Cu), and iron, may change over multiple orders of magnitude in a few years or less. Therefore, pit-lake predictive models should use the finest temporal discretization that is reasonably possible while not becoming computationally impractical. Generally, pit-lake model time steps should correspond to those utilized in the groundwater flow model that governs the water balance (again while not becoming computationally impractical). Time steps should not exceed 5 years, and 1-year time steps are optimal

in many instances. For lakes in which detailed limnological predictions are warranted, shorter time steps (e.g., weekly or monthly) may be required to assess stratification and mixing. Temporal discretization is also a key factor in solute-transport modeling (Konikow, 2011), which is one type of model that could incorporate geochemical processes. Solute-transport modeling should also utilize the finest reasonable temporal discretization.

Finally, the spatial discretization of solute-transport models, and the groundwater flow models on which they rely, must be considered in analyses. Refer to the Division's Guidance for Hydrogeologic Groundwater Flow Modeling for specific spatial discretization requirements. Spatial discretization is also important in coupled limnologic/geochemical models of pit lakes (in this instance the spatial discretization represents the vertical dimension in the water column). If required, such hydrodynamic models should use a vertical discretization appropriate for the site.

7. Sub-Models

The use of sub-models has the potential to increase the overall predictive uncertainty of geochemical models. This concept was discussed above in regard to incorporating groundwater flow model results into geochemical models. Sub-models are codes or other means of prediction that are used to evaluate a particular reaction or process. The results of these sub-models are then used as input variables or parameters to the overall geochemical model. Sub-models are also discussed in Bredehoeft (2003), where they are termed "cascading models." As described by Bredehoeft (2003) sub-models each contain some degree of uncertainty, and the linking of models into a cascade results in calibration problems with the uncertainty of one model being incorporated into the predictions of another, and an overall increase in the predictive uncertainty of the final model results. Sub-models may be necessary in some instances however to place bounds on processes which could not be quantified rigorously without the use of a sub-model. In addition to error and uncertainty cascades, sub-models are also likely limited by our actual understanding of the processes at work. This concern is described by Drever (2011), wherein the issue is raised that our ability to create numerical codes has outpaced our ability to understand physical processes and to collect data to compare to the predictions of numerical codes. Geochemical models that employ sub-models must include an evaluation of the contribution of the sub-model to the overall model uncertainty. Stochastic modeling methods offer another method of assessing model uncertainty, as discussed further in section 8 below.

7.1 Sulfide Oxidation and Reactive Rock Mass

One example of a critical sub-model in geochemical modeling reports submitted to the Division is a model that predicts the extent of sulfide oxidation, typically pyrite, in the domain of interest. Pyrite oxidation is a complex process that is controlled by a variety of factors (Jerz and Rimstidt, 2004; Williamson and Rimstidt, 1994), and this process is an important control on the composition of waters impacted by mining (Nordstrom, 2011). There are a variety of methods to simulate pyrite oxidation, including those summarized by Davis and Ritchie (1986; 1987), Davis et al. (1986), Fennemore et al. (1998), Sunkavalli et al. (2013), and Wunderly et al. (1996). The mathematical formulation and prediction methods of the sulfide oxidation process are beyond the scope of this guidance, but modelers are encouraged to consult the representative literature prior to modeling.

In practice, the goal of most sulfide-oxidation modeling is to determine the mass of reactive rock that can contribute solutes to mine-impacted waters. An alternative method to sulfide-oxidation modeling for calculating the mass of reactive wall rock is to assume a uniform fracture depth and density. Although there are some studies of fracture networks in environments similar to Nevada mines (e.g., Case and Kelsall, 1987; Chakraborty and Jethwa, 1994; McCloskey et al., 2003; 2005; Siskind and Fumanti, 1974), these studies cannot be applied to all sites without accounting for site-specific

attributes such as lithology, primary porosity and permeability, blasting method (frequency, spacing, magnitude), structural complexity and variability throughout the mine, and various other factors. Also, the method of assuming a temporally static reactive wall rock mass does not account for the time period over which the wall rock is oxidized.

The main issue with either of the methods of estimating reactive rock mass is that these predictions commonly underestimate the loading of solutes to pit lakes, in some instances by up to a factor of 10 (Kempton and Atkins, 2009). These under-predictions of solute loading appear to be at least partially related to under-prediction of reactive wall rock mass. Estimates of reactive wall rock thicknesses reported to the Division (which can be related to mass using the density of the material and the three-dimensional geometry of the pit) are commonly on the order of 3-10 feet. These estimates are in contrast to observational evidence from Nevada mine sites summarized in Kempton and Atkins (2009), where appreciable O_2 concentrations were reported at depths up to 45 feet in highwalls. Although O_2 concentration is not a direct measurement of sulfide reactivity, the two are generally positively correlated, see Williamson and Rimstidt (1994). Similar to the results presented in Kempton and Atkins (2009), McCloskey et al. (2003; 2005) found evidence of blast-induced fracturing up to approximately 50 feet deep in wall rock of an open pit hosted by sedimentary rock in Montana. The findings of Kempton and Atkins (2009) and McCloskey et al (2003; 2005) therefore indicate that reactive wall rock mass may be significantly underestimated in many studies. Under-prediction of solute loading related to pyrite oxidation could also be caused by the assumption in many models that all pyrite oxidation and metal mobilization ceases when wall rocks are submerged, which is not necessarily the case in some pit lakes (Gammons, 2009). It also important to note that controlling characteristics may vary widely from site to site, and potentially from fracture to fracture. Because the thickness of reactive zones is highly variable and site-specific, a sensitivity analysis is required to estimate the possible range of solute concentrations entering the pit from the reactive rock mass (in applicable pit-lake studies).

Several other processes also impact reaction rates including grain size, morphology, and paragenetic relations of ore and gangue minerals. These factors impact reaction rates in ways that may be unclear without detailed analysis. Petrographic examination of mineralogic relationships may be required to determine the extent of reactivity in the rock masses.

The above discussion is not meant to preclude sulfide-oxidation modeling from being incorporated into geochemical studies, but only to highlight that the modeling, or any other method of solute-release estimation, must incorporate site-specific characteristics and must include an uncertainty analysis. In the future, more mine sites should incorporate testing to more accurately determine wall rock oxidation depths, in-situ oxidation rates, and metal release (Kempton and Atkins, 2009; Kempton et al., 2009). In some instances, the Division has determined that these types of assessments will be required in the applicable WPCP. Additionally, all assessments of solute loading should incorporate an analysis of the underlying geochemical reactions occurring in the applicable geochemical testing, as these can be informative for both the conceptual and numerical models of solute-release at the site (Kempton et al., 2009; Maest and Nordstrom, 2017).

8. Sensitivity and Uncertainty Analyses in Geochemical Predictions

Geochemical modeling calculations contain inherent uncertainty. Types of uncertainty include uncertainty in the value of input parameters (intrinsic error) and uncertainty caused by incorrect model structure or lack of applicability of the model to the site (epistemic error). Intrinsic errors may be due to inaccurate thermodynamic data or analytical errors in input water chemistry data, and epistemic errors may be caused by simplification of the distribution of minerals in the environment, assumptions of equilibrium, and the length of the empirical dataset applicable to the site. Because of these

uncertainties, geochemical models must assess potential error in their predictions. One of the most common methods of assessing uncertainty is a sensitivity analysis (Alpers and Nordstrom, 1999). A more mathematically robust method to evaluate uncertainty and potential outcomes uses Monte Carlo methods or other probabilistic or stochastic analyses (Drever, 2011; Kempton et al., 1997; Lapakko, 2015; Lauzon et al., 2011).

8.1 Sensitivity Analysis

Sensitivity analysis is the process of systematically altering model input values to examine the impact on simulation results. Sensitivity analysis has been utilized in various ways in geochemical modeling of pit lakes (Castendyk and Webster-Brown, 2007a; 2007b; Davis et al., 2006), mining-contaminated groundwater (Glynn and Brown, 2012), and other environments as summarized in Nordstrom and Campbell (2014).

The physical and chemical parameters or inputs that should be considered for sensitivity analysis vary according to the needs of the model and the environment to be simulated. For example, mineral precipitation may be thermodynamically predicted but may not occur for a variety of reasons (Nordstrom, 2009b). Conducting a sensitivity analysis on mineral solubility is therefore an effective means for determining the different solution chemistries that would result from two end-member situations, one in which all predicted mineral precipitation is allowed to occur and one in which the precipitation of one or all minerals is suppressed. Neither of these simulations is necessarily what will occur in reality, but they provide quantitative bounds to the predictions, which is one of the major goals of sensitivity analysis (Drever, 2011). The sensitivity analysis with all mineral precipitation suppressed also provides the appropriate input chemistry for ecological risk assessments (ERAs) directed at calculating risk to terrestrial and avian species from ingesting both dissolved and suspended constituents from a pit lake (see Section 10 below).

Other processes that could be considered for sensitivity analysis include sorption reactions, gas exchange, pit-lake turnover, climatic factors (e.g., evaporation, highwall runoff, etc.), fracture depth and density near the pit walls, particle size and reactivity for pit backfill models, groundwater flow rates and influent geochemistry, and effective porosity (for solute fate and transport models). Not all of these parameters are required to be included in sensitivity analyses for all geochemical models, as the parameters included should be site-specific and focused on the areas of greatest uncertainty in the input data. The one required sensitivity analysis for all submitted pit-lake geochemical models is the suppression of all mineral precipitation as described above. Alternatively, mineral equilibrium may be evaluated in a stochastic analysis. The results of this sensitivity or stochastic analysis must be explicitly reported in geochemical modeling documents and evaluated via an ecological risk assessment (and/or elimination of exposure pathway[s]) if a Division Profile 3 reference value exceedance is predicted. Additionally, most pit-lake models should consider completing a sensitivity analysis on sorption reactions (e.g., by changing surface charge or available sorption sites). This is because sorption reactions appear to be commonly over-predicted in pit-lake models submitted to the Division.

It is important to note that some sensitivity analyses will inevitably result in the sensitivity model failing to calibrate (if sufficient data are available for calibration). A lack of calibration is still an informative result of the analysis, provided that the failure to calibrate is stated in the model report (and provided that the base-case model is calibrated), given that a failure to calibrate indicates the degree to which observed conditions agree or disagree with the specific parameter set utilized. However, if sensitivity analysis models do calibrate, they provide additional information regarding the wide range of input values that can reproduce the observed conditions.

8.2 Probabilistic Analysis

In addition to sensitivity analyses, which essentially produce rough estimates of alternative deterministic outcomes (while not necessarily maintaining model calibration), incorporation of stochastic modeling approaches allows for a broader and more rigorous understanding of the quantitative probability of various outcomes. A variety of different parameters could be considered for inclusion in stochastic approaches applied to geochemical modeling including climatic parameters, variability in groundwater composition, solute release from waste rock and highwalls, and mineral precipitation. Some stochastic geochemical modeling codes are freely available (e.g., De Lucia and Kuhn, 2013; McGraw and Hershey, 2016), although advanced code capability still likely requires further development. To date, the Division has not specified a particular confidence interval for reporting the results of probabilistic models, although the 95 percent confidence interval is widely used in other fields of application for statistical analysis.

The Division recommends the use of probabilistic modeling approaches in geochemical models when applicable dependent upon site-specific considerations. If a probabilistic model that incorporates sufficient complexity in the conceptual model is computationally practical and not cost-prohibitive, such an approach may provide a superior predictive tool. Of specific importance to this discussion is the requirement from section 3 above that, regardless of what method is used, the conceptual model should be the simplest description of the system possible that includes all significant processes while still containing enough complexity to represent important system behavior. Comparative studies of probabilistic models and deterministic models may be helpful in the near term to evaluate the practicality and reliability of probabilistic models for Nevada mines.

9. Geochemical Model Evaluation

Unlike groundwater flow models, which are subject to rigorous assessment of how well predictions emulate observations (commonly via both steady-state and transient calibration to observed fluxes and groundwater elevations), geochemical models are not commonly assessed for predictive agreement. One of the primary reasons for this is that many geochemical models are created to predict future conditions for which no known comparison point currently exists (although analog sites may be available). This is not the case for all geochemical models however, as there are examples of predictive studies at sites with currently existing pit lakes (Davis et al., 2006; Hanna et al., 2016; Savage et al., 2009; Tempel et al., 2000). Although some analyses of geochemical model agreement have been completed, there is currently no widely-used method to evaluate geochemical predictions mathematically and quantitatively. Therefore, in instances where the geochemistry of existing pit lakes has been predicted into the future, geochemical model evaluation has tended to be qualitative in nature.

All model reports must contain some prediction assessment, be it a comparison to observed regional groundwater or surface water quality, or to existing pit lakes in similar geochemical, hydrologic and climatic environments. Modelers should also be aware of the International Network for Acid Prevention (INAP) pit lakes database (Johnson and Castendyk, 2012; INAP Pit Lakes Database). The INAP pit lakes database contains analytical data from pit lakes around the world (including Nevada) in different geologic environments, hydrologic regimes, and ore deposit types. The INAP pit lakes database could therefore prove useful in geochemical model evaluation. Use of analogs from the INAP pit lakes database can be very helpful, but the burden is on the modeler to show that the proposed open pit and consequent pit lake will be similar enough in lithology, mineralization, structure, climate, hydrogeology, and geochemical processes to be comparable to the selected analog. In addition, Eary and Schafer (2009) contains a summary of the various factors that should be considered during model evaluation.

The reliability of future predictions for existing pit lakes is related to the availability of applicable field data, and it is ideal in modeling to be able to perform a history match (Bredehoeft, 2005). When the historical data are not available (i.e., because no pit lake exists), predictive modeling is severely limited in its ability to provide certainty, but evaluation of various potential scenarios can be helpful. Scenario predictions are educated, non-unique guesses. The range of scenario possibilities should be presented with justification for selection of each scenario and discussion of the range of uncertainty in that particular outcome. An example of the difficulty in predicting recharge rates from well-calibrated models is described by Moeck et al. (2018) who show how different conditions for the calibration period and the independent historical test period adds substantial uncertainty to the model.

Although there are no strictly quantitative established methods to evaluate deterministic geochemical modeling predictions, there are several basic methods to evaluate simulation results. First, all geochemical solutions must display mass balance as described above. A solution that does not obey mass balance represents a system that cannot exist as simulated. In practice, mass-balance calculations for geochemical models submitted to the Division may be difficult to compute rigorously as a secondary check because the system simulated is generally not closed (i.e., there are processes that remove mass from the aqueous system that are difficult to compute by hand).

Second, all predictions should be checked for charge balance. In analytical procedures, acceptable charge-balance error (CBE) may be greater than 10% (Appelo and Postma, 2005). All model results submitted to the Division should display similar or better charge balance, or else the solution would be questionable. Evaluating mass balance and charge balance requires, at a minimum, that all major cations and anions, pH, and electrical conductivity are measured. The method of McCleskey et al. (2011) can be used to evaluate the direction of the charge imbalance (and determine whether cations or anions need adjusting), and the conductivity imbalance. Using these two measures, the dominant cation or anion concentrations can be adjusted to meet acceptable Division CBE.

An additional consideration that should be made regarding geochemical model evaluation, even in the case of predictions that compare favorably with observations, is that geochemical models are non-unique. Non-uniqueness means that there are other combinations of variables that satisfy the same basic constraints set by the modeler. As a result, models may appear to represent reality, when in fact an alternative conceptual model or different numerical model inputs could achieve similar agreement with observations (Bethke, 1992; Nordstrom, 2012).

10. Geochemical Model Reporting

Ultimately, the methods and results of geochemical models must be reported in a way that promotes transparency and an understanding of the model assumptions, uncertainties, and predictions. Among other considerations, this means that the model report must be written in a technically rigorous but simple and straight-forward manner that is understandable to scientifically-inclined non-modelers (Nordstrom, 2012).

Unlike groundwater flow models, for which there are a variety of widely-accepted resources discussing the appropriate contents and detail of model reports (e.g., Reilly and Harbaugh, 2004), no guidance related to the structure and content of geochemical model reports is currently available in the literature. One aspect that is somewhat unique to geochemical modeling as compared to groundwater flow modeling is the lower degree of reproducibility of the results. For groundwater modeling, the laws that control groundwater flow contain fewer degrees of freedom than the laws governing geochemical reactions. This is not to say that groundwater flow lacks complexity, but it can generally be simulated with greater reproducibility and agreement between observations and simulations than geochemical reactions. Therefore, it is important for geochemical modeling reports

to indicate the sources of uncertainty in their predictions and conclusions (Drever, 2011). It is also desirable for the magnitude of the uncertainty to be described (e.g., using standard deviation or other statistical measures).

Specific requirements and considerations for model reporting to the Division are described in Attachment A. This list is not meant to be overly prescriptive; each item included in Attachment A need not appear with the exact same title in modeling reports, or in the same order. Additionally some reports may include sections not listed in Attachment A. However, outright omission of any items applicable to the specific project included in Attachment A will likely result in the geochemical model report being deemed incomplete. The template that the Division will use to review geochemical models is also supplied in Attachment A. This template may serve as a review record for each geochemical model submitted to the Division.

Additionally, an important aspect of model reporting is that pit lake predictions that include mineral precipitation cannot be used as inputs to ERAs. In contrast to geochemical models intended to predict potential impacts to groundwater quality, ERAs are aimed at evaluating ecological risk due to ingestion of pit lake water (and other exposure pathways). Therefore, the predictions used in ERAs must use geochemical model results with mineral precipitation suppressed, as terrestrial or avian life could reasonably be expected to ingest both dissolved and suspended solids in pit-lake waters, including precipitated minerals in the upper water column. The only exception to this is when site-specific data (from the pit lake under investigation) are available to clearly document that bioavailability of certain constituents of concern is less than the total available mass of each given constituent. By using model predictions with mineral precipitation suppressed ERAs will be environmentally conservative, in that these model predictions will likely result in slight over-prediction of the bioavailability of constituents of concern.

11. Conclusion

The environmental geochemistry of mine sites is often complex, requiring geochemical models of varying sophistication. In some instances the Division requires the submittal of geochemical models to assess the potential for groundwater degradation, in accordance with NAC 445A.424, or the potential for adverse health effects from pit lakes pursuant to NAC 445A.429. The predictions or analyses included in these models serve as a tool for creating an understanding of what has occurred at a mine site in the past, and what may occur in the future. These modeling studies may also be used by other interested parties in a variety of other decision-making avenues such as mining feasibility unrelated to regulatory authority. In addition, model results must be understandable to non-modelers (Nordstrom, 2012).

The range of conditions, both best- and worst-case scenarios, should be reported, because of the large uncertainties inherent in these calculations. If a probabilistic model that incorporates sufficient complexity in the conceptual model is computationally practical and not cost-prohibitive, such an approach should be considered to constrain the model predictions to a reasonable confidence interval. Some of the most well-bounded geochemical model predictions will be based on a well characterized and well documented evolution of an existing pit lake system. Comparing the predicted water quality with monitoring data over time and examining the modeled and monitored results to understand why previous predictions did not compare well with observations will likely create a more reliable pit-lake model. With enough well-characterized and modeled pit lakes over a substantial period of time, a database of pit-lake analogs will also gradually help to improve predictive capabilities.

Geochemical models are commonly linked to other predictive models, most notably groundwater flow models. In these instances, the geochemical model should rely on a Division-approved

underlying groundwater flow model, and the conceptual models applied to both should be consistent. The reader is referred to the Division's Guidance Document for Hydrogeologic Groundwater Flow Modeling at Mine Sites for further details on groundwater modeling.

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Attachment A: NDEP-BMRR Geochemical Model Review and Report Checklist

Part 1 – Report Information

Project Name:

Permit #:

Code:

Part 2 – Contents of Report

Text Sections

Report Section:	Response: (Y/N)	Notes:
1. Title, project name, permit number, preparer, and date		
2. Executive summary		
3. Site background		
4. Study objectives and application/need for geochemical modeling		
a. Application of modeling methods, to include a consideration of stochastic versus deterministic approaches		
b. Numerical code(s) used, and reasoning for application		
i. Databases used (thermodynamic, kinetic, etc.), and any modifications made		
c. Performance assessment of previous model iteration (if applicable)		
5. Description of system of interest		
a. Geologic framework		
i. Mineralogic character of ore deposit and host rocks, including discussion of hydrothermal alteration and associated geochemical changes (if applicable)		
d. Current and past hydraulic and geochemical conditions		
6. Description of the conceptual model and applicability to the site		
7. Description of the numerical model (if applicable)		

Report Section:	Response: (Y/N)	Notes:
a. How the conceptual model was translated to the numerical model		
8. Description of boundary conditions (gases, solid phases, etc.)		
9. Summary of any previous geochemical modeling performed at the site (if applicable)		
10. Summary of predictions (if applicable)		
11. Summary of sensitivity/uncertainty analyses (if applicable)		
a. Quantitative comparisons of results of the base-case model with sensitivity analyses/stochastic predictions, and discussion of the likelihood of the alternative scenarios, and how these likely scenarios affect long-term management/outcomes		
b. Monte Carlo or other stochastic methods used?		
c. Was calibration maintained or not?		
12. Conclusions of the study		
13. Appendices		
a. Results of applicable geochemical testing if applicable (e.g., ABA, HCT, etc.), reported in accessible numerical format (e.g., CSV, Excel, etc.)		
b. Model input files		

Figures

Report Figure:	Response: (Y/N)	Notes:
1. Geologic map and cross section(s), with scale, north arrow, and legend, as applicable		
2. Locations of geochemical parameter measurement points (i.e., monitoring wells, stream monitoring stations, etc.)		
3. Sample locations for geochemical testing in plan-view and cross section		
4. Any prevalent geochemical testing results (if applicable)		

Report Figure:	Response: (Y/N)	Notes:
5. Calibration and predictive results of any applicable sub-models (e.g., pyrite oxidation, etc.; if applicable)		
6. Predicted concentrations of all applicable geochemical parameters over time, compared to the appropriate Division reference values (e.g., Division Profile 1 for groundwater or Division Profile 3 for pit lakes)		

Tables

Report Table:	Response: (Y/N)	Notes:
1. Climatologic characteristics		
2. Proportions of various lithologies and hydrothermal alteration styles exposed in the ultimate pit surface (UPS), if applicable		
3. Statistical summary of site groundwater chemistry, to include all applicable parameters (e.g., Division Profile 1 or Division Profile 3) and appropriate statistical measures (e.g., mean, median, maximum, minimum, and number of analyses)		
4. All input parameter values to applicable sub-models (e.g., D_1, D_2, sulfide contents, etc. for pyrite oxidation modeling)		
5. Pit-lake water budget(s) including quantities of inflow and outflow to different hydrogeologic units (if applicable)		
6. Mineral(s) included in equilibrium calculations (if applicable)		
7. Predicted concentrations of all applicable geochemical parameters over time, compared to the appropriate Division reference values (e.g., Division Profile 1 for groundwater or Division Profile 3 for pit lakes)		
8. Parameter values used in sensitivity or stochastic analyses		

Part 3 – Model Review

General Considerations

Consideration:	Response: (Y/N)	Notes:
1. Are the objectives of the study and the level of confidence clearly stated?		
2. Are the uncertainties associated with the model clearly stated?		
3. Are all required sections of the report present (including figures and tables)?		

Modeling Approaches

Consideration:	Response: (Y/N)	Notes:
1. Is the overall approach (inverse model, predictive model, etc.) clearly stated and appropriate?		

Conceptual Model

Consideration:	Response: (Y/N)	Notes:
1. Is the conceptual model reasonable and not unnecessarily complex for the system under investigation?		
2. Are all relevant physical processes and features within the model domain incorporated into the conceptual model?		
3. Is the conceptual model supported by representative data?		
4. Are there alternate conceptual models that could be reasonably applied?		
5. Has a reasonable methodology been applied to estimate scaling factors from empirical testing (if applicable)?		

Model Discretization

Consideration:	Response: (Y/N)	Notes:
1. Is the temporal and spatial discretization fine enough to represent potentially important changes in chemistry over time and distance?		

Boundary Conditions

Consideration:	Response: (Y/N)	Notes:
1. Are geochemical boundary conditions (e.g., gas partial pressures, mineral phases, concentration boundaries, etc.) reasonable for the objectives of the study?		
2. Do the boundary conditions of the model overly constrain the model results so that the calibration is insensitive and the predictions are not realistic?		

Uncertainty and Sensitivity Analysis

Consideration:	Response: (Y/N)	Notes:
1. Has the sensitivity or stochastic analysis included enough potential controlling factors to encompass possible conditions on the site?		
2. If the model report is for a pit lake, has a sensitivity analysis been conducted with all mineral precipitation suppressed (or a similar analysis been performed)?		
3. Are the sources of uncertainty discussed?		
4. Has some quantitative or qualitative assessment of uncertainty been made?		
5. Have suggestions to reduce uncertainty in future models been included?		
6. Has a probabilistic approach been utilized?		

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