Use of water quality models for design and evaluation of pit lakes

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Abstract

This paper provides an overview of water quality model approaches that can be applied to pit lakes. Water quality models are tools that can be used from the early stages of mine development to design and promote waterbodies that will meet end-use objectives. Models assist in planning the filling period of pit lakes, up to initial release into the receiving aquatic environment, and beyond into the post-closure phase. This paper first describes the application of water quality models to pit lakes, including typical implementation steps to follow, the possible spatial discretization of the waterbodies with the models, the typical hydrodynamic water quality components assessed with the models, and the geochemical analyses usually undertaken to support the modelling effort. The challenges and limitations of water quality models are then presented, notably data sources, sensitivity and uncertainty. This paper concludes with a case study of a multi-phase water quality model being developed for pit lakes in the oil sands region of Northern Alberta, Canada.

1 Introduction

The environmental and engineering studies that are typically required for permitting, mine planning and mine closure require an estimation of water quality during all stages of life of mine. Pit lakes are a key component of mine closure and aquatic reclamation for many existing and planned open pit mines. As ultimate discharge points from a reclaimed mine, the design and evaluation of these waterbodies is essential to the overall success of the mine closure plan.

Forecasting and evaluating pit lake water quality poses a challenge because of the variety of geological environments, ore deposits and mine waste types that may be encountered. Furthermore, many planned pit lakes will not be constructed until decades after the initial mine design. Due to these challenges, the most practical way to obtain estimates of pit lake water quality is generally through predictive modelling. Water quality modelling can be completed as part of the design stage for the mine development, with increasing model complexity according to the level of design details.

Development of a conceptual pit lake model (e.g., Figure 1) is a key component of the preliminary design phase to ensure that an appropriate set of field data is collected. Based on the physical dimensions, geology and catchment area of the open pit, inflow rates and chemistries may be characterized for natural and reclaimed areas within the catchment area. Model inputs may be estimated from geochemical testing, baseline sampling, proxy systems or other literature sources. Mechanistic models can then be used with this information to simulate water quality under the anticipated closure scenarios defined in the conceptual model.

This paper discusses the use of models for predicting water quality in pit lakes. The discussion covers: basic steps in a modelling application; model frameworks; variables of interest; limitations; uncertainties and sensitivities. It concludes with a case study of a recent pit lake model being developed for the Cumulative Environmental Management Association (CEMA). The case study describes a multi-phase lake, sediment and gas modelling software that has been developed for use by oil sands mining operators for pit lake planning, assessment and design.
2 Modelling framework

2.1 Why model?
One objective in developing a mine closure plan is to identify and implement mitigation strategies that may be required to achieve long-term sustainability and to minimize aquatic impacts on receiving streams. For many open pit mines, pit closure is accomplished by actively or passively filling the final pit with water to create a pit lake (Castro and Moore, 2000). It is generally in the best interests of both operators and regional stakeholders to design and construct a “walk away” lake if possible that meets end-use goals without the need for perpetual, active treatment. Depending on the jurisdiction and type of mine, pit lakes may be expected to have water quality that is within the range of natural levels of regional lakes, meet water quality guidelines for the protection of aquatic life and human health and/or provide habitat for valued ecosystem components such as sport fish.

From the early stages of the mining development, several years and often decades may pass before the pit lakes are developed in the mine area. However, assessment of pit lake water quality is required for each stage of the mining development to evaluate the adequacy of the proposed closure and reclamation plans. Water quality modelling allows such an assessment in the early stage of the mining development. As the closure period approaches, modelling will provide support for the detailed design of pit lakes. In the later stages, modelling can be used to predict long-term outcomes of the post-closure pit lake with increasing levels of confidence.

2.2 Modelling steps
General modelling advice is given below, following the themes laid out in more detailed guidance documents (e.g., Anderson and Woessner, 1992; Castendyk and Eary, 2009; Kuipers et al., 2006; Maest et al., 2005; USEPA, 2002; USEPA, 2009). In addition, most model software packages have very detailed user manuals that lay out the steps for setting up modelling applications. A common theme of these guidance documents is the general workflow that should be followed when modelling, regardless of stage or complexity. Although there are subtle differences in the recommendations of the documents listed above, modelling of pit lakes should follow these fundamental steps:

- **Define the objectives for modelling.** All subsequent modelling tasks should be completed with a clear aim of meeting these objectives. Among other things, the objectives will determine the type of modelling that is required. For example, sensitivity analyses can be completed to determine key driving variables, without putting too much weight on absolute values. In contrast, stochastic modelling can be used for risk assessment modelling, where each output value or consequence is attached to a frequency or likelihood of occurrence.

- **Develop a conceptual model.** Define the inputs to the lake and physical characteristics of the system. Describe the key processes that will influence the possible water quality of the pit lake. Process diagrams or schematics can be helpful to visualize the relevant physical and chemical processes in the conceptual model, as shown in Figure 1 and Section 4.

- **Select the appropriate model software.** The model software selection will be a function of physical and chemical factors that could influence pit lake chemistry, model objectives, the conceptual model and available data. Consider domain, dimensionality, functionality, input data requirements, reliability and computational effort. More than one model software package may be necessary to simulate all key processes. For example, it may be necessary to employ a groundwater model, a geochemical model, a hydrodynamic model and a water quality model. If an appropriate model is not available that fits the conceptual model, development or modification of an existing model may be necessary.

- **Establish key output metrics.** Examples of output metrics are water concentration, turnover rate, outflow rate or water level. The model must be able to predict and report key metrics.
• **Establish screening criteria in advance of model runs.** Examples of screening criteria are applicable regional water quality guidelines, concentrations of natural lakes and aquatic health benchmarks. Choosing the appropriate screening criteria to meet the objectives of the modelling will allow the modeller to view preliminary results in context, and to adjust assumptions and inputs throughout the modelling exercise.

• **Gather input data.** Compile and assemble all necessary input data for the selected model. Data could include surface water and groundwater flow, surface water and groundwater chemistry, geochemical characterization of the main rock types that will be exposed in the pit walls, climate data or analogue data from comparable sites. In many cases, the pit lake in question may be decades from construction, so input data may be unavailable. If data are not available, the modelling exercise may need to be delayed while data are collected, or a simpler model may need to be developed. Methods for dealing with lack of data will vary, depending on the stage of modelling and objectives, as discussed in the following subsections.

• **Implement quality assurance procedures.** Screen input data for outliers, unit conversion errors, analytical or instrument malfunctions and other perennial pitfalls. An important consideration in geochemical models is charge balance of the input solutions; as a general best practise, input solutions should be charge-balanced prior model simulations with geochemical speciation software. Another useful procedure is to view graphs of all model input time-series along with the raw data used to generate the formatted inputs. Additionally, graphing inputs and outputs on the same figure can be done to compare the model software response with the expectations of the conceptual model. For example, graphing meteorological input data next to simulated water temperature can indicate whether a model software is responding appropriately.

• **Calibrate and validate, if possible.** If the lake is in the filling stage, compare model predictions with observed data. If a future lake has not been filled, validate and refine inputs to the model whenever information becomes available. Validation can also be done at a smaller scale using bench-top physical models, or by evaluating surrogate systems such as pit lakes with similar characteristics.

• **Conduct an uncertainty or sensitivity analysis.** Quantify confidence limits and identify key sensitivities, as discussed in the following subsections.

• **Compare results to criteria.** If the model predicts concentrations that are less than the screening criteria, the modelling exercise may be finished. If not, changes to the closure drainage plan or additional mitigation may be required.

• **Continue improvement loops.** Once changes have been made to the closure plan, the updates should be fed back into the process and modelling can be resumed. Depending on the type and magnitude of change, the feedback may warrant updates to the conceptual model, additional data collection and revisiting the model software selection.

• **Conduct a post audit.** Once the lake develops, compare predicted values to observed values and calibrate the prediction model as needed to match observations (Andersen and Woessner, 1992).

### 2.3 Model frameworks

The model framework should be rigorous enough to consider all key geochemical, hydrological and limnological processes that could contribute to pit lake water quality over time. Several complex, contemporaneous processes occur during pit lake development, such as exchange of water between the pit lake and the surrounding hydrologic system, development of vertical density profiles in the lake, geochemical interactions that occur within the damaged rock zone of the pit walls and within the water column, as well as biological growth and decay cycles. It may be necessary to use several numerical models to address the individual processes occurring within a pit lake, using the results of one model to define the basis of a model of an interdependent process (Castendyk and Eary, 2009).
The number of dimensions used to define the geometry of a waterbody is an important component that differentiates one model from another. Several publicly- or commercially-available water quality models exist that allow a 0-, 1-, 2- or 3-dimensional definition of a waterbody. Table 1 summarizes model characteristics according to dimensional capability. Compendia of water quality models, with their capabilities, are available in USEPA (1997) and WERF (2001).

Geochemical models may be included in a zero-dimensional model (0-D) capacity, consisting of a coupled water and mass balance. These models are often used to check processes that may be occurring to influence the water quality of the pit, such as chemical speciation, mineral dissolution, mineral precipitation, oxidation, reduction and surface adsorption. Furthermore, geochemical models may also consider exchanges of gases with the atmosphere, which may influence the chemical composition of near-surface lake water.

Geochemical models are developed based on assumptions related to the hydrodynamic properties of the pit lake, using the output from other geological, limnological and hydrological models. To apply these models to a stratified pit lake, the models can be set up in separate cells to simulate vertical stratification. Alternatively, they can be coupled with hydrodynamic models of higher dimensions.

Lake hydrodynamics, including the possible formation of meromixis within the pit lake, are important determinants of water quality. Hydrodynamic models will consider variables that affect water density and circulation, such as temperature, total dissolved solids (TDS) and total suspended solids (TSS). If an evaluation of lake hydrodynamics is required to evaluate the pit lake water quality, a 1-D, 2-D or 3-D model will be required.

Other distinguishing components of water quality models are their capability to characterize specific groups of water quality constituents, and the interrelations between these groups. Typical groups would include the constituents required to characterize: oxygen dynamics; nutrient cycles; pH and alkalinity; specific species of concern; and generic conservative and degradable constituents. These water quality components are addressed in Section 2.4.

Figure 1    Example of conceptual pit lake model
Table 1 Description of options for pit lake modelling

<table>
<thead>
<tr>
<th>Model type</th>
<th>Description</th>
<th>Capabilities</th>
<th>Limitations</th>
<th>Example of models</th>
<th>Considerations</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-D chemical</td>
<td>Water and mass balances assuming full mixing of water within the lake; balances can be made within separate cells to account for stratification</td>
<td>These tools are usually user-developed, made on a case-by-case basis, and should normally be quick to run</td>
<td>No spatial representation; applicable to fully-mixed systems such as shallow lakes</td>
<td>Excel or general simulator such as Goldsim, Matlab or Stella; may be coupled with geochemical model, such as PHREEQC (Parkhurst and Appelo, 1999)</td>
<td>Ease of use</td>
</tr>
<tr>
<td>1-D physical and chemical</td>
<td>Modelling formulations that allow discretization of geometry as a function of depth</td>
<td>Will typically provide basic representation of lake hydrodynamics (including stratification) and water quality, are relatively quick to run</td>
<td>Lack of horizontal discretization makes these mainly applicable to lakes with small surface area relative to depth</td>
<td>DYRESM coupled with CAEDYM (Hipsey et al., 2006), or any 2-D and 3-D model reduced to 1-D; PHREEQC may simulate 1-D changes in composition</td>
<td>Computational demands</td>
</tr>
<tr>
<td>2-D physical and chemical</td>
<td>Two modelling formulations are available: laterally-averaged and depth-averaged</td>
<td>Models available with relatively detailed representation of lake hydrodynamic and water quality components</td>
<td>Laterally-averaged models are applicable mostly to long and narrow lakes; depth-averaged models are applicable to shallow lakes</td>
<td>Laterally averaged CE-QUAL-W2 (Cole and Wells, 2008), depth average MIKE21 (DHI, 2011), or any 3-D model reduced to 2-D</td>
<td>Ability to simulate complex interactions</td>
</tr>
<tr>
<td>3-D physical and chemical</td>
<td>Models provide longitudinal, lateral and depth discretization, and therefore can be used for any geometry.</td>
<td>Models available with detailed representation of hydrodynamic and water quality processes; geochemical models can be coupled to 3-D hydrodynamic models</td>
<td>Requires significant user and computational time to operate and develop; existing data not always sufficient for 3-D representation</td>
<td>ELCOM coupled with CAEDYM (Hipsey et al., 2006), EFDC coupled with HEM3D (Ji, 2008), MIKE3 (DHI, 2011), GEMSS (Buchak and Edinger, 1984), MODFLOW (Harbaugh et al., 2000)</td>
<td>Ease of use, Computational demands, Ability to simulate complex interactions</td>
</tr>
</tbody>
</table>
2.4 Modelling components

While there are many processes that affect water quality in pit lakes, there are three main categories of models that simulate these processes. Hydrodynamic models simulate the density, circulation and stratification of water and the resulting advective transport of constituents. Geochemical models simulate chemical reactions among minerals, water and substrates, such as oxidation/reduction, dissolution/precipitation and sorption/desorption. Water quality models simulate the fate and transport of oxygen, nutrients and other constituents that can settle or degrade in the water column. As mentioned, some models can be coupled together to simulate physical and chemical behaviour; some models are internally coupled. The following sections list some considerations for each type of model.

2.4.1 Hydrogeological considerations

The local and regional hydrogeological conditions can influence pit lake water quality in both the short and long-term. A groundwater model can be used to simulate the movement and quality of groundwater both upgradient and downgradient from a pit lake. Specific processes and considerations that will require a groundwater model are as follows:

- **Groundwater table recovery**: Groundwater will generally be depressurized and drawn down for some distance away from an open pit mine in advance of mining operations. Transient groundwater modelling may be used to determine the time to re-establish a stable groundwater table, and steady-state modelling may be used to predict the final water table elevation.

- **Groundwater discharge and recharge**: In some areas, groundwater flow to the pit lake will comprise the largest inflow. Thus, groundwater inflows will affect the residence time of the pit lake, which in turn affects water quality. Recharge of the groundwater system from the pit lake is also an important consideration for groundwater resources downgradient of the lake.

- **Groundwater quality**: Mass loading associated with groundwater solutes can directly affect pit lake water quality. This is especially true if the local groundwater system has been impacted by mining operations. Likewise, poor pit lake water quality can impact downgradient water resources. Solute transport and particle tracking may be used to simulate both of these interactions.

Hydrogeological conditions may include an evaluation of the short and long-term influence of surface water feedback to the groundwater system. Depending on the conceptual model, a separate model may be required to quantify the surface water inputs to the groundwater system. An evaluation of the potential formation of feedback loops between surface and groundwater systems should be considered during the development of the hydrogeological conceptual model.

2.4.1 Hydrodynamic considerations

Characterizing the hydrodynamics of a lake, primarily the velocity and density fields in the waterbody, is essential for modelling any waterbody that is not fully mixed. The hydrodynamic component of the modelling effort determines the movement of masses, including water and water quality constituents, in the lake. This component also determines whether stratification occurs in the lake, at which periods it occurs, and how it affects movement of masses and oxygen aeration. Many water quality models include hydrodynamic modules in their formulation. Water quality models that do not have such inclusion must then have the capability to read and use results from a separate hydrodynamic model. Below are additional considerations for a hydrodynamic model:

- **Ice cover**: For modelling lakes in a Nordic environment, the hydrodynamic component of a model must incorporate the formation and thawing of an ice cover on the lake. An ice cover will provide thermal insulation and shielding against wind, which will impact movement of masses in the lake, and will also prevent aeration, thus temporarily eliminating the oxygen supply to the waterbody.
Ideally, the ice cover should also account for salt rejection, which can affect the concentrations of all species in a lake and the overall mixing regime.

- **Mass transport**: Chemical mass transport into and out of the lake can include contributions from pit wall runoff (as detailed above), surface water flow and groundwater flow. Surface water flows typically affect the epilimnion of the lake by the transport of acidity, alkalinity and dissolved metals. Groundwater inflows can influence the whole lake.

- **Dilution/concentration**: Direct precipitation on the lake surface can result in dilution of dissolved constituents. Evaporation and salt exclusion, on the other hand, increase concentrations of salinity and dissolved constituents. In net evaporative climates, pit lakes may become meromictic and/or terminal due to long-term evapo-concentration.

- **Mixing**: Mixing of the pit lake during annual or biannual lake turnover, or by wind and wave action can contribute to processes that may affect lake chemistry, such as vertical homogenization of dissolved chemical parameters, vertical distribution of dissolved oxygen stored in the epilimnion, sediment re-suspension and vertical distribution of carbon dioxide stored in the hypolimnion followed by ex-solution at the lake surface.

### 2.4.2 Geochemical considerations

The chemogenesis of a pit lake is a function of many geochemical processes that can occur within a pit lake. Each of these processes must be quantified with respect to its contribution to the ultimate pit lake water quality. A brief summary of some of the key geochemical processes that should be considered in a pit lake model is provided below. The reader is referred to Castendyk and Eary (2009) for a detailed description of the layers in each pit lake where these processes may occur, and the effect of each process.

- **Reactions within the damaged rock zone**: The damaged rock zone of a pit lake includes the shell of highly fractured rock or sediment around the pit perimeter. Mineral reactions, such as sulphide oxidation or dissolution of soluble mineral phases, result in the addition of acidity, sulphate and trace metals to pit wall runoff. The rate of reaction of these mineral phases in the range of conditions defined by the conceptual model is of key importance to the pit lake water quality predictions.

- **Mineral precipitation**: Dissolved mineral phases may precipitate from mixed pit lake waters, which can reduce the concentrations of some chemical parameters and provide surfaces for metal adsorption. The reader is referred to Nordstrom and Alpers (1999) in mine pit lakes.

- **Metal adsorption**: Surface adsorption of metals to hydroxide precipitates, clay minerals or organic material with reactive surfaces in solution can decrease concentrations of metals and metalloids.

- **Speciation and redox**: The speciation and redox state of anions and metals in solution can be influenced by geochemical processes that occur within the pit lake, resulting in transformations of one species to another, oxidation or reduction reactions, precipitation or dissolution of mineral precipitates, or desorption / adsorption onto surfaces. Vertical changes in redox conditions are common in meromictic lakes.

Geochemical predictions of pit lake water quality must quantify each source in terms of its contribution to the overall system. The post-mining hydrologic system, including anticipated future geochemical and limnological conditions, must be considered in order to estimate post-closure pit lake water quality. The geochemical conceptual model will define the key processes that should be accounted for in the numerical model during the various stages of pit lake formation. However, simplifying assumptions should be verified with field monitoring data as the pit lake forms over time. Field data should then be used to adjust the conceptual model to reflect actual field conditions.
2.4.3 Water quality considerations

Understanding the end use of the water body will influence the type of water quality model and degree of complexity of the modelling effort. If it is clear through simple mixing models that constituents will concentrate or degrade with time in the pit lake, or that active mitigation measures such as treatment will be required, then it may not be necessary to conduct more detailed modelling. In most instances the goal is to create a pit lake that will eventually become productive habitat. To design such a lake, it is necessary to investigate specific aspects of water quality, such as nutrients and key parameters of concern. General purpose water quality models are available for a wide range of applications, including characterization of the components detailed below:

- **Generic constituents**: Most water quality models also include the ability to model user-defined constituents. These can be conservative constituents, meaning they do not undergo fate processes, or settleable or degradable constituents. Settling and decay rates are normally set according to first-order or constant rates. These constituents do not interact with other components of the model, except in the case of biochemical oxygen demand (BOD) constituents. This category of model constituents can be used to simulate the concentration any number of toxic and non-toxic substances of interest.

- **Oxygen cycle**: Oxygen consumption, production and replenishment are important processes that should be included in any water quality modelling effort, because the dissolved oxygen (DO) status of a pit lake will affect the fate and behaviour of a host of other constituents. For example, the redox state will affect most geochemical processes described above, as well the aerobic degradation of organic compounds, nitrification, denitrification, iron reduction, and sulphate reduction. A basic oxygen balance will consider atmospheric aeration and inflows as sources, and biochemical, chemical and sediment oxygen demand (SOD) as sinks. More complex models will account for photosynthesis and respiration at one or more trophic levels.

- **Nutrient cycle**: The nutrient cycle forms the primary basis of many water quality models, as it determines the trophic status of the aquatic system. Nutrients consist of inorganic and organic forms of nitrogen, phosphorus and carbon. Sources of nutrients include loadings in inflows and available fractions of sediment and dissolved and particulate organic matter. Nutrients may be lost through uptake, adsorption or settling. Interaction with primary producers includes consumption through photosynthesis and release through respiration.

- **Primary production**: The nutrient and oxygen cycles are primarily related through the growth and decay of phytoplankton, periphyton and macrophytes. Typical formulations of growth and decay of these organisms are incorporated in water quality models and are dependent mainly on temperature and the availability of light, oxygen and nutrients. Algae loss is usually defined in terms of mortality (i.e., transformation into dissolved and particulate organic matter), settling for phytoplankton, burial for periphyton, and grazing by zooplankton.

The geometric domain of pit lake water quality models is often limited to the water column in the waterbody, although interactions do occur at interfaces such as the water surface and lake bed. Features are often included in the models to incorporate loadings from sediment. Precipitation and evaporation at the lake surface is often incorporated in the modelling formulation, and chemical loadings associated with precipitation may also be defined. Precipitation loadings should account whenever possible for impacts of aerial emissions from industrial activities if there are any near the pit lake.

3 Challenges and assessment of limitations

3.1 Data sources

The development of a database for pit lake modelling should be initiated from the early stages of the mining project. Climate, hydrometric, surface and groundwater water quality, and geochemical baseline
studies will normally be undertaken to determine the environmental setting of a mining project. The data from these studies and the mine plan of the project are generally used to populate the database for pit lake modelling. Continuing monitoring during the planning, construction and operational stages of the project should be completed to refine the database and fill in any data gaps identified during the preliminary modelling stages. Thus, as the mining project progresses, so does the ability to model and design the desired pit lake. The types of data described below are normally required as model inputs:

- **Geological model:** The geological block model for the open pit is typically available in the early stages of a mining project. The geological block model provides important information about the rock types that will be exposed at the various levels of the open pit. This information forms the basis for defining the geochemical characteristics of pit wall runoff.

- **Lake geometry:** Pit geometry will typically be available in the early stages of the mining project, as part of the ore evaluation assessment. In the initial stage of modelling, the pit geometry may be represented in the model as a simple shape, such as a cylinder or cone. Such simple shapes should provide a reasonable approximation of the expected geometry of the pit, notably surface area, depth and volume. A more exact geometry will be required in 2-D and 3-D models, if more refined modelling is required in the early stages of the project and later once a final pit geometry is established.

- **Climate:** Long term climate characteristics for the mine area will normally be developed from climate and hydrological studies in the early stages of the project. Climate change forecasts should be incorporated into these predictions. It is recommended that an onsite meteorological station will be installed and operated in the mine area from the early stages of the project to provide local climate characteristics, then be maintained and operated through the mine life, including during the closure and post-closure stages. Climate variables that are expected to affect the hydrodynamic and consequently water quality of the pit lake include precipitation and evaporation; air temperature; dewpoint; solar radiation; cloud cover; and wind speed and direction.

- **Inflow rates:** Establishing inflow rates for all water sources is required to assess the water quality and hydrodynamics of pit lakes. Sources may typically be divided into surface water and groundwater, as determined from their expected point of entry into a pit lake. Surface water inflow rates may be determined from a hydrologic assessment of the watersheds draining into the lake and overland flow, and may also consist of diverted waters from adjacent watersheds. Groundwater inflow rates will be evaluated from a hydrogeological assessment determining flow pathways through the ground using a model such as MODFLOW. The inflow rates should be combined into an overall pit lake water balance to evaluate the rate of filling, the relative volumetric proportion of each source of water contributing to the lake, the long-term water level, and outflow rates.

- **Inflow temperatures:** Water temperature affects the hydrodynamics of lakes, including stratification, and therefore will influence water quality. Temperature time series must be assigned as part of the modelling effort to all water sources to a pit lake. These time series should be established from observations of water temperatures in the mining areas, although it is not unusual for such data to be scarce in the early stages of the project. Climate data, notably air temperature, and regional water temperature data may assist in deriving water temperature for surface sources to the pit lake. Seasonal variations of groundwater temperature are not expected to be as high as those of surface waters. Time series for groundwater may be derived from regional groundwater temperature data, and will vary more with depth than with time.

- **Inflow total suspended and dissolved solids:** These two general water quality parameters affect water density and will therefore affect the hydrodynamics of a pit lake. Time series of these parameters must be developed as part of the modelling efforts for all water sources. Except in rare cases, groundwater sources can safely be assumed to contribute negligible suspended solids.
Assessment of these two parameters should normally be part of monitoring programs through all stages of the mine development. The levels of these parameters may vary significantly on a seasonal basis and depending on the watershed characteristics.

- **Oxygen characteristics**: Two components of the oxygen balance should be considered for each inflow source. First, the DO concentration in the inputs will be a direct source of oxygen to the pit lake. Second, chemical oxygen demand and BOD in inflow sources will lead to DO consumption within the lake. Dissolved oxygen is easily measured in the field, and this task should normally be incorporated into monitoring programs throughout the stages of the mine development.

- **Geochemical characteristics**: Chemical weathering of rock exposed in the damaged rock zone of the open pit can contribute acidity, alkalinity, sulphate and metals to pit wall runoff. The results of the geochemical characterization are required to assess the relative contribution of each rock type that is exposed in the pit walls. An understanding of the geochemical characteristics of pit wall rock, namely the rate of acid generation and metal leaching from the main lithologies, can have important implications with respect to mitigation strategies for the pit lake.

- **Inflow chemistries**: A chemical profile or time series will need to be developed for all inflow sources. This category of data can vary widely, and will depend on the objectives of the modelling and the parameters of concern. The list may include general parameters such as: pH, alkalinity, acidity and redox potential, major ions; nutrients and algae; organic compounds; and metals. Monitoring programs through the stages of the mine development constitute one source of data for constructing these time series. Deep groundwater inflow chemistry is particularly important in Canadian Shield waters as it is difficult to obtain but may substantially influence the major ion chemistry and TDS of the pit lake.

- **Sediment characteristics**: Loadings from sediments may impact water quality, particularly in the lower layers of pit lakes, and should therefore be incorporated in the model formulation. Sediment oxygen demand is an important driver of DO and is notoriously deficient from model input data. Metals, ions, nutrients and biogenic gases constitute typical loadings from sediment, which may be assessed from water quality analytical results from samples and geochemical analysis. The model described in Section 4 was developed to deal with these issues.

Data within the lakes themselves, if available, including general chemistry, nutrients, water temperature, TDS, TSS, DO, BOD and generic and toxic constituents, are also required. Such data will not be available in the early stage of the mining development, when the pit lake is not yet created. Therefore, data from similar lakes may serve for comparison with model predictions, in order to check the validity of the model until data from the pit lake itself are collected. Expert judgment is required to determine the adequacy of surrogate data.

### 3.2 Sensitivities

In the early stages of pit lake modelling, input data are limited; however, models may be used to identify key sensitivities. In a sensitivity analysis, one input variable is modified per model scenario, and the model results are compared to show a relative change in one or more output variables. For example, a sensitivity analysis might ask “if this pit lake is 10% larger, how will that change the salinity of the outflow compared to the base case?”, or “if this pit lake is filled in 10 years rather than 50 years, how will that change the overall chemistry of the pit lake compared to the base case?” The results of a sensitivity analysis can be used to define the design criteria to be applied to the pit lake at future stages of modelling. The sensitivity analysis serves also to identify the most sensitive input variables, which indicates that these variables are key drivers of the overall outcome of the pit lake.

Suggested input variables to use in a sensitivity analysis are listed below, along with their possible effects on water quality:
• **Lake residence time:** A long hydraulic residence time may enable appreciable aerobic decay of degradable and toxic constituents, and may serve to smooth seasonal variability in concentrations. Too long of residence times may lead to excessive evapo-concentration, which could contribute to meromixis and lack of outflow.

• **Lake depth, shape, and orientation:** The depth of a pit lake will normally be determined by the characteristics of the final mining pit and the amount of waste material to be disposed of at the bottom of the pit. Where flexibility exists, lake depth may be varied to optimize the balance between evapo-concentration in shallow lakes and meromixis in deep lakes. Meromixis may be favourable if the intention is to isolate waste from the outflow, but may be unfavourable if the intention is to promote aerobic degradation of constituents.

• **Lake filling time:** The desired rate of pit lake filling is dependent on site specific conditions. When rock with a high acid generation potential or metal leaching potential is exposed in the damaged rock zone of the pit walls, it is generally preferable to fill the pit rapidly to reduce the geochemical reaction rates. Conversely, in the case of oil sands pit lakes, longer filling periods will likely improve water quality at the time of initial discharge because of the additional time for degradation of toxic constituents.

• **Excavate or cover reactive wall rock:** When rock with a high acid generation potential or metal leaching potential is exposed above the projected final lake surface or within the watershed, it may be possible to cover this rock with a permanent geotechnical liner.

• **Water sources for lake filling:** Depending on local restrictions, natural background flows from local streams may be used to supplement inflows into a pit lake if the lake is to be filled more quickly than the rate that could be supported by the lake’s catchment. Filling with background water sources may also provide dilution to improve the quality of water at the time of initial release. The placement of different water types with different salinities may also be used to promote or inhibit meromixis.

• **Deposition of mine wastes in the open pit:** Deposition of mine wastes, such as tailings or waste rock, at the bottom of pit lakes can result in a reduction of lake volume and depth and the introduction of contaminant sources through pore water release and geochemical fluxes. Deposition of potentially acid generating tailings or waste rock below a water cover is a commonly used practise for mine waste management, as the water cover could reduce the rate of mine waste oxidation. In-pit disposal of mine wastes should be considered as part of the conceptual model, to ensure that the potential range of geochemical implications of deposition of mine wastes in a saturated environment is appropriately assessed in the pit lake model.

Other model parameters that are representative of natural processes impacting lake hydrodynamics and water quality (e.g. wind sheltering from topography, shading from surrounding vegetation, constituent decay rates, and reaction rates of rocks exposed in the pit walls) may also be incorporated in a sensitivity analysis. Further field studies and design criteria can then be developed to support a more precise definition of the range of values applied to sensitive parameters.

### 3.3 Uncertainty

The goal of water quality modelling for pit lakes is to determine the characteristics of a lake (e.g. concentration of water quality constituent) under a reference assessment case (e.g. best, worst or likely case). The intent of uncertainty analysis is to develop confidence bands around the results of the assessment case as a function of the uncertainty of the inputs fed to the model. A standard approach for uncertainty analysis is Monte Carlo simulations (see Figure 2), which consist of running and processing a large number of simulations (e.g., 200 to 1,000), each with its own sets of probable inputs. For this approach, probabilistic formulations must be defined for each input. These formulations are then used to develop a set of inputs for each simulation.
Examples of probabilistic formulations are given below for specific group of inputs:

- **Process inputs**: These inputs consist of model coefficients such as geochemical reaction rates, decay rates, nitrification rates, mortality rates and settling rates. Variations of these inputs may be defined according to a standard distribution, such as a uniform and normal distribution. The central value of that distribution may consist of the average or median of values available in the literature for the associated parameters. The upper and lower bounds forced on the distribution may be based on extreme values found in the literature or other calibrated models or expert judgment.

- **Flow and water temperature inputs**: If possible, flow and water temperature time series should come from hydrological and hydrogeological models. Sets of time series would result from an uncertainty analysis conducted with these models. Otherwise, variations of the characteristics (e.g., mean and standard deviation) of the time series of flow and water temperature time series of the assessment case may be defined according to standard statistical distributions. These distributions can then be sampled to develop one unique set of flow and water temperature time series per simulation.

- **Water quality inputs**: These consist of time series of water quality constituent concentrations, including TDS and TSS. Like flow and water temperature, water quality inputs may be characterized, and variations of the characteristics can be used to develop one unique time series per simulation.

4 **Case study – modelling oil sands pit lakes**

Several case studies exist with respect to hard rock mining applications of pit water quality modelling (Castendyk and Eary, 2009; Maest et al., 2005). Provided below is an alternate scenario whereby the principals as discussed above are applied to modelling an oil sands pit lake.
The oil sands of Alberta, Canada represent the world’s second largest reserve of oil, much of which is presently being or will be mined by conventional strip mining techniques. Similar to other mining operations discussed earlier in this paper, oil sands mines will include pit lakes in their closure and reclamation strategy. In some of these pit lakes, mature fine tailings (MFT) will be placed in the pit before it is flooded with water to create a lake. The MFT poses challenges to reclamation because it contains organic substances as well as dispersed clay materials that settle very slowly (Mikula et al., 1996).

4.1 Oil sands pit lake model

The inclusion of MFT in a pit lake carries the implication of several processes that are not covered in existing water quality models. In particular, observations on operational tailings ponds indicate that physical and chemical processes within the sediment layer may have important implications for lake water quality (Holowenko et al., 2000). Physical effects include deepening of the lake as time progresses and the tailings consolidate and re-suspension of sediments when biogenic gas production leads to bubble ebullition. Chemical effects include the direct release of pore water to the water column, diffusion of gases from biogenic bubbles and consumption of oxygen as reactions take place at the sediment-water interface. A schematic of the conceptual model is presented in Figure 3. Because there is presently no model that accounts for the processes in the conceptual model, an Oil Sands Pit Lake Model (OSPLM) was developed as a regional initiative by CEMA.

![Schematic of the processes added to the CE-QUAL-W2 under the present phase of OSPLM development](image)

The OSPLM is currently being developed for predicting sediment and water quality in oil sands pit lakes that contain MFT. Although OSPLM is designed specifically for oil sands pit lakes, it could be applied to other systems. Its primary focus is to incorporate chemical reactions within MFT that may result in the release of aqueous and gaseous compounds into the water column, leading to changes in pit lake water quality. The model simulates the anaerobic decay of these compounds and production of gases such as methane, which could alter the physiochemical nature of the pit lake water column.
4.1.1 Model platform

The OSPLM is being developed by programmatic adding processes relevant to oil sands pit lakes to the freely-distributed hydrodynamic and water quality model CE-QUAL-W2 Version 3.6 (Cole and Wells, 2008). The additional programs are added in the form of modules written to separate FORTRAN files to preserve the original CE-QUAL-W2 code.

4.1.2 Model setup

Several key processes were identified for the present development phase of OSPLM. The key processes can be categorized by the layers where these processes occur. These two compartments are the MFT bed and the overlying water column. CE-QUAL-W2 does not include a sediment transport model and thus the MFT bed was added as a separate sediment bed compartment to the existing CE-QUAL-W2 modelling framework. Additional constituents were added to the existing water column compartment within the CE-QUAL-W2 framework.

4.1.2.1 Sediment bed

The additional processes added within the sediment bed compartment for OSPLM include the bed consolidation, pore water release, sediment diagenesis, oxygen demand exerted on the overlying water column, gas production and release, and oxygen-demanding constituent decay. The sediment compartment added to the existing framework of CE-QUAL-W2 calculates the MFT bed consolidation and updates lake bathymetry for subsequent hydrodynamic calculations by adding active model grid layers below the lake bed. This approach provides a dynamic linkage between the hydrodynamics and the lake deepening. Consolidation of the MFT bed also adds expunged pore water to the overlying water column.

Methanogenesis has been found to be an important process within the oil sands pit lakes (Fedorak et al., 2002). To estimate the amount of methanogenesis and other gas production, a detailed sediment diagenesis model based on DiToro (2001) formulations was added to the module. The framework for this diagenesis formulation is shown in Figure 4. The gases produced during diagenesis processes build pressure within the MFT bed until the cracks appear. The bubble formation formulae were based mainly on the work of Boudreau et al. (2001). At the onset of crack formation, the produced gas is released into the water column. The diagenesis process consumes DO from the overlying water column, increasing the net SOD.
4.1.2.2 Water column

The dissolved diageneric products released through pore water and gases released through ebullition enter the overlying water column. In the water column, OSPLM links with existing CE-QUAL-W2 generic constituents to track the dissolved constituents that may consume oxygen. The movement of gasses released as bubbles from the MFT bed are also tracked through the water column until they reach the water surface where these gas bubbles burst to release gasses to the atmosphere. Gasses can also go through dissolution process while in the water column based on their solubility.

4.2 Modelling steps

In Section 2.2, we presented a series of steps a modeller should follow when setting up a pit lake model. We now revisit these steps using the OSPLM as a case study:

- **Define the objectives for modelling.** The objectives for modelling oil sands pit lakes are to understand the key drivers of water quality to inform pit lake design, particularly with respect to submerged tailings. In this example, the objective is to understand sediment processes and their effects on water quality in the water column.

- **Develop a conceptual model.** The conceptual model of sediment and water interactions is presented in Figure 3, and the sediment diagenesis processes are presented in Figure 4. The conceptual model was prepared through a literature review of relevant processes and through consultation with mine operators and researchers.

- **Select the appropriate model.** In this case, there was no existing model that could mechanistically model the processes of interest. Therefore, the OSPLM was developed specifically for oil sands pit lakes.
• **Establish key output metrics.** Several output metrics have been identified for the OSPLM. The model will output concentrations and fluxes of all relevant constituents, such as methane, hydrogen sulphide and ammonia, shown in Figure 4.

• **Establish screening criteria in advance of model runs.** At the present stage of development, the model will be used for sensitivity runs. Once the predictive ability of the model has been further developed, screening criteria will be established against which simulation output can be compared.

• **Gather input data.** Data compilation will be a major undertaking for the OSPLM because there are many rates and constants that will need to be obtained. The first step will be to conduct a literature survey for available rates and constants. Then, field and laboratory studies will be completed to isolate and estimate specific rates and constants. Data for inflow quantities and chemistry, meteorology and other inputs can be gathered from the numerous baseline studies that have been completed for oil sands projects.

• **Implement quality assurance procedures.** Quality assurance procedures will be completed as specified in Section 2.2.

• **Calibrate and validate, if possible.** While there are no oil sands pit lakes as yet, there are experimental reclamation waterbodies on existing oil sands leases. These waterbodies may be used to calibrate part or all of the OSPLM. As oil sands pit lakes, or demonstration pit lakes, begin to fill, the model can be calibrated and validated in full.

• **Conduct an uncertainty or sensitivity analysis.** One of the main purposes for this model is to complete sensitivity analyses on sediment processes. The focus at this stage of development is experimental modelling, meaning that the mechanistic model will inform our conceptual model and vice-versa.

• **Compare results to criteria.** Once final and calibrated, the model will be used to assess pit lake performance against desired outcomes, such as maintenance of water column DO, low rate of sediment resuspension, attainment of sulphide and ammonia guidelines, etc.

• **Continue improvement loops.** At this stage, the feedback loops are mainly occurring in the first three to five steps listed above. As the model becomes fully refined and developed, the next steps will be to focus on the validation and sensitivity analyses.

5 **Summary and conclusions**

Forecasting and evaluating pit lake water quality poses a challenge because of the variety of geological environments and ore deposit types that may be encountered. Furthermore, the lakes generally will not be constructed until decades after the initial mine design. For these reasons it is critical that each pit lake model be tailored to the specific conditions that influence the pit. Conditions that can strongly influence the pit model include: geochemistry, hydrogeology, hydrology, limnology, mine planning, pit backfilling, input water quality, and flow rates amongst others.

Predictive modelling is required in order to identify and implement mitigation strategies for the various stages of a mine development. Modelling allows an assessment of the potential range of water quality resulting from processes that may take years to occur. This paper provides guidance with respect to modelling considerations. Model development starts with the setting of model objectives. Then, a conceptual model of the pit lake can be constructed that identifies key processes and inputs. A model can be selected to represent these processes, considering dimensionality and complexity of the system. If an appropriate model is not available, model development may be required to represent the processes of interest. The model must be able to report key metrics that can be screened against relevant criteria.

The outcome of a model can form the basis for water quality monitoring protocols. Monitoring data can be used to validate the results of a modelling effort. Long-term predictions can gain confidence and credibility
if it is calibrated and validated, though this is not always possible with pit lakes. In the case of pit lakes that will not be constructed until well into the future, inputs to the model can be validated and refined throughout the mining period based on the results of operational monitoring, so that a robust database is available for pit lake design when it is time to fill the lake. During this period, model refinements can result in iterative loops to previous modelling steps. At all stages, quality assurance procedures can be completed to maximize confidence in model predictions.

While many water quality models are available publicly and commercially, and have been the subject of development and refinement for decades, opportunities for additional development and improvement remains available with these tools. Current and future areas of development that may be beneficial for pit lake water quality models include the coupling of hydrodynamic, water quality and geochemical models, as has been done to some extent in models such as ELCOM and OSPLM.

The case study of OSPLM discussed in this paper provides an example of how models can be used to investigate key drivers of pit lake water quality. While preliminary, OSPLM provides a model framework for future refinements that can be completed as part of subsequent validations. As much as field and laboratory research will feed into model development, it is anticipated that the model will feed back into field and laboratory research by identifying knowledge gaps and key sensitivities.

Acknowledgements

The authors wish to thank Ken DeVos for reviewing this paper, and the Cumulative Environmental Management Association (CEMA) for funding development of the Oil Sands Pit Lake Model.

References


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