

# Water quality prediction of mining waste facilities based on predictive models

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Front cover: Waste rock pile at the closed Hannukainen mine site in 2009.  
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In mining activities, management of mine wastes is a critical issue as improper waste disposal often results in liability for mining operators with the risk of financial consequences. Of primary concern is the low quality drainage from mine waste that leads to adverse effects on the surrounding environments and ecosystem. This drainage usually results from the weathering of mine wastes, and in particular sulphide-rich waste deposits that are disposed after extracting the valuable metals, upon their exposure to the atmosphere. In the last decades, extensive research efforts have been dedicated to understand the acid generation processes as well as to accurately quantify and predict acid mine drainage, which has led to the development of various prediction techniques. This report reviews all the major processes that influence drainage quality in mine waste dumps. In particular, this review includes geochemical processes concerning acid generation and neutralization mechanisms, microbiological activity and its relevance on mineral weathering reactions, electrochemical processes, heat transport mechanisms, water flow and solute transport, and gas transport processes. Additionally, existing water quality prediction methods based on laboratory and field scale tests, including mineralogical, physical, and geochemical characterisation, static tests, chemical extractions, leaching tests, and kinetic tests, are reviewed. Moreover, this report also includes a comprehensive review of all the available predictive modelling tools, including general modelling principles, different model types based on their formulation, and available computer codes, in mining environmental simulations. The scope and capability of predictive models are demonstrated by presenting three different published case studies from the literature focusing on waste rock pile and tailings systems. Additionally, this document also presents the important aspects that are relevant to predictive modelling, such as major sources of uncertainties and challenges in numerical modelling, limitations in model calculations, scaling factors for model input parameters, data requirements, basis for a code selection, and applicability of the presented modelling approaches under Nordic climate conditions. Besides the review of the literature methods, this review also focuses on the potential approaches to enhance the prediction accuracy by using integrated methodologies to properly describe the multifaceted processes occurring in mine wastes. Furthermore, this work specifically highlights the importance of conducting predictive calculations at the early phase of a mine even before the initiation of actual waste disposal.

**Keywords:** Mine waste, drainage quality, predictive modelling, reactive transport modelling

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## 1 INTRODUCTION

### 1.1 Background

Management methods for mining wastes (KaiHaMe) is a 3-year project funded by the European Regional Development Fund (ERDF) that aims at developing methods to increase the raw material value of gold and base metal ore deposits and to reduce the environmental impact of mining waste, as well as the amount of disposed hazardous waste. This will be done by modifying gold ore tailings with mineral processing techniques and by seeking new options for the use of waste rocks from base metal mining. In addition to ERDF, the project has been co-funded by the Geological Survey of Finland (GTK), Boliden Kevitsa Mining Oy, FQM Kevitsa Mining Oy, Kemira Oyj and Endomines Oy.

One of the main objectives of the project is to provide tools for predicting the effluent quality of mine wastes to reduce their environmental impacts. This is because low-quality mine drainage from wastes is one of the biggest concerns related to the management of mining wastes (e.g. MEND 1991, Price 2003, Heikkinen 2009). This particularly applies to base metal, precious metal, uranium and coal mining, in which the mine wastes usually contain easily oxidizing sulphide minerals. Sulphide minerals are prone to oxidation once the waste is disposed on the ground surface under the influence of atmospheric oxygen and water (e.g. Singer & Stumm 1970, Blowes & Ptacek 1994). Sulphide oxidation produces acidity, which results in the dissolution of minerals in the waste and mobilisation of elements and compounds harmful to the environment (e.g. Blowes & Jambor 1990, Lottermoser et al. 1999). The transport of mining-influenced waters into the receiving water body may deteriorate water quality and cause harm to the biota (e.g. Kihlman & Kauppila 2010, 2012).

The effluent quality of mine wastes largely depends on the mineralogical and chemical composition of the wastes (e.g. Blowes & Ptacek 1994). Other influencing factors include the disposal type and structure of the waste facility, climatic condi-

tions, the biological content of the mine waste, the availability of oxidizing agents, as well as mining and mineral processing methods. Mine drainage may be acidic or neutral and contain elevated concentrations of harmful elements and compounds, such as trace metals, metalloids, sulphate and iron (e.g. Younger 1995, Pettit et al. 1999, Cravotta et al. 1999). The acidity of the drainage depends on the ratio of acid-producing and -neutralising minerals in the waste. Sulphide minerals, especially iron sulphides such as pyrrhotite and pyrite, are acid-producing minerals, whereas carbonates are the most effective neutralizing or acid-buffering minerals (e.g. Blowes & Ptacek 1994, Ptacek & Blowes 1994).

In order to assess the potential environmental impact of mine wastes and to design relevant management methods for the waste facilities and their water treatment, the drainage chemistry should already be predicted in the planning phase of a mine. Estimates of the drainage quality are needed especially in the environmental impact assessment procedure and in the environmental permit application to facilitate mine planning, i.e. planning of waste facilities and water treatment systems in particular, and to prevent negative impacts on the watersheds. Data on the expected water chemistry is also required when planning the monitoring programme to identify the key substances that need to be observed. In operating mines, water quality prediction is needed to adjust the existing effluent control measures and to plan for the closure of waste facilities. At closed or abandoned mine sites, water quality prediction is also important to assess the long-term impact of the wastes and necessary water treatment methods. (e.g. Kauppila et al. 2013)

The prediction of effluent quality is, however, a challenging task due to several reasons. For example, mineral weathering processes resulting in low-quality drainage from mining wastes are very complex and long term (e.g. Blowes & Jambor 1990, Blowes & Ptacek 1994). The evolution of poor-

quality drainage may take years or decades from the start of the operations, and may continue over decades or even hundreds of years unless managed properly. However, the mineral weathering processes are site-specific, as each mining site is unique with respect to the deposit geology, and thus waste composition, and local environmental and climatic conditions, even if the overall chemical processes are the same. Basically, the excavated and generated wastes also show a heterogeneous composition within a site. Additional challenges arise because the drainage chemistry may change during the operation period of a mine once mineral weathering evolves (e.g. Dold 2014). Therefore, effluent quality prediction should also include an estimate of the type and timing of the changes to properly dimension the management methods. However, since modelling should be performed in a phase for which no data on the modelling conditions yet exist, model calibration for proposed waste piles is not possible (Tremblay & Hogan 2000, Maest et al. 2005).

As a result of these challenges, considerable research effort during recent decades has been put into improving understanding of the long-term behaviour of mining wastes and the development of prediction tools for their effluents (e.g. Morin & Hutt 1994, White et al. 1994, White et al. 1999, Blowes et al. 2007, Sapsford et al. 2009). For instance, a series of investigations and reports on the long-term behaviour and effluent prediction tools to improve the management of mining wastes have been documented by the MEND (Mine Environment Neutral Drainage) programme for the Natural Resources of Canada and the MiMi

(Mitigation of the environmental impact from mining waste) programme in Sweden (cf. Höglund et al. 2004, MEND 2017). In addition, the International Network for Acid Prevention (INAP) has compiled an internet-based global guide on acid and neutral rock drainage and its prediction, prevention and mitigation (INAP 2009). Currently, a variety of forms of guidance and tools are available, ranging from simple laboratory tests and analyses to field-scale tests and simple geochemical or more sophisticated reactive-transport modelling (e.g. Lawrence & Day 1997, Maest et al. 2005, INAP 2009, Price 2009, Parbhakar-Fox & Lottermoser 2015). A comprehensive prediction usually combines data from all these sources (Lawrence & Day 1997).

However, during the planning of a mine, the data available for the prediction are typically quite limited. Therefore, it is not sensible to develop models for the prediction that are too complex. Instead, the predictive model should be in accordance with the complexity of the available data, the scale of the addressed problem and the requirements set by the regulatory decisions made at that point (e.g. Maest et al. 2005). As information on the operations, waste materials and their effluents increases and becomes more reliable during mining operations, the predictive model should be re-evaluated and updated in later phases. It should be noted that no matter how complex and detailed a model is, some uncertainty will remain in the prediction, even at its best, due to the heterogeneity of the excavated materials and sites. Therefore, the predicted water quality is typically a range of concentrations rather than precise single values (Price 2009).

## 1.2 Objectives and content of the literature review

The purpose of this report is to review the existing modelling approaches applied to predict drainage quality from mine wastes. Following the examples by Maest et al. (2005) and Nordstrom (2017), the terms code and model are separated in this review. By code, we refer to a computer program applied to solve mathematical equations describing natural processes in mine waste, whereas by model, we refer to “a simplified representation of the site-specific conditions at a particular site, which may be a conceptual model or one created using a computer code” (Maest et al. 2005). The focus of the report is especially on the early-stage prediction of drainage chemistry, i.e. on the plan-

ning phase of a mine, where waste disposal has not yet occurred.

The review first provides a short description of the key processes in mine wastes influencing drainage quality (Chapter 2) and of typical laboratory and field methods (Chapter 3) used to predict the water quality and to provide background information. Chapter 4 includes the modelling approaches by presenting insights into the general aspects of predictive modelling, common codes and models used to evaluate mine drainage, and the principles of selecting a code to be applied, as well as by describing case studies using reactive transport modelling to predict the evolution of drainage from

mine wastes. The last section of Chapter 4 further discusses the uncertainties involved in modelling. In addition, Chapter 5 presents an overview of the data requirements for predictive modelling. As a

conclusion of the review, recommendations are made on the effluent prediction modelling of mining waste facilities.

## 2 KEY PROCESSES INFLUENCING DRAINAGE QUALITY IN MINING WASTES

Drainage quality in mining environments is collectively affected by different physical, geochemical, microbiological and electrochemical processes (e.g. Nordstrom et al. 2015). Of primary concern is the effect of geochemistry, as it is typically the key source of poor quality drainage containing a high specific conductivity and elevated concentrations of major ions, toxic trace metals and/or metalloids. Depending on the major processes, such mine drainage waters can be acidic, circumneutral, basic or saline in terms of pH and salinity, and are usually termed as acid mine drainage (AMD), neutral mine drainage (NMD), basic mine drainage (BMD), or saline drainage, respectively.

The most dominant processes affecting the ultimate drainage quality are completely site-specific and usually determined by the characteristics of waste materials and the prevailing environmental conditions in a particular mining site. Table 1 presents a list of typical processes, which are further illustrated in the following sections. In addition to these processes, the drainage quality is also influenced by chemicals and reactants used in ore excavation and mineral processing. For example, notable  $\text{SO}_4^{2-}$  in the drainage may also originate from the use of sulphuric acid in ore processing (e.g. Heikkinen et al. 2002, 2009).

Table 1. Physical, biogeochemical and electrochemical processes affecting the drainage quality of mining wastes (modified after Tremblay & Hogan 2000).

Physical and thermal processes	Biogeochemical and electrochemical processes
<i>Hydrology/Meteorology</i> (precipitation, evapotranspiration, wind, barometric effects)	Oxidation of sulphide minerals
<i>Unsaturated/saturated water flow</i>	Dissolution of buffering minerals
<i>Aqueous phase transport of dissolved <math>\text{O}_2</math> and other oxidation products</i> (advection, diffusion/dispersion, sorption)	Redox reactions
<i>Gas phase transport of <math>\text{O}_2</math> and other reaction product gases</i> (advection, diffusion/dispersion)	Secondary mineral precipitation and passivation
<i>Gas-pore water partitioning</i>	Ion exchange
<i>Heat transport</i> (conduction, convection, spontaneous exothermic reactions)	Surface complexation
	Catalysis by microorganisms
	Radioactive decay
	Galvanic effects
	Coulombic interactions

### 2.1 Acid generation and neutralisation processes

The generation of acid mine drainage is best illustrated as a result of the oxidation of reactive sulphide minerals when they are exposed to an oxidant (e.g.  $\text{O}_2$ ,  $\text{Fe}^{3+}$  or  $\text{MnO}_2$ ) and water under oxic or anoxic conditions, depending on the oxidant. The oxidation of pyrite, the most abundant sulphide mineral in the Earth's crust, is considered to be the most common mechanism responsible for acid generation in mining wastes (e.g. Blowes et al. 2014). Upon exposure of the pyrite-bearing mine waste to atmospheric oxygen, pyrite is oxidized, leading to the release

of dissolved ferrous iron, sulphate and protons (Table 2). This ferrous iron can be further oxidized to ferric iron if the oxidizing conditions persist (e.g. Nordstrom 1982). The iron oxidation mechanism is usually sustained by microbial activity. Ferric iron forms hydrated iron oxyhydroxides (e.g. goethite, ferrihydrite), which may precipitate. This secondary mineral precipitation may form coatings on sulphide mineral surfaces and can potentially reduce the mineral oxidation rates by limiting the exposure to the reactants. Pyrite can also be oxidized by the

dissolved ferric iron species, especially under low pH conditions. The rate of such pyrite oxidation by  $\text{Fe}^{3+}$  has been shown to be significantly higher than by  $\text{O}_2$  (e.g. Williamson & Rimstidt 1994, Mylona et al. 2000). These simultaneous reactions, i.e. the dissolution of pyrite by ferric iron and the oxidation of

ferrous iron, constitute a cycle of pyrite dissolution (e.g. Singer & Stumm 1970). The net consequence is an increase in the total dissolved solutes (e.g.  $\text{Fe}^{2+}$ ,  $\text{SO}_4^{2-}$ ) and the release of acidity in the drainage water associated with mining wastes.

Table 2. Reactions of sulphide oxidation and (oxy-)hydroxide precipitation in mine wastes (e.g. Seal et al. 2003, Dold 2010).

Minerals	Reactions
Pyrite	$\text{FeS}_2(s) + \frac{7}{2}\text{O}_2 + \text{H}_2\text{O} \rightarrow \text{Fe}^{2+} + 2\text{SO}_4^{2-} + 2\text{H}^+$
	$\text{Fe}^{2+} + \frac{1}{4}\text{O}_2 + \text{H}^+ \rightarrow \text{Fe}^{3+} + \frac{1}{2}\text{H}_2\text{O}$
	$\text{Fe}^{3+} + 3\text{H}_2\text{O} \rightarrow \text{Fe(OH)}_3(s) + 3\text{H}^+$
	$\text{FeS}_2(s) + 14\text{Fe}^{3+} + 8\text{H}_2\text{O} \rightarrow 15\text{Fe}^{2+} + 2\text{SO}_4^{2-} + 16\text{H}^+$
	$\text{FeS}_2 + \frac{15}{4}\text{O}_2 + \frac{7}{2}\text{H}_2\text{O} \rightarrow \text{Fe(OH)}_3 + 2\text{SO}_4^{2-} + 4\text{H}^+$
Pyrrhotite	$\text{Fe}_{1-x}\text{S}(s) + \left(2 - \frac{x}{2}\right)\text{O}_2 + x\text{H}_2\text{O} \rightarrow (1-x)\text{Fe}^{2+} + \text{SO}_4^{2-} + 2x\text{H}^+$
	$\text{Fe}_{1-x}\text{S}(s) + (8-2x)\text{Fe}^{3+} + 4\text{H}_2\text{O} \rightarrow (9-3x)\text{Fe}^{2+} + \text{SO}_4^{2-} + 8\text{H}^+$
	$2\text{Fe}_{1-x}\text{S}(s) + \left(\frac{1}{2} - x\right)\text{O}_2 + (2-4x)\text{H}^+ \rightarrow \text{FeS}_2 + (1-2x)\text{Fe}^{2+} + (1-2x)\text{H}_2\text{O}$
	$\text{Fe}_{1-x}\text{S}(s) + (2-2x)\text{H}^+ + x\text{H}_2 \rightarrow (1-x)\text{Fe}^{2+} + \text{H}_2\text{S}$
(where x can vary from 0 to 0.125)	
Chalcopyrite	$\text{CuFeS}_2 + 4\text{O}_2 \rightarrow \text{Cu}^{2+} + \text{Fe}^{2+} + 2\text{SO}_4^{2-}$
	$\text{CuFeS}_2 + \frac{17}{2}\text{O}_2 + 5\text{H}_2\text{O} \rightarrow 2\text{Cu}^{2+} + 2\text{Fe(OH)}_3 + 4\text{SO}_4^{2-} + 4\text{H}^+$
Sphalerite	$\text{ZnS} + 2\text{O}_2 \rightarrow \text{Zn}^{2+} + \text{SO}_4^{2-}$
	$\text{ZnS} + 8\text{Fe}^{3+} + 4\text{H}_2\text{O} \rightarrow \text{Zn}^{2+} + 8\text{Fe}^{2+} + \text{SO}_4^{2-} + 8\text{H}^+$
	$\text{ZnS} + 2\text{H}^+ \rightarrow \text{Zn}^{2+} + \text{H}_2\text{S}$
Galena	$\text{PbS} + 2\text{O}_2 \rightarrow \text{Pb}^{2+} + \text{SO}_4^{2-}$
	$\text{PbS} + 8\text{Fe}^{3+} + 4\text{H}_2\text{O} \rightarrow \text{Pb}^{2+} + 8\text{Fe}^{2+} + \text{SO}_4^{2-} + 8\text{H}^+$
Arsenopyrite	$4\text{FeAsS}(s) + 13\text{O}_2 + 6\text{H}_2\text{O} \rightarrow 4\text{Fe}^{2+} + 4\text{SO}_4^{2-} + 4\text{H}_2\text{AsO}_4^- + 4\text{H}^+$
	$\text{FeAsS} + \frac{7}{2}\text{O}_2 + 6\text{H}_2\text{O} \rightarrow \text{Fe(OH)}_3 + \text{SO}_4^{2-} + 4\text{H}_2\text{AsO}_4^- + 3\text{H}^+$

In addition to pyrite, another common acid-generating iron sulphide mineral in the mining wastes is pyrrhotite (e.g. Thomas et al. 1998, Janzen et al. 2000). Weathering of pyrrhotite by oxygen leads to a similar acidifying process as pyrite, but the dissolution rate of pyrrhotite is usually found to be much higher (approximately 20 to 100 times) compared to that of pyrite in atmospheric conditions (e.g. Nicholson & Scharer 1994). Pyrrhotite dissolution can follow oxidative or non-oxidative pathways, depending on the pH conditions (Table 2). The non-oxidative mechanism is found to be orders of magnitude faster than the oxidative pathway (Thomas et al. 1998).

Besides iron sulphides, the oxidation of other metallic sulphides (e.g. chalcopyrite, sphalerite, pentlandite, galena or arsenopyrite) can also be an important mechanism controlling the quality of mine waste drainage. The dissolution of these sulphide minerals may or may not lead to acid generation, depending on the chemical conditions as well as the oxidant. For instance, the oxidation of chalcopyrite, sphalerite or galena by oxygen generally does not produce acids, but coupling with ferrous iron oxidation, ferrihydrite hydrolysis or the presence of dissolved ferric iron may initiate acid-generating processes (e.g. Dold 2010, Blowes et al. 2014). Nevertheless, the oxidation of these minerals has severe implications for mine waste weathering, as they may release hazardous toxic elements such as Zn, Ni, Pb, Cd, Ti, Cu or As, which can impact on the surrounding natural systems, as well as human health (Table 2). Arsenopyrite dissolution releases both sulphur and arsenic species. In this dissolution the oxidation of As(V) to As(III) is found to be more rapid compared to iron oxidation (e.g. Buckley & Walker 1988, Nesbitt et al. 1995). Table 2 summarizes the reactions involving the oxidation of sulphides particularly relevant in mining environments.

The acid generated in the sulphide mineral oxidation processes mentioned above can result in an extremely low range of pH (1.5–4), and such pH can even reach negative values under exceptional conditions within mining waste environments (e.g. Nordstrom et al. 2000). The increased acidity in the aqueous phase promotes the dissolution of acid-neutralizing minerals along the migration pathways of pore water containing low pH solutions. Such acid-neutralization reactions usually result in the progressive buffering of pH, often accompanied by the precipitation of metal-bearing oxyhydrox-

ides and oxyhydroxide sulphates, facilitating the removal of dissolved metals from the migrating pore water (e.g. Dold 2010). The most common pH-buffering minerals in mine settings are carbonates, aluminium and ferric hydroxides, and aluminosilicates. The pH of the drainage ultimately depends on the balance of acid and neutralizing minerals, their spatial variability, and their reaction kinetics in the waste.

Calcite, dolomite, ankerite and siderite, or their mixtures, are the most common carbonate minerals in mine wastes. The dissolution of these minerals leads to the release of alkaline earth and metal cations, such as Ca, Mg, Fe and Mn (e.g. Blowes et al. 2014). Among these carbonate minerals, calcite is found to be not only the most common, but also the fastest reacting carbonate mineral in the mining environment context. The dissolution of calcite neutralizes acidity as a result of hydrogen ion complexation with the released carbonate ion ( $\text{CO}_3^{2-}$ ) to form bicarbonate ( $\text{HCO}_3^-$ ) or carbonic acid ( $\text{H}_2\text{CO}_3$ ) (e.g. Blowes & Ptacek 1994). The rapid dissolution of calcite has the potential to buffer pH in a near-neutral range (6.5–7.0). However, the dissolution capacity of calcite has been shown to be pH dependent and generally increases under low pH conditions (e.g. Dold 2010) (Table 3). As the pH increases due to neutralization processes, calcite may also precipitate as a secondary mineral.

Besides calcite, another carbonate mineral observed in mine wastes is siderite, which can act as both an acid neutralizer and acid producer, depending on the chemical conditions (e.g. Dold 2010). Siderite may follow different reaction pathways, especially with the combination of ferrous iron oxidation and ferrihydrate precipitation. The dissolution of siderite buffers the pH of the system at around 5. The depletion of carbonate minerals typically leads to a drop in pH, which facilitates equilibrium with the next soluble phases, hydroxide minerals (Table 3). The dissolution of aluminium hydroxides (i.e. amorphous  $\text{Al(OH)}_3$  or crystalline form, gibbsite) maintains the pH in the region of 4.0–4.5, whereas the following soluble Fe hydroxide phases (such as ferrihydrite or goethite) buffer the pH values in the range of 2.5–3.5 (e.g. Blowes et al. 2014). Consequently, these mineral dissolution processes complement a buffering sequence starting with calcite (pH = 6.5–7.0) and followed by siderite (pH = 5.0–5.5). Upon the consumption of all carbonate minerals, the buffering is controlled by gibbsite (pH = 4.0–4.5), followed by iron hydrox-

ides ( $\text{pH} = 2.5\text{--}3.5$ ) (Ptacek & Blowes 1992, Blowes & Ptacek 1994). The dissolution of aluminosilicate minerals (e.g. chlorite, smectite, biotite, muscovite, plagioclase and amphibole) also has the potential to neutralize acidity and to mobilize a range of elements in pore water, including Al, K, Na, Ca, Mg and Mn. These silicates can undergo simultaneous

dissolution with carbonates and oxyhydroxides, but their reaction rate is usually kinetically controlled (except at a very low pH, it is generally much slower than that of carbonates) and their pH buffering is not constrained to a specific pH range (e.g. Amos et al. 2015).

Table 3. Acid neutralization reactions in mine wastes (Seal et al. 2003, Dold 2010).

Minerals	Reactions
Carbonates	$\text{CaCO}_3 + \text{H}^+ \rightarrow \text{Ca}^{2+} + \text{HCO}_3^-$
	$\text{CaCO}_3 + 2\text{H}^+ \rightarrow \text{Ca}^{2+} + \text{H}_2\text{CO}_3^0$
	$\text{FeCO}_3 + \text{H}^+ \rightarrow \text{Fe}^{2+} + \text{HCO}_3^-$
	$\text{FeCO}_3 + \frac{1}{4}\text{O}_2 + \frac{5}{2}\text{H}_2\text{O} \rightarrow \text{Fe(OH)}_3 + \text{H}^+ + \text{HCO}_3^-$
Hydroxides	$\text{Al(OH)}_3 + 3\text{H}^+ \rightarrow \text{Al}^{3+} + 3\text{H}_2\text{O}$
	$\text{Fe(OH)}_3 + 3\text{H}^+ \rightarrow \text{Fe}^{3+} + 3\text{H}_2\text{O}$
	$\text{FeO(OH)} + 3\text{H}^+ \rightarrow \text{Fe}^{3+} + 3\text{H}_2\text{O}$
Silicates	$\text{KAlSi}_3\text{O}_8 + \text{H}^+ + 7\text{H}_2\text{O} \rightarrow \text{K}^+ + 3\text{H}_4\text{SiO}_4 + \text{Al(OH)}_3$
	$\text{CaAl}_2\text{Si}_2\text{O}_8 + 2\text{H}^+ + \text{H}_2\text{O} \rightarrow \text{Ca}^{2+} + \text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$
	$\text{CaAl}_2\text{Si}_2\text{O}_8 + 8\text{H}^+ + \text{H}_2\text{O} \rightarrow \text{Ca}^{2+} + 2\text{Al}^{3+} + 2\text{H}_4\text{SiO}_4$

## 2.2 Microbiological processes

Microbiological processes can significantly affect the acid rock drainage problem by catalysing sulphide mineral oxidation reactions (e.g. Nordstrom 2000). In particular, bacterial species such as *Thiobacillus* and *Acidithiobacillus* are known to accelerate acid generation in waste rocks and tailings impoundments (e.g. Nordstrom & Southam 1997, Blowes et al. 2014). These microorganisms obtain energy from the oxidation of Fe(II) or reduced S species and are capable of deriving cellular carbon from the fixation of atmospheric carbon dioxide through the Calvin cycle (e.g. Dold 2010).

*Acidithiobacillus ferrooxidans* is the best known and most extensively studied species that plays a major role in the oxidation of  $\text{Fe}^{2+}$ , which is the rate-limiting step in pyrite oxidation under acidic conditions (e.g. Singer & Stumm 1970). The reaction rate in such microbially mediated pyrite oxida-

tion under field conditions is reported to be several orders of magnitude higher compared to the abiotic laboratory rate (e.g. Kirby et al. 1999, Nordstrom 2003). However, in mine environments, the specific microbe species responsible for microbial oxidation have also been found to change over time during the course of acidification (e.g. Leduc et al. 1993, Southam & Beveridge 1993, Blowes et al. 1995, Elberling et al. 2000, Moncur et al. 2005).

The detailed role of microorganisms in sulphide mineral oxidation, as well as in the overall geochemistry of mining environments, has been widely described and reviewed by Colmer and Hinkle (1947), Evangelou and Zhang (1995), Nordstrom (2000), Baker and Banfield (2003), Johnson and Hallberg (2003, 2005) and most recently by Blowes et al. (2014), among others.

## 2.3 Physical processes

Although the genesis of acid mine drainage is primarily related to the geochemical reactions occurring within the mined sediments, different physical processes also crucially control the quality and quantity of drainage. For instance, the amount of water available for the oxidation of acid-producing minerals is determined by hydrological processes such as precipitation and evapotranspiration. The abundant supply of oxygen, which is a controlling reactant for the sulphide mineral oxidation, is a function of water flow, gas transport and heat transport. Figure 1 represents a schematic diagram of the processes affecting drainage quality and how they are interconnected at a mine site.

### 2.3.1 Water flow and solute transport

The mechanism of water flow through mining waste facilities is controlled by the characteristics of the waste material (e.g. particle-size distribution, permeability, fractures and heterogeneity), the tim-

ing and extent of net infiltration, and the capillary pressure conditions in the porous matrix. The leachate quality of mine drainage and the transport of dissolved solutes (i.e. reactants and oxidized products) through waste materials is ultimately linked to the movement of the pore water.

Depending on the distribution of hydraulic conductivity, fracture networks and/or water saturation, fluid flow and solute transport in such systems can be dominated by different physical processes. For example, in waste rock piles, solute migration can typically be controlled by advective matrix flow or channelized preferential flow due to the presence of a mixture of coarse- to fine-grained rocks, as well as due to a wide distribution of void spaces (e.g. Smith & Beckie 2003, Nichol et al. 2005, Fretz et al. 2011, Blackmore et al. 2012, Neuner et al. 2013). In contrast, tailings impoundments generally contain fine-grained materials with a relatively high water content, typically resulting in a relatively

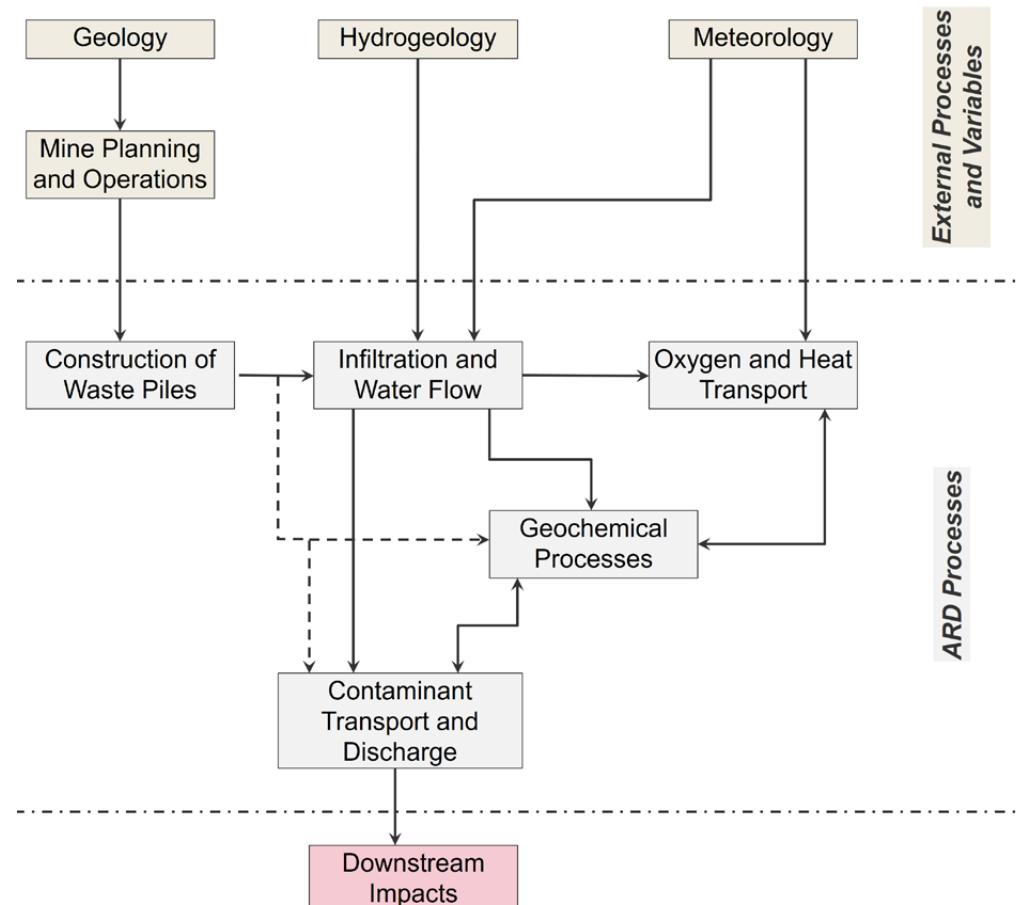


Fig. 1. Processes affecting the quality of drainage from waste piles (modified from Tremblay & Hogan 2000).

lower hydraulic conductivity than in the waste rocks (e.g. Blowes & Jambor 1990, Johnson et al. 2000, Moncur et al. 2005). The water migration rate in such settings is usually slow and can be affected by capillary forces. Therefore, in addition to advective processes, molecular diffusion and hydrodynamic dispersion can also play an important role in solute transport in these systems.

Furthermore, the transport of metals and metalloids, released from the sulphide oxidation and/or dissolution of other minerals, is also significantly affected by sorption or sorption-like mechanisms such as ion exchange and/or surface complexation (e.g. Appelo & Postma 2005, Dzombak & Morel 1990). The sorption of these metal ions is mainly induced from the surface charge, which originates from the ionization of surface functional groups of oxides, oxyhydroxides, and silicate minerals in contact with water (e.g. Davis & Ritchie 1986, Brown et al. 1995). Such processes usually take place at the solid–liquid interface and may form mineral–species complexes, providing the potential for removing dissolved species from the drainage water. The extent of sorption effects is dependent on the net surface charge, pH, temperature, dissolved metal concentrations and residence time (e.g. Parks 1990, Dzombak & Morel 1990, Stumm & Morgan 1996).

### 2.3.2 Gas and heat transport

Gas transport is another controlling factor determining the quality of drainage from waste piles, as it brings the potential reactants (e.g. oxygen) into contact with reactive sulphide minerals. In mining wastes, the transport of gases can take place by different mechanisms, including advective transport in the gas phase, diffusion in the gas phase, and/or advective and diffusive/dispersive transport of dissolved gases in infiltrating water.

Advective gas transport can generally occur due to the wind-driven air flow, pressure gradients resulting from the consumption of O<sub>2</sub> because of sulphide oxidation reactions within the waste piles, thermally driven density gradients, and/or barometric pressure changes (e.g. Amos et al. 2015). Diffusion is typically driven by concentration gradients (or more accurately chemical potential gradients) and leads to the net movement of a solute from a region of higher concentration to a region of lower concentration (e.g. Grathwohl 1998, Haberer

et al. 2015). In waste rock piles or tailings impoundments, this process can be the principal gas transport mechanism, especially in low permeability settings where advective processes are considerably inhibited (e.g. Pantelis & Ritchie 1992, Lefebvre et al. 2001a, 2001b).

Besides transport within the gaseous phase, the infiltrating water is also generally loaded with dissolved oxygen. Consequently, dissolved gases can undergo advective and diffusive/dispersive transport within the aqueous phase in porous media. Such solute transport processes can also be important in the supply of oxygen in sulphide oxidation reactions. However, the transport mechanisms in the water phase are often significantly slower (sometimes by orders of magnitude) compared to gas phase transport. For example, the transport of oxygen in water is almost 10,000 times slower than in air (e.g. Tremblay & Hogan 2000). The net capacity of oxygen (and other atmospheric gases) loading in water is also generally limited by the aqueous solubility limit. The maximum concentration of dissolved oxygen in water is known to be around 30 times less than in the atmosphere (e.g. Tremblay & Hogan 2000).

In unsaturated waste deposits, gas transport is often found to be tightly coupled with the heat transport process, as the movement of gases can carry a considerable amount of heat (e.g. Amos et al. 2015). This flow of heat in connection with seasonal temperature variations can lead to temperature gradients, which can influence sulphide oxidation rates and limit water flow through waste piles, between the pile centre and the external environments. The main heat transport mechanisms in mine wastes include convective (also termed advective) and conductive (also known as diffusive) transfer. The former is usually driven by air pressure gradients and it dominates in high permeability settings, whereas the latter refers to heat transfer through the bulk matrix by temperature gradients and is usually the dominant process in low permeability waste materials. Furthermore, sulphide oxidation reactions are exothermic and can generate a considerable amount of heat during the oxidation process. Therefore, such mechanisms may also lead to temperature gradients within wastes, facilitating thermally driven air flow into the waste facilities (Lefebvre et al. 2001a, 2001b, Pham et al. 2013).

## 2.4 Electrochemical processes

In addition to the processes discussed above, the final drainage quality in a mining environment can also be substantially affected by electrochemical processes. As such, electrochemical reaction steps or transfer of electrons, which occur at the mineral–water interface, can control the dissolution rate of sulphide minerals (e.g. Holmes & Crundwell 1995, 2000, Crundwell 2013). Galvanic effects are other well-known phenomena that can significantly modify the reactivity of pyrite and other sulphide minerals (e.g. Byerley & Scharer 1992, Subrahmanyam & Forssberg 1993, Salomons 1995, Lin 1997, Cruz et al. 2001, 2005, and Liu et al. 2008). Such galvanic reactions generally occur between conductive/semi-conductive minerals in water by forming a galvanic couple, which induces an electrical potential between the two contacting sulphide minerals (e.g. Kwong et al. 2003, Shuey 2012). As a result, the dissolution rate of a specific sulphide mineral is enhanced or hindered, depending on that particular sulphide being the cathode or anode of the developed galvanic cell (e.g. Mehta & Murr 1983, Holmes & Crundwell 1995). For instance, through

electrical coupling with other sulphides such as chalcopyrite or sphalerite, pyrite oxidation has been found to be significantly delayed, leading to supposedly long-term contamination in waste rock drainage, due to cathodic protection (e.g. Cruz et al. 2005). In contrast, the dissolution of other involved sulphides (chalcopyrite and sphalerite) is accelerated in the presence of pyrite (e.g. Cruz et al. 2005, Chopard et al. 2017). Moreover, the transport of dissolved ions can also be fundamentally controlled by electrochemical behaviour, as the sorption of H<sup>+</sup> and other ionic species occurs through electrical double layers at the mineral–liquid interface (e.g. Hiemstra et al. 1989, Appelo 1994, Kent et al. 2007, Prigobbe et al. 2014, McNeece & Hesse 2016). Furthermore, Coulombic interactions between different charged species can extensively modify fluxes, as well as the migration of individual ionic species, including protons, in a multi-ionic environment (e.g. Lasaga 1979, Giambalvo et al. 2002, Appelo & Wersin 2007, Appelo et al. 2010, Rolle et al. 2013, Muniruzzaman et al. 2014, Muniruzzaman & Rolle 2015).

## 3 LABORATORY AND FIELD TESTS IN WATER QUALITY PREDICTION

Several laboratory and field methods have been developed to characterise mine waste materials and to predict their long-term behaviour (cf. e.g. Lawrence & Day 1997, Meast et al. 2005, Price 2009). Thorough mineralogical and geochemical characterisation of wastes forms the basis for the prediction, prevention and management of their environmental impacts, and the collection of input data for the predictive modelling. Assessment of the potential of mine wastes to produce harmful mine drainage (i.e. AMD or NMD) is needed, especially in the planning of waste facilities as well as effluent treatment systems, and in selecting suitable methods for the closure of waste facilities.

In order to better prevent environmental impacts, mine waste characterisation already needs to be carried out during the exploration and planning phase of a mine, when no waste yet exists, and such characterisation should cover all the features of the generated waste fractions. In these phases, representative samples of waste rocks and tailings can be collected from exploration drillings and benefi-

cation tests, respectively. The waste rock samples should represent all different excavated waste rock types of the ore deposit. Block models are usually developed to define different geological units in the deposit in order to quantify and characterise the ore and the waste types. In the later phases of mining, such data on characterisation are updated and complemented to enable more detailed predictive modelling of the effluents and to determine appropriate waste management actions (e.g. Maest et al. 2005).

A typical waste characterisation scheme includes the determination of the mineralogical, geochemical, acid production and leaching properties of waste materials (Fig. 2), including possible analysis of mine waste's physical properties, e.g. particle-size distribution (PSD). These are needed to predict water quality from waste piles/facilities and to assist in the evaluation of quality of source term leachates that could be used as inputs for geochemical modelling. Nordstrom (2017) stressed that for background perquisites for modelling, one of the most useful aspects of geology is to identify minerals,

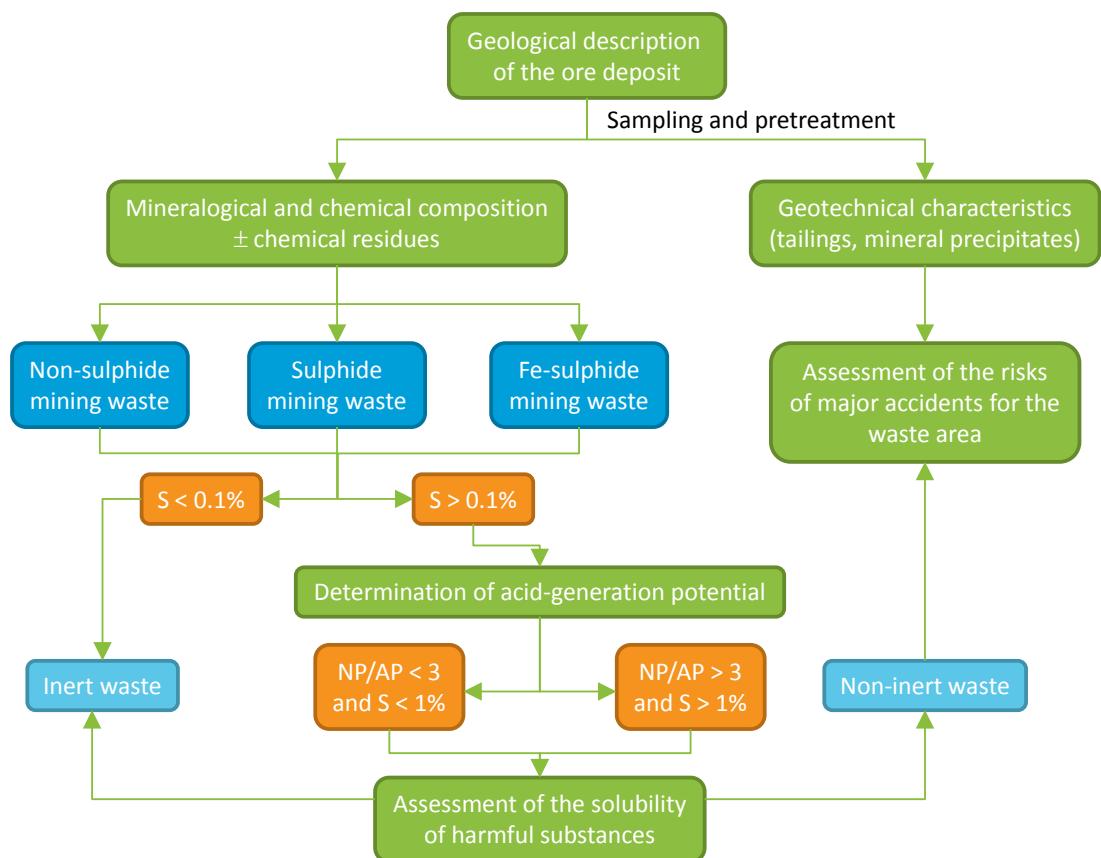


Fig. 2. Typical scheme for the characterisation of mining wastes (Kauppila et al. 2013).

their chemical composition, and relative solubilities and stabilities, as well as to understand rock types or lithologies, their main minerals and their mode of formation. Based merely on geological data (i.e. ore type, mineralogy) on the deposit, a preliminary assessment of the acid generation potential, neutralizing capacity and the occurrence of harmful elements in the waste can already be made.

Characterisation methods to assess the acid production potential and leaching properties of waste can be divided into two types: static and kinetic tests. Static tests are short-term laboratory analyses, usually good for preliminary investigation and screening. The results of static tests together with geochemical analyses can be used to select suitable samples for kinetic testing, and they can also provide threshold data for modelling (e.g. whole rock composition). The samples for kinetic tests should represent the different mine waste types and the range of leaching characteristics anticipated for the waste material (Declercq et al. 2017). Kinetic tests are longer-term tests, which reveal information on the leaching behaviour over time. These tests are usually more expensive, time consuming and with larger test settings. They are often used to provide

benchmarked data and verification of the modelling results. Static and kinetic test results can be coupled with information from the mine plan and water balance to develop numerical predictions of future seepage and runoff water quality associated with different mine waste facilities. Static and kinetic test data are usually used in mine drainage prediction in itself, without feeding the data to any additional computer model (e.g. White et al. 1999, Lapakko 2002, Maest et al. 2005, Price 2009).

Mine waste characterisation data can be utilized in drainage quality prediction, e.g. by the widely used thermodynamic equilibrium modelling approach, or the kinetic modelling approach (see e.g. Declercq et al. 2017). In thermodynamic equilibrium modelling, the geochemical data from static and kinetic tests is first scaled (for scaling, see chapter 4.2) to field conditions using the planned physical characteristics of the mine waste facility, which include the amount of waste, surface area, height, and grain size. Climate data can be coupled with this information to calculate mass balance predictions of leachate quality as a function of time. The scaled and mass balanced leachate chemistry can then be equilibrated using modelling tools, e.g.

PHREEQC, where thermodynamically favoured, potentially existing phases are allowed to precipitate, to assess the drainage quality in field conditions (Declercq et al. 2017). In the kinetic modelling approach, the dissolution and precipitation of the possible mineral phases present in the waste are allowed over a selected time period, on the basis of mineralogy, the reactivity equations for each mineral, temperature, particle-size distribution and reactive surface area parameters (Declercq et al. 2017).

A concise summary of the most common mine waste characterisation methods is presented in the following sections and in Table 4. For kinetic testing, special attention is paid to humidity cell testing (HCT), which is the most commonly used and the only standardized kinetic test method (Lapakko 2002). For more detailed information on the individual methods, several reviews and guidebooks are available, including Lawrence and

Day (1997), Maest et al. (2005) and Price (2009). In Europe, a standard for the characterisation of mining wastes has been published by the European Committee for Standardization (CEN/TR 16376:2012: *Characterization of waste – Overall guidance document for characterization of wastes from extractive industries*, Technical Committee 2012), and recommendations on the characterisation methods are included in the BREF document for mine wastes (*Reference Document on Best Available Techniques for Management of Tailings and Waste-Rock in Mining Activities*, EC 2009b; to be updated in 2018). Additional information on the methods is also available via a Wiki page of the Geological Survey of Finland (GTK): Mine Closure Wiki ([mineclosure.gtk.fi](http://mineclosure.gtk.fi); GTK 2017), which is an open internet resource on the technologies and approaches used in mine closure (Kauppila et al. 2016), including a section on mine waste characterisation (Karlsson & Punkkinen 2017).

### 3.1 Mineralogical and physical characterisation

Mineralogical characterisation can be used to determine the mineralogical composition, i.e. relative abundances of minerals in mine wastes. The main objective of the mineralogical characterisation of mine wastes is to identify the acid-generating and neutralizing minerals, potentially harmful substances containing minerals, and easily weathering minerals, e.g. salt minerals (e.g. Kauppila et al. 2013). Mineralogical methods can also be used to determine the relative degree of weathering of mineral grains. These analyses are essential in interpreting the results of static and kinetic tests. Thorough descriptions of the relationships between mineralogy and static and kinetic tests are presented, for example, by Jambor (2003) and Williams and Diehl (2014).

The physical characterisation of mine waste is essential for many modelling approaches (Declercq et al. 2017), and includes the determination of the mass, moisture, particle-size distribution and reactive surface area. The physical properties of mine waste and the physical differences between laboratory settings and the field size mine waste facility also affect the scaling up of laboratory test results to the field scale (Malmström et al. 2000, Kempton 2012, Kirchner & Mattson 2015), which is often done before actual modelling to provide more detailed information on the reaction kinetics (Nordstrom 2017).

Various methods are available to quantify the mineralogical composition of mine wastes, and other mineralised and non-mineralised materials. Common methods for mineralogical analysis include optical microscopy (OM), scanning electron microscopy (SEM) and X-ray diffraction (XRD). In addition, microprobes can be used to identify the chemical composition of individual minerals and to gain information on the sorption of different elements, in particular toxic trace metals in mine wastes.

In OM, a detailed investigation of a thin section prepared from a mine waste sample is carried out with a petrographic microscope, i.e. using transmitted light microscopy or reflected light microscopy. OM is typically used to define the quantitative mineralogical composition of waste rocks, whereas the tailings are generally so fine-grained that their mineralogical composition is more practical, rapid and reliable to measure with the SEM technique. If a sample contains opaque minerals such as oxides and/or sulphides, as mine waste samples often do, polished thin sections and reflected light (ore microscopy) is used. The mineral abundances can be determined, for instance, by a standard point-counting method with 600 points, when the general grain size and the occurrence of opaque minerals of the sample make this possible. After the calculation of mineral abundances, the rock type is classified

**Table 4.** Examples of common characterisation methods for mine wastes. (PSD = particle-size distribution).

<b>Method</b>	<b>Description</b>	<b>Reference / Standard / Guide</b>
<b><i>Mineralogical methods</i></b>		
Optical microscopy (OM)	Transmitted/reflected light microscopy, point-counting of minerals	EN 932-3:1996 and amendment A1:2003
Scanning electron microscopy (SEM)	Information on e.g. mineral abundances, chemical composition, grain size and microstructures	e.g. Swapp 2014
X-ray diffraction (XRD)	Quantitative and qualitative mineralogy for crystalline samples, especially clay minerals	e.g. Reynolds 1989
<b><i>Particle size measurements</i></b>		
Sieving	PSD for particles >0.063 mm	SFS-EN 933-1
Wet method laser diffraction	PSD for particles <0.063 mm, based on scattering of a laser beam	e.g. Cepuritis et al. 2017
X-ray sedimentation	PSD for particles <0.063 mm, based on particle sedimentation speed and equivalent Stokes diameter	e.g. Cepuritis et al. 2017
<b><i>Static tests and related determinations</i></b>		
Modified ABA test	Quantifying the potential of a sample to produce and neutralize acid	CEN/EN 15875 (CEN 2011), Sobek et al. 1978
Total sulphur for acid production potential (AP)	S combustion in e.g. a LECO furnace	ISO 15178 (ISO 2000)
Neutralisation potential (NP)	Titration by HCl to pH 2.0–2.5	CEN/EN 15875 (CEN 2011), Lawrence & Wang 1997
Net acid generation (NAG)	Acid generation based on the reaction of a sample with hydrogen peroxide	Miller et al. 1990, AMIRA 2002
<b><i>Chemical extractions</i></b>		
XRF	Total element concentration	Criss & Birks 1968
Aqua regia	Leaching of sulphide fraction	ISO 11466 (ISO 1995), Doležal et al. 1968, Heikkinen & Räsänen 2009
Ammonium oxalate	Leaching of Fe(III)oxyhydroxides, Fe(III)oxides	Räsänen et al. 1992a, Dold 2003, Heikkinen & Räsänen 2008
Ammonium acetate	Leaching of exchangeable and carbonate fractions	Gatehouse et al. 1977, Sondag 1981, Dold 2003, Heikkinen & Räsänen 2008
Ammonium chloride	Leaching of physically adsorbed, easily leachable, bioavailable fractions	Heikkinen & Räsänen 2008
<b><i>Leaching tests</i></b>		
Two-stage batch leaching test	Leaching of water-soluble fraction	SFS-EN 12457-3
Column leaching test	Leaching of water-soluble fraction	CEN/TS 14405 (CEN 2017)
<b><i>Kinetic tests</i></b>		
Humidity cell test (HCT)	Small-medium scale laboratory test	ASTM 2013, CEN/TR 16363 (CEN 2012)
Field scale lysimeter test	Non-standardized medium- to large-scale field test	Hansen et al. 2000
Large-scale test pile	Non-standardized large-scale field tests	INAP 2009, MEND 2012

according to the recommended nomenclature. A simplified petrographic description, of which OM is a part, can be made in accordance with the European Standard EN 932-3:1996 with the incorporation of its amendment A1:2003.

SEM produces superficial images of a sample by scanning it with an accelerated and focused beam of electrons. The electrons interact with the sample, revealing information concerning the texture, chemical composition, and crystalline structure and orientation of the sample material. The geological applications of SEM are widely used, e.g. in determining mineral abundances, grain sizes and microstructures. The SEM method is rapid and accurate in identifying environmentally hazardous minerals, i.e. typically sulphide minerals, as well as those minerals providing neutralizing capacity in mine wastes. It is also optimal in studying the weathering state of minerals, particularly sulphide minerals, and their weathering products. In addition, SEM can provide information on the mineral associations of various minerals and element distributions within the minerals. In preliminary mine waste characterisation, SEM can provide information concerning overall mineralogy, the grain-size distribution and elemental deportments, to make an initial assessment of the environmental properties of mine waste and to produce essential information for modelling purposes. Several types of SEM setups and variations exist, with the differences being mainly in the amount and characteristics of the attached detectors (BSE, SEI, CL), spectrometers (EDS, EDX) and software (e.g. MLA, QEMSCAN, AMICS, INCA, Aztec). (e.g. Swapp 2014, Karlsson & Kauppila 2017)

XRD can be used for the reliable, swift quantitative and qualitative identification of minerals, mineral abundances and the most technical products. However, this method is most suitable

for crystalline samples, and especially useful for clay mineral determination. For mine wastes, this method is typically used to define their preliminary modal mineralogy or to identify the mineralogical composition of secondary precipitates or sludges. XRD studies are commonly complemented with SEM studies, and occasionally also with other methods, e.g. thermal analysis or infrared spectrophotometry (Reynolds 1989, Karlsson 2017).

The particle-size distribution of a mine waste sample can be obtained, for example, by sieving according to the standard SFS-EN 933-1. The standard sieving method is suitable for particle sizes ranging from a few hundred millimetres to 0.063 mm. Estimation of the particle-size distribution in a waste rock pile is challenging, as very large-scale sieve analyses, which are needed for boulders with diameters up to thousands of millimetres, are difficult to perform. Some widely varying waste rock PSD estimations from previous studies have been presented by Kempton (2012). Particle sizes below 0.063 mm can be analysed by several methods, for example with wet method laser diffraction or with X-ray sedimentation. The former is based on the scattering of a laser beam passing through a dispersed particulate sample, while the latter is based on the particle sedimentation speed and equivalent Stokes diameter (Cepuritis et al. 2017). According to Cepuritis et al. (2017), these two methods are recommendable, since a large amount of surface area is concentrated among the very small particles (even below 5 µm). However, in many cases, sieving may need to be combined with one of these measurements to cover the whole range of particle sizes in the waste material. The surface area of a sample can be calculated, for example, based on the PSD and by using MDAG Grain 3.0 software, which can be accessed from <http://www.mdag.com/grain30.html> (Declercq et al. 2017).

### 3.2 Geochemical characterisation

The geochemical characterisation of mine wastes is carried out to identify the primary contaminants and other elements of concern in the wastes and to assess the leachability of substances from the wastes. Analytical methods for determining the element concentrations in rock samples can generally be categorized as destructive or non-destructive. Non-destructive methods leave the sample intact, whereas destructive methods dissolve the sample. A common non-destructive method is X-ray fluores-

cence spectrometry (XRF), which is used to analyse the total chemical composition of wastes. In this method, a sample is subjected to short wavelength X-rays, which in turn induce the emission of longer wavelength X-rays from the sample. In some XRF methods, the sample is fused into lithium borate glass and would therefore be considered as destructive (Crock et al. 1999, Lapakko 2002).

Destructive methods for total element concentrations include the use of multiple strong acids,

e.g. a combination of hydrofluoric, hydrochloric, nitric and perchloric acids, to digest the sample (e.g. Briggs 2002, Briggs & Meier 2002). Certain minerals, e.g. spinels, zircon and chromite, are resistant to acid digestion and must be subjected to sintering or fusion and subsequent acid digestion to bring them into solution. The resulting solutions are usually analysed with atomic absorption spectroscopy (AAS), inductively coupled plasma–atomic emission spectroscopy (ICP–AES), and/or inductively coupled plasma–mass spectrometry (ICP–MS) (Hall 1995, Rautiainen et al. 1996, Crock et al. 1999, Lapakko 2002).

As the total element concentrations do not reveal information concerning element mobility, various extractions and short-term leaching tests have been developed to evaluate whether potentially harmful elements or compounds are prone to mobilizing from mine wastes. A wide range of selective extraction methods, targeting a particular chemical fraction in the mine wastes, is available with an objective to simulate the mobilisation of elements in specific environmental conditions. The chemical compositions of the leachate solutions are usually measured with ICP–AES and/or ICP–MS (e.g. Hall et al. 1996, Dold & Fontboté 2001, Kauppila 2017).

Commonly used selective extractions include hot aqua regia (Niskavaara 1995) to determine the concentrations of acid-soluble elements. The aqua regia method reflects the element concentra-

tions bound to mica, clay, salt and sulphide minerals (Doležal et al. 1968, Räisänen et al. 1992b). Weaker leaching methods can be used to investigate, for example, elements adsorbed to the surface of minerals and mineral precipitates, with either a sequential or single extraction. Weaker extract solutions include distilled water for the water-soluble fraction (Dold 2003), ammonium chloride for physically adsorbed, easily leachable and bio-available fractions (Heikkilä & Räisänen 2008), ammonium acetate for exchangeable and carbonate fractions (Gatehouse et al. 1977, Sondag 1981, Dold 2003, Heikkilä & Räisänen 2008), and ammonium oxalate for Fe(III) oxides and oxyhydroxides (Räisänen et al. 1992a, Dold 2003, Heikkilä & Räisänen 2008).

According to the European Commission Decision on the characterisation of waste from the extractive industry (EC 2009a, Decision 2009/360/EC) and the Finnish Government Decree on mining waste 190/2013 (Government Decree 2013), the leachability of elements should be evaluated with the pH dependence leaching test, percolation test, time-dependent release and/or other suitable testing. Such tests recommended by the European mining waste characterisation standard (Technical Committee 2012) include the two-stage batch leaching test/shake-flask test according to CEN/EN 12457-3 (CEN 2002) and the column leaching test CEN/TS 14405 (CEN 2017). Distilled water is used as a leaching solution in both of these tests.

### 3.3 Static tests

Static characterisation tests are short-term and relatively low-cost tests for the classification of different waste types and estimating the capacity of mine wastes to produce acidic drainage. Static tests are commonly used as a screening tool, as these tests do not consider, for example, the availability of acid-producing or neutralizing minerals, or differences between the respective dissolution rates of minerals (Lapakko 2002).

The most commonly used static test is the acid-base accounting (ABA) test, which includes several variations such as the modified Sobek method (Sobek et al. 1978) and a test based on the standard CEN/EN 15875 (CEN 2011). The ABA tests aim at quantifying the potential of mine waste material to produce and neutralize acid (Sobek et al. 1978, Price 1997, Price et al. 1997, Lapakko 2002). The acid production potential (AP) is based either on the total sulphur

content of a sample, measured, for example, using a combustion furnace (the so-called LECO furnace, ISO 2000), or on the sulphide sulphur content. The latter is often determined by removing the non-sulphide sulphur phases from the sample and measuring the difference between the total sulphur content and the removed sulphur phases (Lapakko 2002). Determination of the neutralization potential (NP) can be challenging, as a variety of minerals neutralize acidity (cf. chapter 2.1) and these minerals dissolve with variable intensity in different static tests, depending on the reagents used and the duration of the test period. Therefore, different static tests may produce markedly different results for the same sample (e.g. Jambor 2003, Räisänen et al. 2010). A commonly used NP determination method is the titration method EN15875, which is a modification of the method by Lawrence and Wang (1997).

Based on the ABA test results, the potential risk of acid production is estimated based on the ratio of NP and AP ( $NP/AP =$  neutralization potential ratio NPR) or their subtraction ( $NP-AP =$  net neutralization potential NNP). Mine waste is considered as potentially acid generating if  $NPR < 1$  or  $NNP < -20$ , in the uncertainty zone if  $NPR$  is  $1-3$  or  $NNP$  is  $-20 - +20$ , and non-acid generating if  $NPR > 3$  or  $NNP > 20$  (Sobek et al. 1978, White et al. 1999, Lapakko 2002, Price 2009). These limit values for the acid generation potential should be considered as rough guidelines and risks should still be evaluated site specifically, although non-acid-generating values have been obtained from the bulk analysis of mine waste. Pedretti et al. (2017b) estimated, for example, that 40% of waste rock piles with a bulk NPR of 4 can be expected to generate acidic drainage after 100 years.

Another test to assess the acid production potential of rock material is the net acid generation (NAG) test (Miller et al. 1990). The NAG test is based on the

reaction of a sample with hydrogen peroxide, which accelerates the oxidation of sulphide minerals in the sample. During this test, acid generation and acid neutralisation reactions can occur simultaneously, with the end result representing a direct measurement of the net amount of acid generated by the sample (AMIRA 2002). This test does not separately estimate the neutralisation potential. Therefore, the AMIRA guidebook (2002), for example, recommends the use the net acid production potential (NAPP) together with NAG for more detailed classification of acid generation. The acid production potential of a sample can be obtained from the NAGpH and NAPP value. The material is considered non-acid forming if  $NAGpH > 4.5$  and NAPP is negative, and potentially acid forming if  $NAGpH < 4.5$  and NAPP is positive (AMIRA 2002). The NAG test can also be classified as a kinetic test, when the pH and temperature are monitored during a single-addition NAG test (Morin & Hutt 1999, Räisänen et al. 2010).

### 3.4 Kinetic tests

In kinetic testing, mine waste material is subjected to leaching, usually with an objective of observing the long-term acid generation behaviour of the mine waste and assessing whether it will generate poor quality drainage, posing hazards to the environment. Kinetic tests are also used to determine mineral oxidation and dissolution rates. In kinetic laboratory tests, mineral weathering is generally accelerated beyond that observed in the field (excluding some wet tropical environments). In kinetic laboratory tests, the effects of weathering can be better observed compared to field observations, for instance due to the relatively large fraction of the rock mass exposed to oxygen and large amount of water per unit mass of rock (Lapakko 2002, Gautama et al. 2015).

Kinetic tests can be carried out in the laboratory or at the field scale. Both approaches have advantages and disadvantages. In the laboratory, measured parameters (e.g. the interval and volume of flushing water, temperature, leachate quality) are generally more controlled than in the field. In contrast, field tests require a longer observation time and have larger costs, but they are considered to give more realistic results (Lapakko 2002, Gautama et al. 2015). However, the results of field tests are highly dependent on the local environmental conditions. A technical report by the European Committee

of Standardization (CEN) provides detailed guidance on kinetic laboratory tests (CEN/TR 16363, CEN 2012).

The objectives of studies related to the different kinetic tests define the testing data to be obtained. According to the CEN/TR 16363, the key parameters to be measured during a kinetic test commonly include the weight of the sample, pH, alkalinity, sulphate, total dissolved solids, key metals (e.g. copper for copper mines, etc.) and element concentrations (anions and cations) in the leachate (CEN 2012). To understand the geochemical processes taking place within the test, other relevant information may include the flow rate of air and water, oxygen/carbon dioxide concentrations during the test run under sealed conditions, temperature, mineralogy/speciation before and after testing, speciation/element availability before and after testing, and grain size or surface area evaluation before testing (CEN 2012).

The results from kinetic testing are typically presented as the concentration or accumulated concentration plotted against time, and are used with the data from static tests, mineralogical and geochemical analyses and geochemical/reactive transport modelling in predicting the effluent quality of mine wastes under a range of conditions. To obtain a more realistic evaluation of the loadings and the

potential impact on the environment, kinetic test results are typically scaled up (cf. section 4.2) and used with water balances (Kempton 2012, INAP 2009).

### 3.4.1 Humidity cell test

The humidity cell test is the most common kinetic laboratory test method (Lapakko 2002), and is the only kinetic method normalized by the American Society for Testing and Materials (ASTM). Although the HCT is widely used in industry and research, it is not currently commercially available in Finland. The method was designed to enhance the weathering of mine wastes to conveniently produce and collect soluble weathering products (ASTM 2013). HC testing is used for assessing of rate of oxidation under laboratory conditions and long-term rates of acid generation (especially when a static test suggests that the ability of a mine waste sample to produce acid drainage is uncertain) and metal mobilisation (Maest & Nordstrom 2017, CEN 2012). A commonly used HCT procedure is the ASTM D5744-13 method (ASTM 2013), which is modified from the laboratory weathering procedure originally developed by Caruccio (1968) and revised by Lawrence (1990) and Ferguson and Morin (1991) (ASTM 2013, Maest & Nordstrom 2017, Punkkinen et al. 2017).

In the HCT, 2 to 5 kg of crushed sample material is commonly subjected to several tens or even hundreds of weeks of HC testing, including the collection of weekly effluents and their analysis for a range of laboratory parameters, in addition to the major and trace element chemistry (CEN 2012). The recommended duration of the test in the original ASTM HCT standard (ASTM 1996) is 20 weeks. The recent ASTM versions (2007, 2013) do not define a specific length for the test. Instead, they state that the solutes should be measured weekly for at least the first two weeks, every other week until week 20 and less frequently thereafter. According to the MEND publication (Price 2009), HCTs should be continued until  $\text{SO}_4^{2-}$  and metal leaching rates stabilize for at least five weeks, which could take from 40 weeks to even several years. According to Maest and Nordstrom (2017), the minimum length of a HCT should be at least a year.

While the HCT method is standardized, a substantial challenge is related to the interpretation of the test results. For example, no specific requirements or expert qualifications exist for authorities for conducting or interpreting the HCT results,

even though the environmental risk assessment of mine waste facilities and the assessment of whether water quality standards are met is often based on HCT results (Maest & Nordstrom 2017). Based on the ASTM standard (2013), the HCT would be suitable for simulating site-specific leaching conditions. However, according to Maest and Nordstrom (2017), it can only be used to determine changes in drainage quality with changing composition for a particular rock type. This, together with the lack of guidance in using HCT results, might cause certain dubiousness for practitioners (Maest & Nordstrom 2017).

In evaluations connected with mine permits, drainage quality assessments are usually based on the use of “steady state” or “stable” values and concentrations (Maest & Nordstrom 2017). They are usually defined as the average of the last five weeks of testing (Price 2009). There are, however, some problems related to the use of steady state values. For example, differing steady state conditions have been noticed to occur at several time periods in a test that has been running for long enough. Furthermore, predictions based on steady state rates tend to ignore the conditions producing highest solute concentrations (e.g. heavy rainfall events, snow melt; Maest & Nordstrom 2017). In addition to steady state values, Maest and Nordstrom (2017) suggest that more attention should be paid to the “early flush”, which is typically ignored (Price 2009), and to the maximum sulphide oxidation rates. “Early flush” refers to the early portion of HCTs, wherein soluble salts tend to be flushed out. Maximum sulphide oxidation rates can be obtained from the change in dissolved  $\text{SO}_4^{2-}$  concentrations over the time that Fe and  $\text{SO}_4^{2-}$  concentrations are increasing most rapidly (Maest & Nordstrom 2017).

In the HCT, special attention is typically paid to the oxidation rate of sulphide and neutralizing minerals by observing changes in Fe,  $\text{SO}_4^{2-}$  and major element concentrations and pH (Maest & Nordstrom 2017). Samples producing acid drainage typically have neutral initial pH values, which drop below 6 as the test progresses, while Fe and  $\text{SO}_4^{2-}$  concentrations increase. Partially weathered sulphide-bearing samples typically show elevated initial  $\text{SO}_4^{2-}$  concentrations in the early flush (together with other substances, e.g. Ca, Cu, Ni, depending on the sample material), which decrease rapidly followed by a later increase in these concentrations before the values level off. Although the sulphide mineral oxidation rate is strongly dependent on Fe- and S-oxidizing bacterial activity, the microbial influ-

ence is rarely monitored or assessed in HCTs (Maest & Nordstrom 2017).

The mineralogy of the tested material should be thoroughly investigated before and after HC testing, also taking into account secondary minerals. In particular, the behaviour of the secondary minerals, such as relatively soluble sulphate salts (Jambor et al. 2000), is largely ignored when interpreting the HCT results. In general, when interpreting the changing chemical conditions during an HCT, the iron mineral solubility is a key aspect. Therefore, to understand the main HCT leachate quality controlling reactions, data on Fe(II) and Fe(III) concentrations is necessary. In field conditions, secondary minerals from sulphide oxidation can be present intermittently and repeatedly from year to year, strongly affecting the mine drainage quality, which also advocates for the utilization of early flush HCT results (Maest & Nordstrom 2017).

Based on the mineralogical information and measured concentrations of, for example, Fe, SO<sub>4</sub> and possible metals in the leachate, the most likely minerals responsible for the leachate quality changes can be pinpointed. Possible dissolving phases controlling the leachate quality can be assessed, for instance, by inverse modelling with PHREEQC using the WATEQ4F database (Maest & Nordstrom 2017).

The assessment of which minerals are dissolving can be based on the mineral stoichiometry and leachate molar concentrations (Price 2009). For example, the Fe:S ratio in some common sulphide minerals such as pyrite (FeS<sub>2</sub>) and chalcopyrite (CuFeS<sub>2</sub>) is 1:2, and the ratio in pyrrhotite (Fe<sub>1-x</sub>S) is close to 1:1. If the leachate Fe:S ratio is notably low, Fe loss can be expected, e.g. by Fe hydroxide precipitation. In this case, SO<sub>4</sub> might be a better constituent for oxidation rate calculations than Fe (Maest & Nordstrom 2017). If the SO<sub>4</sub> concentration is notably high, dissolution of gypsum can be suspected. The masking of sulphide dissolution by gypsum dissolution can be confirmed by inspecting Ca concentrations, especially if no easily leachable carbonates are present. If gypsum dissolution is confirmed, the leachate SO<sub>4</sub> concentration can be corrected to present sulphide dissolution by subtracting the Ca molar concentration in relation to the SO<sub>4</sub> molar concentration, according to gypsum stoichiometry (Ca:SO<sub>4</sub> in gypsum is 1:1) (Maest & Nordstrom 2017).

For more detailed information on the HCT geochemistry, the publication "A geochemical examina-

tion of humidity cell tests" by Maest and Nordstrom (2017) is recommended. Some suggestions by Maest and Nordstrom (2017) that might improve the HCT procedure and prediction quality are listed here:

- More guidance is needed for more consistent interpretation of HCT results.
- Early flush concentrations and maximum sulphide oxidation rates should be used more often in environmental models.
- HCT samples should be stored for a sufficient amount of time to allow sulphide oxidation and secondary mineral formation so that the variety of geochemical reactions occurring in the field could be better mimicked.
- Determination of Eh, Fe(II) and Fe(III) concentrations can enhance understanding of geochemical reactions, especially if the leachate pH is below 4.0.
- Plotting major cations and anions in molar units together with pH on a single graph, instead of the commonly used custom of plotting single constituents (e.g. SO<sub>4</sub>) of many samples on the same plot, may enhance the understanding concerning the composition of soluble salts in early flushes and geochemical behaviour throughout the test.
- The quality of analytical chemistry measurements should be systematically evaluated, e.g. by examining charge and conductivity balances utilizing WATEQ4F.
- Information on possible HCT method modifications should be presented, as they affect the leachate chemistry. Strong effects are caused by changes in, for instance, the water-to-rock ratio, particle size and volume of the solution used. It should also be mentioned how the solution was added: i.e. trickle versus flood leaching.
- The scaling of laboratory results to field conditions is a major unresolved problem that limits the usefulness of HCTs. Therefore, further research should be conducted on the comparison of laboratory, pilot and field-scale tests, and to assess the effects of seasonal changes in the field (cf. also Malmstrom et al. 2000)

### 3.4.2 Field-scale kinetic tests

Large-scale field lysimeter (or field column) tests are outdoor leaching or percolation tests, where the test material is placed in a container with an open surface. These tests are carried out under natural field-resembling conditions over a longer period of time. They simulate the actual field conditions

better than laboratory tests and are suitable for verifying the results obtained in the laboratory. Lysimeter tests are useful for scientific studies investigating the fate and movement of water, dissolved elements, and other potential contaminants in waste piles. Lysimeters have also been used in assessing water percolation through and evaporation from soil and waste, and to evaluate solute transport. For ARD prediction and metal leaching assessments, lysimeter tests should be implemented in the early stages of the mining operations, since they require a number of years before meaningful results can be obtained and conclusions can be made (Hansen et al. 2000, Urrutia et al. 2011).

The largest scale of field test setups includes pilot cells, test piles, test plots or test pads, which are constructed for long-term monitoring of large quantities of mine waste material. Large-scale set-

ups facilitate the extrapolation of the test results to full-scale waste facilities, as these tests have more representative sample dimensions and particle size, and they minimize the impacts related to boundary effects, sample heterogeneity and a reduced grain size. The construction and assessment of the effects of different cover structures can, for example, also be carried out on field test piles, although the test piles should be relatively large. MEND (2012) suggested minimum dimensions of 1 ha for a test pile to avoid the influence of boundary conditions while monitoring water and energy parameters. The construction and monitoring of test piles require thorough planning, as a comprehensive understanding of chemical and physical reactions, water balance and water movement, and the role of atmospheric gases is not generally straightforward (INAP 2009).

### 3.5 Summary of the characterisation methods and their use in water quality prediction

The characterisation methods, their relevance for water quality prediction and the data they provide

for predictive modelling are summarised in Table 5.

Table 5. Summary of the use of mine waste characterisation methods in the water quality prediction of wastes (after Maest et al. 2005 and Price 2009).

Characterisation method	Relevance for water quality prediction	Input data for predictive modelling / use in modelling
Mineralogy	Identification of primary and secondary minerals, acid-producing and neutralizing minerals and sources of harmful substances; Evaluation of drainage acidity based on the balance between acid-producing and acid neutralizing minerals, Information on the degree of mineral alteration and occurrence type of minerals (crystal forms, liberation state)	Mineral phases and their abundances, relative reactivity rates of different minerals, availability of minerals to weathering
Whole rock analysis	Total potential load of elements to the environment; identification of substances of concern	Identifying rock types with high total levels of potentially harmful elements, helpful in the determination of sample mineralogy
Short-term leach tests	Determination of readily soluble contaminants to be present in leachate	Indication of leaching of salts and readily soluble components from wastes
Selective/sequential extractions	Evaluation of associations of substances of interest with solid phases and assessment of how easily they will be released from wastes	Understanding the occurrence of harmful substances and geochemical conditions in which they may be released to the environment
Static tests	Preliminary assessment of whether drainage will be acidic; guides the selection of materials for further testing	Estimate of the neutralizing and acid generating content and potential of waste material
Kinetic tests	Evaluation of longer-term acid generation/neutralization balances and leaching of potential substances from wastes; more detailed, site specific data on drainage quality; estimates on the acid generation lag time	Oxidation and dissolution rates of minerals, rates of acid generation and neutralization, steady-state pH values, time to net acidic conditions, drainage chemistry and chemical release rates

## 4 MODELLING APPROACHES FOR THE PREDICTION OF EFFLUENTS FROM MINE WASTES

### 4.1 General principles

Prediction of the long-term quality of mine waste drainage aims at defining the type, magnitude, location and timing of measures needed to prevent environmental impacts (Price 2009). Prediction is typically already required in a phase in which waste facilities or piles do not yet exist, i.e. during mine planning, in the environmental impact assessment or environmental permit procedure, to plan the necessary management actions in order to prevent adverse environmental impacts of waste disposal. During mining operations and mine closure, such a prediction scheme should be reviewed and subsequently updated based on the realized environmental properties of the wastes and the monitoring data on effluent quality (e.g. Maest et al. 2005, Kauppila et al. 2013).

In the context of mining wastes, the term “prediction” means “a suite of integrated approaches used to determine in advance the geochemical behaviour of mining waste” (Trembley & Hogan 2000). Basically, prediction involves a set of different laboratory and field-scale tests that are used as a basis and data input for the predictive modelling (cf. Chapter 3).

The key questions the prediction should be able to answer include the following:

- What will be the quality of water discharging from the waste facilities/piles?
- Is there a risk of AMD/NMD? When is the AMD/NMD expected to start and how long will it last?
- Does the discharge quality pose hazards to the receiving water bodies, biota and the environment?
- How will the water quality evolve during operations?
- What types of control measures are needed to prevent negative impacts on watersheds? (e.g. Lawrence & Day 1997, Tremblay & Hogan 2000, Price 2009)

Addressing these questions is very challenging, as the data for the prediction can often be quite limited in the planning phase of a mine, which increases the uncertainty of the prediction. Typically, the data available for predictive modelling during this phase include background and baseline data on the site, plans for the disposal, mineralogical and chemical

composition of the wastes and the results of static and/or kinetic tests on the wastes. A predictive model can be only as good and accurate as the input data, the conceptual model used, and the modeller's understanding of the hydrogeochemical processes (e.g. Alpers & Nordstrom 1999, Bredehoeft 2005, Seppälä & Tuominen 2005). In addition, uncertainty in the modelling generally increases with an increasing simulation time period; hence, long-term model predictions are usually susceptible to the greatest level of inaccuracy (e.g. Bredehoeft 2005). Consequently, due to the heterogeneity of the waste materials, challenges in estimating rates of mineral weathering in the long-term, and the limited accuracy of the prediction methods, the output of the predictive model will even at its best be a range of contaminant concentrations in the drainage and should be considered as indicating long-term trends instead of providing absolute values (Maest et al. 2005, Price 2009, Pedretti et al. 2017a).

Even though models always involve uncertainty, they can still be useful in helping us to understand how waste facilities function and also to make indicative predictions of their future performance (e.g. Bredehoeft 2005). Nevertheless, one should be aware of that the model applied is representative of the site, and the complexity of the model is in accordance with the available data and the regulatory decisions that need to be made, for example, on the effluent management techniques (Maest et al. 2005).

Predictive modelling of drainage quality from waste materials combines hydrogeological and geochemical modelling approaches and typically follows a general modelling scheme (Fig. 3). In the first step, the purpose or objective of the modelling is defined. This phase also includes the collection of input data for the model. Ideally, there is a large set of data to be used in the modelling, providing information on the variation in the hydrogeological and hydrological conditions and the properties of wastes. In practice, a baseline study is usually the main source of information for the hydrogeology and hydrology of the site, and waste properties are based on the preliminary characterisation studies carried out for the environmental impact assessment. The mine plan provides details for the design

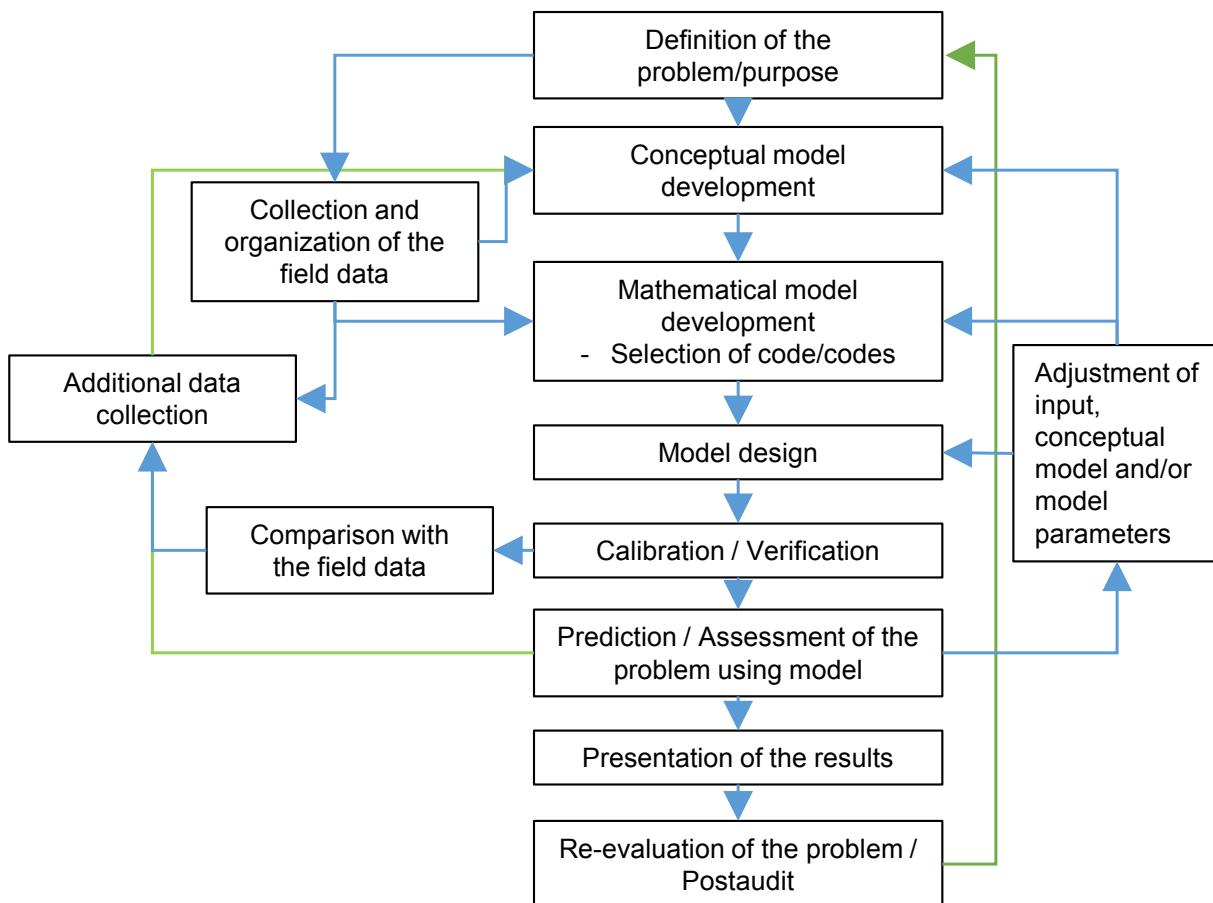


Fig. 3. General modelling process (modified based on Reilly 2001, Anderson & Woessner 2002, Zheng & Bennett 2002).

and disposal type of the waste and for the potential mitigation measures. The data requirements for the predictive modelling of waste materials are discussed in more detail in Chapter 5 of this report.

The next, and the most important, step in the modelling is the development of a conceptual model (e.g. Bredehoeft 2005, Maest et al. 2005, Kresic 2007). Basically, this is a description of the main physical and chemical processes in a system, i.e. the hydrology, hydrogeology and geochemistry of the site (Lefebvre et al. 2001, Maest et al. 2005). In other words, it corresponds to the site characterisation and is the foundation for the model (e.g. Zheng & Bennett 2002, Bredehoeft 2003, Bredehoeft 2005). The conceptual model simplifies the field conditions, promotes the organization of the associated field data and forms the basis for the numerical model (Anderson & Woessner 2002, Seppälä & Tuominen 2005). It should be created as accurately as possible, since errors in the conceptualisation are typically one of the major sources of error in the modelling (Anderson & Woessner 2002, Bredehoeft

2003). In particular, the uncertainty in the conceptual model is intensified in long-term predictive modelling (Bredehoeft 2005). Oversimplification or undersimplification should be avoided in the development of the conceptual model. According to Zheng and Bennett (2002), oversimplification results in a numerical model that is not able to mimic the observed field conditions. In contrast, an outcome of the undersimplification is obviously a too complex model that is computationally too challenging to be used as a practical modelling tool (Zheng & Bennett 2002).

The conceptual model should be continuously updated when new information and data are received on wastes, waste piles and the quality of their drainage as the mining operations progress. For waste piles, the conceptual models usually include 1) understanding and identification of baseline hydrological, hydrogeological and geochemical data (including seasonal and temporal variability) and boundary conditions, 2) defining the extent/size/geometry and material properties of the waste

pile (e.g. mineralogical and chemical composition, geotechnical properties), and 3) identification of the geochemical/physicochemical processes affecting contaminant transport (e.g. precipitation, evaporation, infiltration, advection/dispersion, dissolution/precipitation), as well as 4) the contaminant pathways from the source to the receptor (Fig. 4). In addition, potential impact management or mitigation measures should also be estimated, as they are designed to reduce the transport of contaminants to the receptors (Maest et al. 2005, Kuipers et al. 2006).

The next step after the development of the conceptual model is the selection of an appropriate thermodynamic database and code/codes that will be applied to solve the problem defined by the processes identified in the conceptual model. Several thermodynamic databases and codes are currently available that can be used to address chemical processes and transport of contaminants from mine wastes (cf. e.g. Alpers & Nordstrom 1999, Mayer et al. 2003, Nordstrom 2005, Maest et al. 2005). These codes and the basis for their selection are discussed in more detail in Chapter 4.3 of this review. In many cases, a set of codes may be needed to simulate the processes in mine wastes, as both hydrogeological and geochemical conditions should be combined in the model formulations.

Once the code/codes have been selected, a numerical model is developed to test and improve the appropriateness of the conceptual model and to guide the future data collection (Zheng & Bennett 2002, Bredehoeft 2005). The modelling for effluent quality prediction is performed as forward

modelling using reaction-path modelling or more typically reactive transport modelling (Alpers & Nordstrom 1999). In forward modelling, “an initial water of known composition and a rock of known mineralogy and composition are computationally reacted under a given set of conditions (constant or variable temperature, pressure, and water composition) to produce rock and water (or set of rocks and waters)” (Nordstrom 2005). Basically, forward models simulate the response/results of a system based on a known cause and given set of input parameters. In such modelling, “the products are inferred from an assumed set of conditions (equilibrium or not, phases allowed to precipitate or not, etc.) and thermodynamic and/or kinetic data are necessary” (Nordstrom 2005). Unlike reaction-path modelling, reactive transport modelling has a spatial component. Reactions that can be modelled using reaction-path or reactive transport modelling include mineral dissolution and precipitation, oxidation-reduction, gas evolution and sorption (Alpers & Nordstrom 1999). In addition to predictive modelling of effluent quality, forward modelling is often used to define the requirements and design of the water treatment systems and in assessing remediation alternatives (Alpers & Nordstrom 1999).

Similarly to the conceptual model, the complexity of the numerical model should be in accordance with the objectives and purpose of the modelling task and should not be exaggerated (Zheng & Bennett 2002). In addition, both conceptual and numerical modelling should be iterative processes in which the models are continuously revisited and

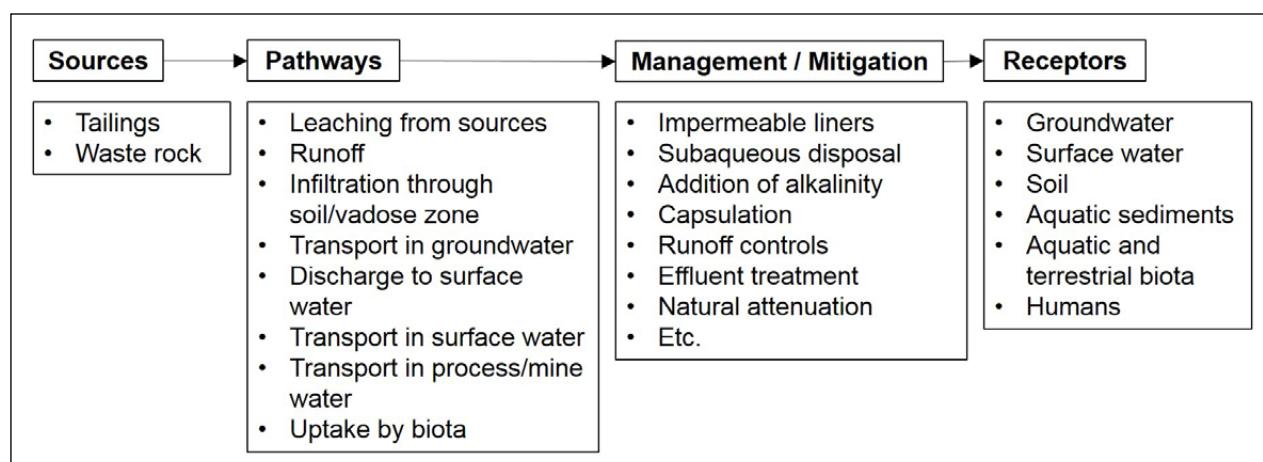


Fig. 4. Generalized conceptual model of the sources, pathways, management/mitigation and receptors of drainage from tailings and waste rocks (modified from Maest et al. 2005).

updated based on new data (Zheng & Bennett 2002, Bredehoeft 2003). Iterative modelling is a way to reduce errors in the conceptualisation and in the model (Bredehoeft 2003).

In the case of flow modelling or solute transport modelling, the next step after the development of the numerical model in the modelling process is calibration. However, a challenge of forward modelling in pre-mining phases is that the results of the modelling cannot be calibrated, as the system to be modelled does not yet exist and there are no field observations that the model could be matched with (Alpers & Nordstrom 1999). Maest et al. (2005) suggested that in these cases, existing analogues could be used to evaluate the degree of uncertainty in the prediction. Estimation of uncertainties is overall one of the key phases in modelling and is discussed in more detail in Chapter 4.6 of this report. At the end of the modelling exercise, results are presented and the problem is re-evaluated if necessary (Fig. 3).

According to USEPA (2003), the results of the modelling used for regulatory purposes should include the following information:

- model description, basis and justification/appropriateness,
- identification of input parameters and assumptions indicating the sources of the parameters (measurement, calculation, or assumption),
- discussion of uncertainties, and
- sensitivity analysis of important input parameters.

Maest et al. (2005) have outlined the specific steps needed in the predictive modelling of water quality from a mine waste facility and its mitigation, as shown in Figure 5. Depending on the modelling purpose and on the determination of the end-point for the modelling, some of the steps may not be needed. The activities involved in each phase have been compiled in Table 6.

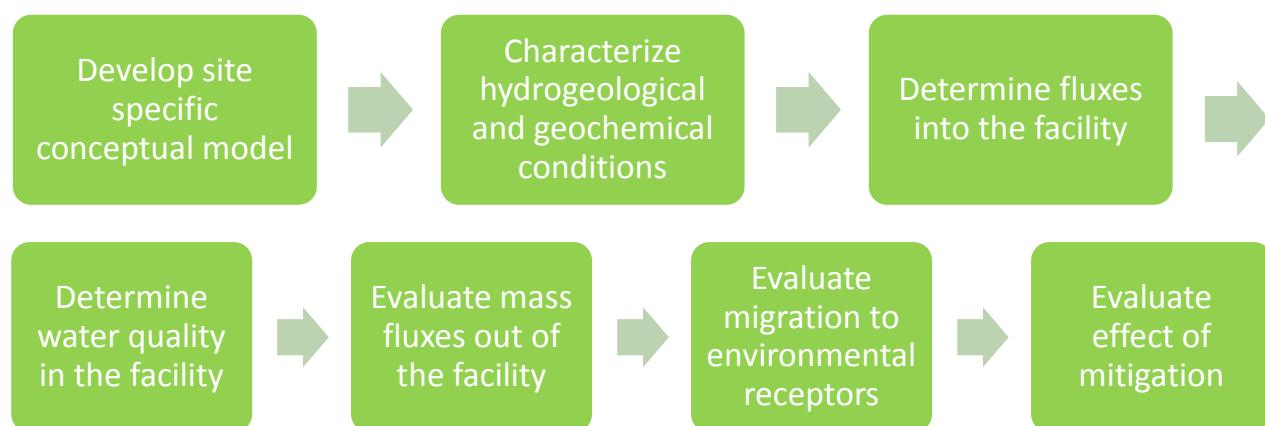


Fig. 5. Steps in water quality prediction in a mine waste facility and in downgradient groundwater and surface water (after Maest et al. 2005).

**Table 6.** Activities involved in each step in developing a water quality predictive model of a mine waste facility (Maest et al. 2005).

Step	Activities needed
1. Develop site-specific conceptual model	<ul style="list-style-type: none"> <li>Develop a conceptual model with all significant processes and pathways that influence water quality</li> <li>Determine the end point of modelling (e.g. water quality in a waste pile; discharge quality from a waste pile)</li> </ul>
2. Characterise hydrogeological and geochemical conditions	<ul style="list-style-type: none"> <li>Estimate how long mine wastes will be exposed to the atmosphere</li> <li>Determine geochemical test units</li> <li>Characterise the geology, geochemistry and hydrology of the waste facility and the disposal site</li> <li>Determine the number and type of hydrogeological units</li> <li>Estimate sulphide mineral oxidation rates during exposure with laboratory tests or with field-scale measurements</li> <li>Evaluate contaminant releases from mine wastes using results from kinetic tests and/or water quality samples</li> <li>Assess chemical loads and the volume of water from other water sources entering the waste facility</li> </ul>
3. Determine mass fluxes into the facility	<ul style="list-style-type: none"> <li>Determine the water balance for the waste facility using meteorological data and numerical or analytical models; Estimate the infiltration of meteoric water into the facility</li> <li>Determine chemical releases to the unit from mined material outside of the facility using short-term and/or long-term leaching data</li> <li>Determine mass flux rates into the waste facility</li> </ul>
4. Determine water quality in the facility	<ul style="list-style-type: none"> <li>Use inflowing water chemistry, releases from mined material and water balance information to determine water quality in a waste facility, if water quality in the facility is a modelling endpoint; use e.g. mass balance</li> </ul>
4. Determine water quality in the facility	<ul style="list-style-type: none"> <li>Use inflowing water chemistry, releases from mined material and water balance information to determine water quality in a waste facility, if water quality in the facility is a modelling endpoint; use e.g. a mass balance geochemical code to mix waters and calculate concentrations; perform uncertainty analysis in the prediction of water quality; consider physical, chemical and biological processes than can change the water quality within the facility</li> </ul>
5. Evaluate mass fluxes out of the facility	<ul style="list-style-type: none"> <li>Evaluate the migration of contaminants from the waste facility (i.e. estimate water and chemical mass fluxes discharging from the bottom or toes of the facility)</li> </ul>
6. Evaluate migration to environmental receptors	<ul style="list-style-type: none"> <li>Use an unsaturated zone flow and transport analytical or numerical codes if mass flux from the waste facility enters the vadose zone rather than groundwater</li> <li>Use groundwater flow and solute transport code to evaluate the downgradient transport of constituents into groundwater</li> <li>Use surface-water-quality code to evaluate transport and mixing processes to assess potential surface water quality impacts</li> <li>Include uncertainty analysis for the prediction of water quality and quantity in the unsaturated zone, groundwater or surface water</li> </ul>
7. Evaluate effects of mitigation	<ul style="list-style-type: none"> <li>Develop a conceptual model for mitigation measures</li> <li>Adjust values for releases of water and constituents from the facility based on the proposed mitigation measures (e.g. the cover)</li> </ul>

## 4.2 From lab scale to field scale – scaling factors

### 4.2.1 Introduction

As described in the previous chapters, the input data used for predictive modelling are based on laboratory analyses and/or field-scale measurements. The usability of the laboratory tests in the long-term prediction of waste behaviour and effluent quality is, however, limited by the scale at which they are

carried out. The sample size in the laboratory tests is generally small, ranging from one hundred grams up to a few kilograms, which should typically be representative of tens or hundreds of million tons of waste material. Therefore, the laboratory results should be scaled to field conditions for drainage predictions. Extrapolation of the laboratory results, is however, a difficult task, since the magnitude of

scaling depends on several complex factors such as the solute being scaled, drainage pH, rock type, mine waste composition, secondary mineral formation, microbial activity, laboratory method and reaction environment variables in both the laboratory and field (e.g. temperature, leachate-to-rock ratio, oxygen availability, grain size) (Kempton 2012, Eary 2015, Kirchner & Mattson 2015, Lapakko & Olson 2015, Pearce et al. 2015).

As all large-scale mine waste sites are more or less unique, the scaling factors cannot be universally quantified. Nevertheless, the scaling factor is typically <100% (Kirchner & Mattson 2015). Several studies have addressed the scaling factors for kinetic laboratory tests and field conditions. These studies have reported rough scaling factors of the order of <1 to 60% (e.g. Morin & Hutt 1994, Andrina et al. 2012, Hanna & Lapakko 2012, Kirchner & Mattson 2015). The scaling factor can, however, vary depending on the different parameters. For instance, Kirchner and Mattson (2015) have noticed that in some cases, the scaling factors for major ions tend to be higher than those for trace elements, which highlights the importance of different water quality modelling for specific ions. According to them, many species also appear to be solubility limited at a larger scale, which should also be taken into account in drainage quality modelling.

In general, drainage prediction by scaling laboratory results tends to have a high degree of uncertainty (Kempton 2012, Kirchner & Mattson 2015, Lapakko & Olson 2015, Pearce et al. 2015). Up-scaling of the results of static tests and chemical analyses, such as leaching tests, is particularly problematic, as these tests do not reveal information on the time span of the potential acidity generation or metal mobilisation (Lapakko 2002).

Several approaches have been used for scaling up kinetic laboratory tests to field conditions. These include water-to-rock ratios, the water contact time, reaction kinetics for individual minerals comprising rock types, particle size and surface area (Eary 2015). It has been recognized that laboratory kinetic tests often tend to overestimate the actual geochemical loads from a field-scale waste pile (Morin & Hutt 1994, Malmström et al. 2000, Kempton 2012). In fact, it has been noticed that laboratory rates for mineral weathering can be up to 1000 times faster than the field rates (Ritchie 1994, Malmström et al. 2000, Smith & Beckie 2003). This is largely due to the physical differences between laboratory kinetic tests and field-

scale waste rock piles (Malmström et al. 2000, Kempton 2012, Kirchner & Mattson 2015). Based on the investigations at the Aitik mine in Northern Sweden, Malmström et al. (2000) reported that the factors affecting lab-to-field scaling, from the most important to the least important, are temperature, particle size, the specific mineral concentration and surface area of minerals. According to Eary (2015), a temperature factor in scale-up calculations should be considered if field temperatures are expected to be around 10 °C higher than in the laboratory. The internal temperature production of a waste rock pile has been noted to affect gas circulation, which might enhance sulphur oxidation rates (Kuo & Ritchie 1999).

As chemical weathering is mainly controlled by the kinetics of mineral surface chemical reactions, the reaction rates are generally proportional to the reacting mineral surface area (Stumm & Morgan 1996, Banwart et al. 2002). As stated by White and Petersen (1990) in their detailed review on the role of the reactive surface area as a scaling parameter for mineral weathering rates, the reactive surface area is, however, sometimes complicated to relate to the physical surface area. Published studies report that sulphide mineral oxidation rates decrease significantly with increasing particle size (Kempton 2012 and references therein). For instance, Davis and Ritchie (1987) demonstrated by modelling diffusion-limited oxidation into shrinking-core spheres that the fragments greater than 200 mm contribute very little to the total waste rock pile oxidation, even after several hundreds of years. More recent studies have noted that practically only waste rock particles below around 20 to 30 mm are flushed by percolating water, limiting the chemical weathering of larger size fractions (Hollings et al. 2001, Stockwell et al. 2003, Kempton 2012). The geochemical significance of smaller size fractions compared to larger particles explains the higher substance concentrations in smaller scale tests compared to field-scale piles.

Typical scale variables and challenges related to scaling are summarized in Table 7. In particular, large differences have been found in the weathering rates of sulphides, liquid-to-solid ratios (L:S), oxidation rates and pH conditions between laboratory tests and field-scale tests (e.g. Shaw & Samuels 2012, Pearce et al. 2015). In general, the weathering rate of sulphides in the field has been observed to be a hundredth or tenth of those in the laboratory. For example, field-scale pyrite, chalcopyrite, biotite

and plagioclase weathering rates have been found to be around 0.01 to 0.2 times those derived from laboratory batch tests on six different particle-size fractions (Malmström et al. 2000). In addition, while studying 8 m × 8 m × 5 m test piles, Wagner et al. (2006) observed sulphate release rates to be 0.3 times those observed in the laboratory kinetic test, suggesting that factors such as temperature and solute transport limited sulphate release under field conditions. Robertson et al. (2012) also noted a sulphate release factor of 0.1 in a 7.6 Mt waste rock pile compared to humidity cell tests.

Similar results have also been recorded for the intrinsic oxidation rate (IOR), i.e. for the oxidation

rate when oxygen is freely available (cf. Bennett et al. 1999). For instance, according to Andrina et al. (2012) and Pearce et al. (2015), there is an order of magnitude difference between IOR rates under field conditions and in laboratory leach columns. At the field scale, it appears that oxygen is usually not the limiting factor, and the main causes for lower observed field IOR rates are probably linked to 1) a restricted water supply and time for “wetting up”, 2) the formation of secondary minerals around sulphide grains as a result of low matrix pore water flow and leachate flushing, and 3) larger particle sizes (Pearce et al. 2015).

Table 7. Scale variables and challenges related to scaling (after Shaw & Samuels 2012, Pearce et al. 2015).

Scale parameter	Laboratory conditions	Example field conditions	Scaling challenges
Particle size	Small	Large	Oxidation and dissolution rates of minerals are higher in the laboratory due to smaller grain sizes and a relatively larger reactive surface area, leading to overestimation of sulphide oxidation and acidity buffering processes
Geochemical system	Open	Open to closed	Open systems discharge acidity, closed systems store acidity, differences in drainage quality
Oxygen consumption measurement	Based on sulphate release	Based on <i>in situ</i> measurement	Sulphate release may not provide an accurate prediction of oxygen consumption
Sample mass	kg	Mt	Mass heterogeneity in waste rock piles not accounted for at the laboratory scale
Air flow / Oxygen supply	Diffusion dominated, unrestricted	Advection dominated, potentially restricted	Unlimited oxygen supply in laboratory tests, field conditions may vary
Temperature	Room temperature	Varies	Field temperatures can be significantly higher or lower, affecting geochemical reaction rates
Liquid: solid ratio	> 1:1 per year	< 0.1:1 per year	Laboratory leachates more diluted, enhanced flushing prevents the development of acidic micro-environments, field reactions may be limited by water supply

In addition to the above-mentioned factors, the liquid-to-solid ratios (L:S ratios), which express the relative supply of water into the waste rock system, have been noted to have a significant impact on scalability. For instance, L:S ratios are typically very low in the field compared to lab-scale tests (Pearce et al. 2015). For example, an AMIRA column (AMIRA 2002) has an annual L:S ratio of around 8:1, whereas typical waste rock storage facilities have low annual L:S ratios, e.g. below 0.1:1. Related to L:S ratios, laboratory leach columns have been observed

to have low levels of stored acidity, and probably underestimate potential drainage quality compared to field conditions (Pearce et al. 2015).

Furthermore, in some laboratory tests, the pH has been higher than under field conditions, and it has been speculated that higher flushing in laboratory kinetic tests enhances the dissolution of neutralizing minerals and prevents the development of acidic micro-environments (Shaw & Samuels 2012).

To summarize, the scaling factor is the ratio of a given solute's release rate under field conditions

to that observed in laboratory tests. The scaling up of laboratory results to field conditions is complicated and site-specific, which limits the usefulness of kinetic testing, e.g. HCTs (Maest & Nordstrom 2017). Defining the suitable scaling factors requires understanding of the overall hydrogeological and geochemical system behaviour of the target site. Further research should be conducted to compare laboratory, pilot and field-scale tests, and to assess the effects of seasonal changes in the field.

#### 4.2.2 A scaling factor concept for waste rock facilities

For the reasons mentioned above, no general method exists for reliably extrapolating laboratory test results to the complexity and physical scale of mine waste facilities. However, in some cases, it is still possible to obtain an order of magnitude estimate of loadings of potentially harmful substances (Banwart et al. 2002, Kempton et al. 2012). Kempton (2012) presented a scaling factor concept for waste rocks generally following the concept described by Malmström et al. (2000), which was demonstrated in a study at the Aitik mine site in northern Sweden. At the Aitik site, investigations on different scales were performed. Small-scale (sample size of 0.15 kg), short-term (20 weeks or longer) kinetic tests carried out at room temperature were scaled to large field columns (1820 kg) and to full-scale field piles ( $9.5 \times 10^{10}$  kg). The large field columns were aerated and irrigated, and operated for 85 weeks at temperature of 4 to 10 °C. In full-scale field piles, effluents were recovered, measured and analysed from drainage ditches with temperatures ranging from 1 to 4 °C (Malmström et al. 2000).

As stated by Kempton (2012), the broad application of the scaling factor approach warrants caution for two reasons: 1) a facility-wide scaling factor only provides facility-wide averages, but waste rock water quality varies spatially and temporally, and 2) some scaling factors might not be entirely independent, and combining them can therefore double count some effects. According to Kempton (2012), geostatistical deposit models should be used to create individual blocks of waste rocks, for which an estimate of the intrinsic solute release rate can be calculated separately. For a single parcel of waste rock, the field substance release rate,  $R_{field}$ , can be calculated from the laboratory rate,  $R_{lab}$ , and several scaling factors, SF (Kempton 2012):

$$R_{field} = R_{lab} \times SF_{moist} \times SF_{size} \times SF_{contact} \times SF_{temp} \times SF_{O_2}$$

The individual scaling factors (presented in this chapter as fractions for field conditions relative to laboratory conditions) of the above equation and discussion of the parameter ranges related to each scaling factor are presented below.

$SF_{moist}$ : This represents the reduction in oxidation caused by a too low moisture content to support chemical oxidation. This scaling factor should be 1, unless *in situ* waste rocks are drier than 2% gravimetric moisture, which is not likely except in the most extreme arid climates (Kempton 2012).

$SF_{size}$ : This is the reduction in field oxidation caused by larger rock fragment sizes. It has been observed that larger waste rock fragments contribute very little to the total waste pile oxidation due to the relatively larger surface area of smaller fragment sizes (e.g. Davis & Richie 1987, Hollings et al. 2001, Aranda 2010, Kempton 2012). In the example presented by Kempton (2012), it was assumed that in a field waste rock pile, the fraction of <20 mm grain diameter was effectively flushed by water (Neuner et al. 2009). Therefore, the kinetic lab test results using <6.4 mm diameter sample material were scaled from <6.4 mm to <20 mm. In the example, Kempton (2012) utilized the results obtained from a surface area study of waste rock at the Antamina mine by Aranda (2010), where 65% of the surface area was in <6 mm material (35% gravimetric fraction) and 88% of the surface area was in material <20 mm (55% gravimetric fraction). The ratio of surface area:mass in the <6 mm fraction was 1.9, which is around 1.2 times the corresponding ratio of 1.6 for the <20 mm fraction, resulting in a  $SF_{size}$  value of around 1/1.2, or 0.83 (Kempton 2012). However, as the fragment sizes identified as carrying the major part of unsaturated flow had high variety (from <5 to <30 mm), as well as the particle-size distribution in a waste rock pile, this scaling factor had large degree of uncertainty (Kempton 2012).

$SF_{contact}$ : This describes the reduction in solute leaching from rock fragments too coarse to be flushed by pore water. Estimates for the fragment size carrying moisture (up to 20 mm in Neuner et al. 2009 and up to 30 mm in Tran et al. 2003) are close to the maximum fragment size contributing significantly to sulphide oxidation. Therefore, the use of  $SF_{size}$  can eliminate the need to correct for the water contact fraction (Kempton 2012). On the other hand, as secondary salts have been noted to

accumulate on the larger size fraction (Tran et al. 2003), the risk of mobilisation is high during infrequent larger rainfall events that produce water flow in larger pores. Therefore, the assumption that the larger size fractions remain isolated from percolating pore water is probably correct in covered waste rock piles, where the cover dampens the water flux (Kempton 2012). In general, Kempton (2012) proposes a wide range for  $SF_{temp}$ , from around 0.1 to 0.65, with higher possible values in waste rock piles with a highly variable water flux.

$SF_{temp}$ : This is the increase or decrease in the oxidation rate caused by higher or lower field temperatures compared to lab temperatures. The temperature effect on the oxidation rate is described by the Arrhenius equation (Arrhenius 1889):

$$k = A \exp\left(-\frac{E_a}{RT}\right)$$

Where:

$k$  = reaction rate constant [1/s, or same unit as used for A]

$A$  = pre-exponential factor, determined at given temperature [1/s]

$E_a$  = activation energy of the reaction [kJ/mol]

$R$  = universal gas constant [0.008314 kJ/mol/K]

$T$  = absolute temperature [K]

From the Arrhenius equation, the  $SF_{temp}$  can be derived by dividing  $k_{field}$  by  $k_{lab}$  (Malmström et al. 2000):

$$SF_{temp} = \exp\left(-\frac{E_a}{R}\left(\frac{1}{T_{lab}} - \frac{1}{T_{field}}\right)\right)$$

According to Kempton (2012), elevated temperatures are typically observed in sulphidic waste rock piles compared to average ambient temperatures. For instance, in the Arctic conditions at the Aitik mine, the internal temperature of the waste rock pile (average gravimetric pyrite content ~1%, rang-

ing from 0 to 5%; Bennett et al. 1994) has been observed to be 1–4 °C, even though the average air temperature is around 0 °C (Kempton 2012). Based on Kempton (2012),  $SF_{temp}$  can range from ~0.3 (or lower) in Arctic conditions to ~6 in well-oxygenated highly sulphidic waste rock.

$SF_{O_2}$ : This represents the reduction in the field oxidation rate caused by limited  $O_2$  availability in pore gas. In general,  $O_2$  is not a limiting factor in waste rock piles (i.e.  $SF_{O_2} = 1$ ), except in zones with a high sulphide concentration and oxidation rates. For scaling calculations,  $SF_{O_2}$  values <1 can be used for rock material with sulphide S concentrations of around 1% and higher. For these high S rock materials,  $SF_{O_2}$  values between ~0.2 and ~0.5 are reasonable, bearing in mind that the inhibition of convective air flow due to the waste rock facility design could cause even lower values (Kempton 2012).

After applying a scaling factor to the kinetic test-derived solute leach rates, the rate of solute release from the field-scale waste rock facility can be estimated (Kempton 2012). The waste rock facility seepage composition can then be roughly calculated by dividing the solute release rate by the waste rock pile seepage flow rate as follows (Declercq et al. 2017):

$$\text{Waste rock seepage water quality} \left[ \frac{\text{mg}}{\text{L}} \right] = \frac{\sum \text{Solute rate} [\text{mg/kg/week}] \times \text{Reactive mass of material} [\text{kg}]}{\text{Total infiltration rate into waste rock pile} [\text{L/week}]}$$

These up-scaled results can then be utilized, for example, in modelling the mineral saturation indices for this predicted solute composition, e.g. using PHREEQC and Minteq.v4 thermodynamic databases.

For more detailed information concerning scaling and the scaling equation presented above, see Malmström et al. (2000), Banwart et al. (2002), Kempton (2012) and Pedretti et al. (2017b).

### 4.3 Model types and codes for modelling mine wastes

In the past, several decades of research efforts have been dedicated to developing quantitative numerical tools in order to describe as well as to predict reactive fluid flow and solute/gas transport not only in the context of mining environments, but also in fluid dynamics in porous media in general. Focusing on the multitude of different geochemical-hydrogeological-microbial problems and depending on the specific applications, as well as objectives, a diverse series of models have been developed and considerable advances have been made in the recent decades (e.g. Barry et al. 2002, Blowes et al. 2014, Amos et al. 2015 and references therein). To date, developments of these models are still an active area in mining and geo-environmental research and will further continue with our increasing knowledge in process-oriented understanding as well as in numerical approaches. Such continuous advancement includes the development of new independent computer codes as well as the addition of increasingly new features to the existing codes (e.g. Steefel et al. 2015).

Based on the formulation and the capabilities of the models typically used to understand and predict the processes in mining environment applications (i.e. mine-waste deposits and decommissioned mines), they can be characterised into three categories:

- a) empirical/engineering models,
- b) geochemical models and
- c) reactive transport models.

The first model type is mainly based on empirical approaches, whereas the other two follow concepts from mechanistic understanding. However, it is rather difficult (if not impossible) to develop a model that is strictly “mechanistic”, as at least some components of the involved process descriptions do not have a theoretical basis but rely on empirical correlations. For example, activity calculations in chemical systems typically use the Debye-Hückel model or its derivatives (e.g. Davies or WATEQ equations), and Darcy’s law in groundwater flow uses parameters such as hydraulic conductivity, which are both often based on empirical equations (e.g. Nordstrom & Munoz 1994, Blowes et al. 2014).

In contrast, the models that are considered “empirical” also have some basis in mechanistic understanding, even though the inputs and/or

outputs of such models may not directly correlate with the involved processes. Therefore, the distinction between “mechanistic” and “empirical” models is usually based on the ‘attempt’ to resolve the involved physicochemical processes rather than the point of view of literal exactness. In the following, an overview of these individual model types is briefly provided.

#### 4.3.1 Empirical and engineering models

Empirical models, which can sometimes also be viewed as so-called “black box” models, are based on the approaches without explicitly taking into account the process-based functional relationships between the input and output parameters. Instead, they use statistical relationships to establish meaningful correlations (e.g. by means of regression analysis) between the parameters of interest in a suite of collected data. In contrast, engineering models can adopt a range of approaches, spanning from empirical to mechanistic, depending on the specific needs (e.g. Perkins et al. 1995). These models usually rely on simplified assumptions regarding the involved processes, and try to reduce the necessary parameters/variables to those that can be easily measured or effectively controlled. The ultimate intent of such formations is to recognize only the important processes in a particular application or decision-making process, and to adopt a suitable model accordingly.

In managing mine waste facilities, both of these models are typically used in assessing the field behaviour of real systems, e.g. to predict annual average or seasonal variation in drainage chemistry, and in predicting the potential risks of contaminated drainage. As they are based on existing monitoring data from field, they are not suitable for predicting drainage chemistry from waste facilities in the planning phase of a mine (Price 2009). However, these predictive methods, in connection with field measurements, can be effective especially when the objective is to identify the dominant processes or to provide support in making practical decisions regarding the potential remediation options during mining activities. Examples of codes incorporating empirical and engineering models, applied in the quantitative prediction and remediation of mine waste drainage at different sites, include but are not limited to RATAP (e.g. MEND 1990), WATAIL

(MEND 1993), MINTOX (MEND 1997) and ACIDROCK (Scharer et al. 1994) (Table 8). In recent years, some of these codes may have become obsolete and might not be available for further updates. Furthermore, with the advent of more powerful codes incorporating more detailed deterministic process-based models, the use of these types of codes has probably become less popular in recent years.

These modelling approaches, however, often lack a theoretical basis in mechanistic understanding, as they do not capture the internal physics or the detailed geochemistry of the relevant processes. Therefore, the predictive capability of these models is also limited to the extent of data and the consistency of prevailing environmental conditions during data collection. The outcomes of such models may also be inapplicable when the prediction is extrapolated to a different system (i.e. different set of conditions compared to that of data collection). Nevertheless, this type of model is normally easy to use, computationally less expensive, and can be useful in examining the effects of controlling factors and in comparing the feasibilities of different management alternatives.

#### 4.3.2 Geochemical models

Geochemical models are widely used in describing mineral–water chemistry, not only in mine-drainage environments but also in natural aquifer systems. These models, usually based on mechanistic formulations, use thermodynamic databases and theoretically derived equations to describe the controlling geochemical processes. Geochemical speciation and mass–transfer models have become seemingly popular over the past decades, and a wide variety of geochemical codes has been developed, including WATEQ4F (Ball et al. 1987), MINTEQA2 (Allison et al. 1991), EQ3/6 (Wolery 1992) and PHREEQE (Parkhurst et al. 1985), among others. The evolution of geochemical codes has been documented, for example, in Alpers and Nordstrom (1999), Mayer et al. (2003), Bethke (2008), Birkle (2012) and Nordstrom and Campbell (2014). Table 8 presents some of the geochemical codes that have been used in mining-related applications.

In mine waste settings, models of this type basically solve the geochemical subproblem without resolving fluid flow and solute/gas transport through the deposits (i.e. as a batch system), and they can be applied to infer chemical reactions affecting the concentrations of dissolved con-

stituents, as well as primary or secondary mineral assemblages (e.g. Mayer et al. 2003, Blowes et al. 2014). Such models can also be used to assist in data interpretation (e.g. concentration of dissolved metals), as well as in predicting the anticipated drainage composition in mine wastes (e.g. Davis & Ashenberg 1989, Blowes & Jambor 1990, Tempel et al. 2000, Eary et al. 2003, Ramstedt et al. 2003, Moncur et al. 2005, Gunsinger et al. 2006) and in adjacent receiving water bodies (e.g. Runkel et al. 1996, Broshears et al. 1996, Runkel & Kimbell 2002, Moncur et al. 2006). The current formulations of geochemical simulators have become increasingly sophisticated, as they are capable of performing a wide range of geochemical reaction calculations, including geochemical speciation, acid–base equilibria, redox reactions, mineral precipitation/dissolution, solid/gas phases, sorption/desorption, ion-exchange, surface-complexation, and microbial reactions over a range of temperature and pressure conditions (e.g. Blowes et al. 2014).

In order to describe ion activities and mineral stability in a highly concentrated electrolyte mixture, which is typical in mine waters due to the high content of dissolved metals as a result of extreme sulphide oxidation and subsequent evaporation, the above-mentioned codes use Pitzer-based formalisms (Pitzer 1973, Pitzer 1991). Such methodologies have been found to be consistent with the observations at different mine sites and have also been suggested by many investigators as a potential approach (e.g. Blowes et al. 2014). The recent versions of these codes also allow capturing kinetically controlled reactions with user-defined rate expressions, and some of them have further evolved by incorporating one-dimensional solute transport (e.g. Parkhurst & Appelo 1999).

#### 4.3.3 Reactive transport models

In recent years, there has been an emerging need for coupling fluid flow, mass and heat transport, and electrochemical processes with the comprehensive geochemistry in the mine environment and subsurface simulations, and this has led to the development of reactive transport models (e.g. Steefel et al. 2015a). This group of models can be considered as a hybrid between hydrogeological models and geochemical models and they are able to simultaneously capture both physical and geochemical processes. Reactive transport models are instrumental investigative tools in understanding and predicting

the ultimate outcomes when multiple dominating processes act concurrently leading to non-intuitive system behaviours. In mine water management, they have been actively used to describe and predict sulphide oxidation and the transport of oxidation products through mine wastes (e.g. Liu & Narasimhan 1989, Wunderly et al. 1996, Bain et al. 2000, Mayer et al. 2006, Acero et al. 2009).

Reactive transport models solve partial differential equations that integrate equations describing the multidimensional physical movement of fluids and dissolved solutes with equations describing biogeochemical reactions. These models are capable of providing a comprehensive approximation of real geochemical systems compared to the other model types. The capabilities of these models include saturated/unsaturated/multiphase flow in multiple dimensions, solute and gas transport processes (e.g. advection, diffusion, and hydrodynamic dispersion), heat transport, and biogeochemical reactions (e.g. equilibrium reactions, kinetic reactions, mineral dissolution/precipitation, and microbial reactions), including thermodynamic databases. Due to the coupled system of partial differential equations and the nonlinearity induced from different reactive processes, a direct solution of a reactive transport problem usually cannot be obtained (e.g. Mayer et al. 2003). Therefore, an iterative scheme is typically adopted to numerically solve such coupled problems.

In the last decade, a suite of reactive transport codes has been developed not only to understand and predict the complex interplay between different physical and geochemical processes in mined and natural sediments, but also to provide quantitative interpretation of experimental observations, both at laboratory and field scales (Barry et al. 2002, Mayer et al. 2003, Steefel et al. 2015a). In fact, the research regarding the developments of these numerical tools is still ongoing and the performance of these codes is constantly being improved. Steefel et al. (2015a) recently presented a comprehensive review of the currently available reactive transport codes along with the specific capabilities, fundamental mathematics, historical developments and numerical solution approaches. The authors pointed out that depending on the formulation, these codes slightly differ from each other in terms of their capability to capture the range of processes, numerical formulations and dimensionality. The evolution of reactive transport codes has also been illustrated in other reviews in the literature, such as Lichtner (1996a,

1996b), Steefel and McQuarrie (1996) and Mayer et al. (2002).

In simulations of mine-waste deposits, the most popular reactive transport codes include, among many others, PHREEQC (Parkhurst & Appelo 1999), Geochemist's Workbench (Bethke 1997), CrunchFlow (Steefel & Lasaga 1994), MIN3P (Mayer et al. 2002), PHT3D (Prommer et al. 2003), HYDROGEOCHEM (Yeh & Tripathi 1990), TOUGHREACT (Xu & Pruess 2001, Xu et al. 2011), PHAST (Parkhurst et al. 2005), PHWAT (Mao et al. 2006), HYTEC (van der Lee et al. 2003), ORCHESTRA (Meeussen 2003), eSTOMP (White & Oostrom 2006), PFLOTRAN (Lichtner et al. 2015), OpenGeoSys (OGS) (Kolditz et al. 2012), and HP1/HPx (Šimunek et al. 2012).

For some of these tools, separate/earlier versions or their derivatives are also available in parallel. Such products have been released as side products or plug-ins over the course of developments, which sometimes involve different combinations of specific features or applicability. These separate versions are also often used to deal with specific reactive transport problems. For instance, the TOUGHREACT family has derivative tools such as TOUGH-2 (Pruess 1991), TOUGH2-CHEM (Xu et al. 2000) and TOUGH-AMD (Lefebvre et al. 2001); CrunchFlow has separate versions such as CRUNCH (Steefel 2005) and CrunchFlowEDL; and MIN3P also exists in some extended versions including MIN3P-DUAL (Cheng et al. 2009), MIN3P-BUBBLE (Amos et al. 2006), MIN3P-DUSTY (Molins et al. 2007), MIN3P-DENS (Henderson et al. 2009) and MIN3P-THCm (Bea et al. 2011).

Table 8 presents a list of the commonly used reactive transport codes and also some of their derivatives. These codes are based on the so-called continuum formulation, which refers to the solution of the transport and reaction problem at a macroscopic Darcy's scale with average local physical and chemical properties in a particular user-defined grid block (e.g. Steefel et al. 2015). For the transport problem, most of these tools mainly adopt Eulerian schemes, whereas some of them (e.g. PHT3D) also allow the use of solvers based on Lagrangian approaches to solve the advection problem (e.g. Steefel et al. 2015a).

Among the above-mentioned codes, the ones that are capable of solving unsaturated/multiphase flow and/or heat transport comprise MIN3P, HYDROGEOCHEM, TOUGHREACT, HP1/HPx, HYTEC, ORCHESTRA, eSTOMP and PFLOTRAN. In order to solve the geochemistry, some codes use other geo-

chemical packages such as PHREEQC (e.g. PHT3D, PHAST and HP1/HPx) or CHESS (e.g. HYTEC) as reaction engines, whereas some of these codes rely on their native geochemical modules (e.g. ORCHESTRA).

Table 8. List of selected codes used for predicting the quality of mine wastes.

<b>Model Type</b>	<b>Codes</b>	<b>References</b>
<i>Empirical/engineering codes</i>	RATAP	MEND 1990
	WATAIL	MEND 1993
	MINTOX	MEND 1997, Bain et al. (2000)
	ACIDROCK	Scharer et al. (1994)
<i>Geochemical codes</i>	WATEQ4F	Ball & Nordstrom (1991)
	MINTEQ/MINTEQA2	Allison et al. (1991)
	MINQL	Schecher & McAvoy (1991)
	PHREEQE/PHREEQM	Parkhurst et al. (1985)/Appelo & Postma (1993)
	GEOCHEM	Parker et al. (1995)
<i>Sulphide oxidation/AMD codes</i>	EQ3/6	Wolery (1992)
	HSC Chemistry	Lamberg & Tommiska (2009)
	CHESS	van der Lee et al. (2003)
	PYROX	Wunderly et al. (1996)
	FIDHELM	Pantelis 1993
<i>Reactive transport codes</i>	TOUGH-AMD	Lefebvre et al. (2001)
	TOUGH-CHEM	Xu et al. (2000)
	RETRASO	Saaltink et al. (2002)
	SULFIDOX	Brown et al. (2001)
	THERMOX	da Silva et al. (2009)
	MINTRAN	Walter et al. (1994)
	PHREEQC	Parkhurst & Appelo (2013)
	CrunchFlow	Steefel & Lasaga (1994)
	MIN3P	Mayer et al. (2002)
	PHT3D	Prommer et al. (2003)
	PHAST	Parkhurst et al. (2005)
	Geochemist's Workbench	Bethke (1997)
	HYDROGEOCHEM	Yeh & Tripathi (1990)
	TOUGHREACT	Xu & Pruess (2001)
	PHWAT	Mao et al. (2006)
	HYTEC	van der Lee et al. (2003)
	ORCHESTRA	Meeussen (2003)
	eSTOMP	White & Oostrom (2006)
	PFLOTRAN	Lichtner et al. (2015)
	OpenGeoSys(OGS)	Kolditz et al. (2012)
	HP1/HPx	Šimunek et al. (2012)
	RICH-PHREEQC	Wissmeier & Barry (2010)

In addition to the multipurpose generic reactive transport codes, as described above, numerical tools have also been developed to exclusively simulate acid mine drainage (AMD) problems. Such codes, specifically focused on kinetic pyrite oxidation and equilibrium/kinetically controlled buffering mineral dissolution/precipitation reactions, are capable of coupling water flow, solute transport, oxygen convection/diffusion and subsequent heat transfer due to exothermic mineral oxidation with sulphide oxidation reactions and pH evolution. Therefore, such sulphide oxidation codes can simulate the generation and release of acid mine drainage in waste rocks, tailings and heap-leach systems. However, these formulations are often limited to only a small number of processes, and hence lack theoretical rigor, especially when a broad range of dominating processes are involved (e.g. Mayer et al. 2003, Amos et al. 2015). Examples of such codes include MINTRAN (Walter et al. 1994), PYROX (Wunderly et al. 1996), SULFIDOX (Brown et al. 2001), THERMOX (da Silva et al. 2009), FIDHELM code (Pantelis 1993) and TOUGH-AMD (Lefebvre et al. 2001b) among others.

Advances in the development of multidimensional multicomponent reactive transport codes also include a fairly new concept of coupling two or more independent codes to form a multipurpose framework in order to rigorously address a complicated problem. For example, coupling of hydrogeological and multicomponent solute transport codes with geochemical codes has been remarkably popular in reactive transport modelling research during recent years (e.g. Wissmeier & Barry 2010, Masi et al. 2016, Muniruzzaman & Rolle 2016). Developments of these coupled simulators were certainly triggered by the release of two recent modules named IPhreeqc (Charlton & Parkhurst 2011) and PhreeqcRM (Parkhurst & Wissmeier 2015) from the United States Geological Survey (USGS).

IPhreeqc (“i” refers to “interface”) is a generic-purpose C++ module of the USGS’s widely used geochemical code PHREEQC (Parkhurst & Appelo 2013). It allows using PHREEQC’s reaction capabilities in

any software programs that are able to interface through Microsoft COM or DLL libraries or in any scripting/programming languages (Charlton & Parkhurst 2011). Besides reactive transport modelling, IPhreeqc can also be used in any other applications involving PHREEQC calculations. In contrast, PhreeqcRM (“RM” stands for “reactive module”) is a specifically designed module that has been devised to incorporate the reaction packages included in PHREEQC with other multidimensional flow and transport codes.

The use of such couplings, which refer to the communication between different codes without modifying their source codes, enhances the flexibility to combine different sets of processes included in different individual software packages. This approach is also particularly convenient for users without extensive programming experience, because the coupling does not require any advanced level coding implementations or the modification of any source codes. Furthermore, the communication between the transport and reaction models in such coupled tools is fast, as information exchange occurs via tight coupling without involving the reading or writing of any external files (Müller et al. 2011).

IPhreeqc has been tested and used by several authors in reactive transport codes written in different scripting platforms such as Python (Müller et al. 2011), FORTRAN and C/C++ (Charlton & Parkhurst 2011), MATLAB (Wissmeier & Barry 2012, Muniruzzaman & Rolle 2016), Visual Basic scripted in Excel (Sieland et al. 2016) and Wolfram Mathematica (Voigt et al. 2017). Recently, different flow and transport codes that have taken advantage of these new modules include COMSOL Multiphysics (e.g. Wissmeier & Barry 2012, Nardi et al. 2014, Nasir et al. 2014, Masi et al. 2016, 2017), UTCHEM (e.g. Korrazi et al. 2015), FEFLOW (Parkhurst & Wissmeier 2015) and OpenGeoSys (He et al. 2015). Furthermore, these tools have also been successfully used in transport models based on the Lagrangian framework (e.g. Engdahl et al. 2017) or on pore-scale network models (e.g. Qin et al. 2016).

#### 4.4 Basis for the selection of a code

The selection of an appropriate code in a particular project should be primarily based on the overall objectives and the exact purpose of modelling studies in that project. Therefore, the specific selection criteria are solely site-specific, and it would not

be feasible to derive a general rule that is applicable for all cases. The selection procedure should follow a workflow starting from the identification of the main processes affecting the system behaviour, followed by the development of a representa-

tive site conceptual model. Afterwards, based on the capability to capture the important processes controlling the system dynamics in the conceptual model, the screening of the codes should be performed among the reviewed and shortlisted computer codes. Emphasis should also be given at this stage to the type and quality of the field supporting data that are available at hand or could be further collected. Such data not only should represent the study site of interest fairly well, but it should also be possible to effectively feed the data into the model to properly calibrate as well as to further adapt it on the basis of possible future observations. Figure 6 illustrates a synopsis of the factors one should consider while selecting a code to perform the prediction of drainage quality at a mine site.

The selected code in a particular modelling task should contain a certain level of complexity that is not only sufficient to rigorously capture all the key processes representing the study area but also appropriate for regulatory decision making. However, the use of a more complex and numerically sophisticated code does not always necessarily lead to better performance in realistic predictions, especially when the conceptual model is not a good representation of the real site. Instead, a relatively less-complex code applied to a better and more representative conceptual model can outperform the former. Data inadequacies may also limit the code application in many cases, and it would not be worth applying a rather complicated code when insufficient data are available to support the complexity of the code. This scenario is very typical at mine sites, as the collected data are often extremely sparse. Nordstrom (2005) pointed out that in modelling mine waste, the advances and level of sophistication in computer software have already significantly outpaced our ability to systematically constrain and test different features of these computer tools. Therefore, by analysing all these factors and the available information, an optimum decision should be taken in choosing a predictive numerical code that is:

- (i) complex enough to capture all the important processes,
- (ii) sufficiently simple to make use of the collected data,
- (iii) able to evaluate uncertainties and to recognize the limitations, and
- (iv) fulfils the main objectives of the modelling project and answers the specific questions the modelling studies aimed for.

Furthermore, care should also be taken if the selected code and its documentation are easily available to the public, and if it has been systematically tested by others in similar applications. A very rare or extremely expensive proprietary code should be avoided. It might also be important to check the user-friendliness, graphical interfaces, and pre- and post-processing features of the selected code. Maest et al. (2005) summarized a list of issues that should be considered when selecting a code to predict mine waste drainage:

- the specific objectives and endpoints of the modelling task
- key processes influencing water quality at the study site
- codes that are capable of simulating these processes
- whether occurring reactions are equilibrium or kinetically controlled (or both)
- whether to use separate codes for hydrogeological and geochemical models or coupled code for both models
- the type and quality of data available (or that can be collected) versus the type of data required for the code
- the influence of microbes and colloids on water quality
- the availability of the code and its resources to the public
- the user-friendliness and the presence of graphical user interfaces.

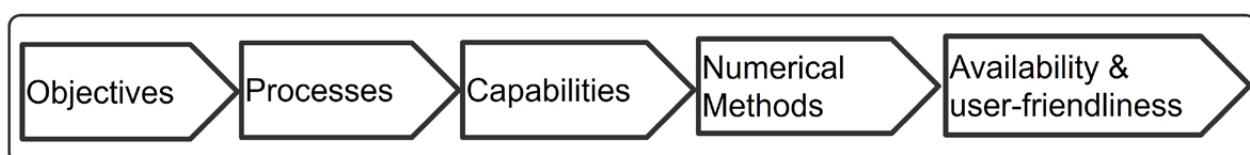


Fig. 6. Factors that should be considered when selecting a computer code to estimate and predict water quality in mine wastes.

Finally, special focus should also be given to the internal numerical methods that are implemented in the mathematical formulation of a code. It is obvious that every numerical method has its own advantages and limitations in relation to the specific problem at hand. Depending on the complexity of the mathematical problem and the presence of exceptional conditions (e.g. steep gradients, non-linearity and discontinuity), certain numerical approaches can be either unstable or susceptible

to numerical errors. Priority should be given to the codes that allow a better formulation to avoid these numerical issues under such conditions. Otherwise, proper measures should be taken in order to systematically handle numerical instability or to minimize numerical errors. Therefore, the modeller should also be aware of these numerical difficulties while selecting a particular code to solve a particular mathematical problem.

#### 4.5 Modelling scenarios: Example case studies

Given the variety of modelling approaches as well as the available numerical codes, as mentioned in the previous section, different types of models can be applied, depending on the specific need of the modelling, to describe sulphide oxidation, acid mine drainage generation, the release of metals and attenuation at a mine site. In the literature, numerous case studies can be found demonstrating the use of different modelling tools to address the long-term behaviour of mine wastes (e.g. Mayer et al. 2002, Molson et al. 2005, da Silva et al. 2009, Fala et al. 2013, Lahmira & Lefebvre 2014, Lahmira et al. 2016, Shokri et al. 2016, Pabst et al. 2017). However, published cases specifically focusing on the actual predictive modelling of proposed future potential wastes in a pre-mining state appear to be scarce, even though consulting companies often perform this type of modelling. One possible reason for the limitation in the availability of such pre-mining modelling studies could be the lack of representative data regarding waste material characterisation, environmental and climate conditions, adjacent hydrogeological pathways, chemical parameters, the spatial variability of different physical/chemical properties, and site-specific background information.

To illustrate the potential applications of numerical models in quantifying the drainage quality from mine wastes, this section presents three case studies. Among these examples, only the first one presents a case describing the assessment of water quality from a proposed waste rock dump in Northern Sweden. In the other two examples, the modelling has been applied to evaluate the chemical processes and the evolution of drainage quality in existing waste piles. The first of these latter examples includes reactive transport simulations in variably saturated tailings impoundments at a Nickel Rim mine site in Sudbury, Ontario, Canada

(Mayer et al. 2002). The last case study is associated with the application of a reactive transport model to a waste rock pile at Doyon mine in northern Québec, Canada (da Silva et al. 2009). Even though these latter examples present modelling simulations from existing sites, the processes included, model formulations and the required overall workflow in the modelling tasks are identical to those at waste facilities under planning. In fact, there is no fundamental difference in model setup or mathematical formulation between the models for an existing waste facility and a planned (i.e. not yet existing) waste facility. Mathematically speaking, one needs to solve the same physicochemical problem and an identical set of equations are used in both cases, while the quantity of site-specific data may vary due to the limited capability to collect detailed data during the planning stage. Therefore, the overall approach typically used in the simulations of existing mining sites can be directly adopted in the predictive modelling of mine sites under planning.

##### 4.5.1 Modelling in a proposed waste rock pile

This example demonstrates numerical modelling and the assessment of long-term seepage chemistry in a proposed waste rock pile at an iron ore deposit at the Aitik mine in northern Sweden (Charles et al. 2016). The study specifically focused on attempting the prediction of source term water quality in terms of drainage concentrations and mass loadings from the waste rock pile into the surrounding receiving surface water bodies. The authors collected a total of 33 waste rock samples, which were identified to be spatially and lithologically representative for this study site, from drill cores. In order to characterise the elemental composition, mineralogical composition and leaching behaviour of the different

rock types, static and kinetic laboratory tests were performed.

The static tests included mineralogical analysis, multi-elemental analysis, aqua regia digest followed by ICP analysis, acid-base Accounting (ABA), net acid generation (NAG) with leachate analysis, and a short-term leach test (BS EN 12457-3, BSI 2002; liquid-to-solid ratio 2:1 and 8:1). Based on the results obtained from the static tests, the authors classified the collected rock materials into two main categories: (i) potentially acid forming (PAF) materials containing >1% of sulphur (28% of the total waste), and (ii) non-acid forming (NAF) materials with a sulphur content of <1% (72% of the total waste). Additionally, kinetic humidity cell tests (HCT) (ASTM D5744-96; ASTM 1996) were carried out on the three NAF and three PAF samples for a duration of 40–60 weeks. During these kinetic tests, leachate samples were collected every week and they were subsequently measured by ICP-OES and ion chromatography.

Based on the background information and site-specific data, conceptual models were developed for the different modelling scenarios during the life of mine (LOM) and post-closure conditions. In par-

ticular, this study explored model scenarios focusing on the following aspects:

- segregated (PAF and NAF blocks) and unsegregated (blended PAF and NAF) wastes,
- annual average and spring snow melt conditions, and
- the application of standard soil and qualified covers in post-closure conditions.

Conceptual models for these specific scenarios are illustrated in Figure 7.

The geochemical modelling was performed using the USGS's geochemical code PHREEQC (Parkhurst & Appelo 2013) by incorporating a modified version of the MINTEQ.v4 database. The infiltration water into the waste dock dump was assumed to have a composition identical to the generic Northern Europe rainwater (Reimann et al. 1997). The infiltration rate was estimated based on the climate monitoring data for this particular site. In order to account for the discrepancies between laboratory and field-scale reaction rates and liquid-to-solid ratios, the authors used scaling factors as suggested by Kempton (2012). Table 9 summarises the physical and chemical scaling factors used in this study.

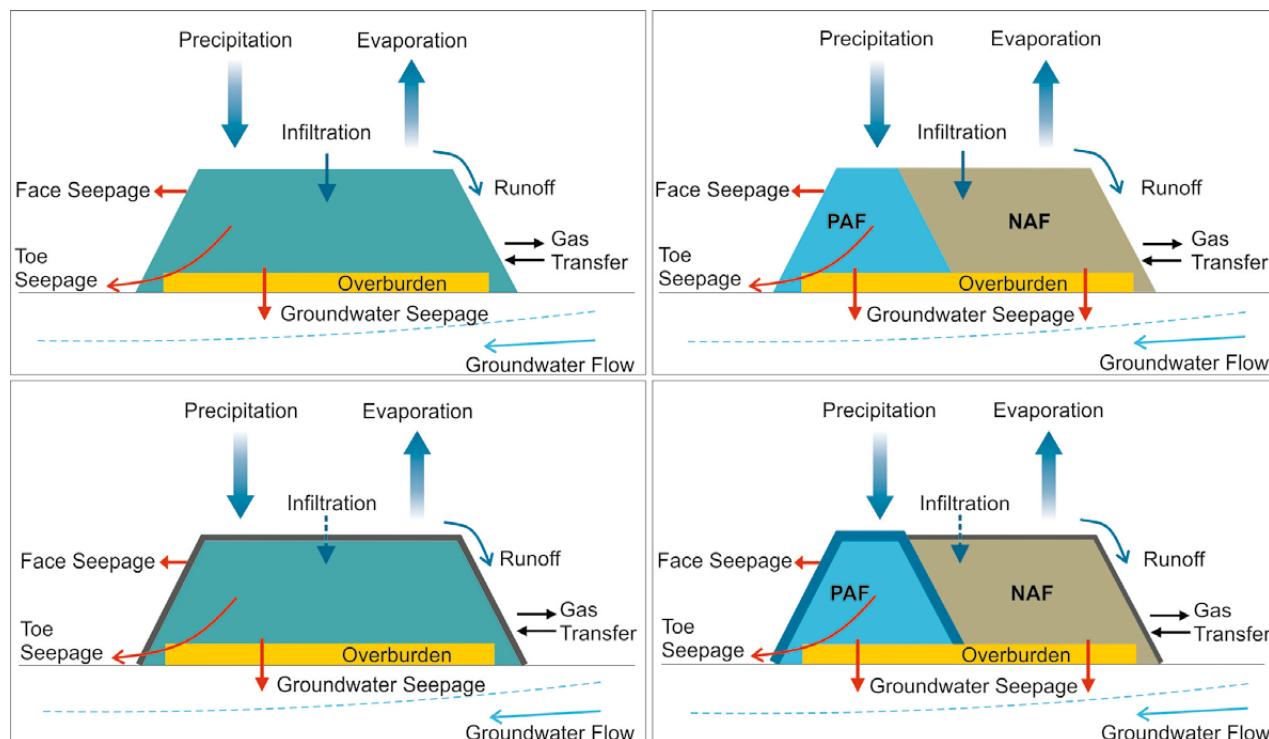


Fig. 7. Conceptual models for blended (left panel) and segregated (right panel) waste rock piles during LOM (top panel) and post-closure (bottom panel) scenarios (after Charles et al. 2016).

Table 9. Summary of the modelling parameters and scaling factors used in the geochemical modelling of the proposed waste rock pile at the Aitik mine (from Charles et al. 2016).

Parameters	Value Applied		
	LOM Average	LOM Spring	Closure
Infiltration (mm/yr)	265	1694	98
Seepage (m <sup>3</sup> /day)	1278	5951	471
Oxygen ingressoin	Based on the ANSTO model <sup>1</sup>		
Scaling factors	NAG	0.001% for all scenarios	
	HCT	No distinct factors used	
Chemical scaling	Temperature	26% for all scenarios	
	O <sub>2</sub> <sup>2</sup>	50% of atmospheric for all scenarios	
Physical scaling	Proportion of fines	20% for all scenarios	
	Proportion of fines flushed	50% for all scenarios	

<sup>1</sup> Convective airflow minimised and O<sub>2</sub> mass transport by diffusion

<sup>2</sup> Average concentration over penetration depth

Numerical simulations were performed for different scenarios, including both LOM and post-closure conditions, utilising the results from the NAG test and HCT. The simulated concentrations of dissolved metals in the source term water appear to be higher when using the NAG test results for all scenarios (Table 10). The predicted concentrations also reveal that the metal loading in the drainage from the waste rock dump is highest during the spring in LOM scenarios, when the infiltration rate (1694 mm/yr) into the dump is also the highest. In contrast, these metal loadings decrease significantly in the post-closure scenarios when the recharge (98 mm/yr) into the waste rocks and the subsequent oxidation of sulphide minerals are effectively inhibited by the applied standard soil and qualified covers.

In addition to the prediction of drainage quality from the proposed waste rock piles, the authors also attempted to assess the possible influence of metal release from the waste rock drainage into an adjacent river for each modelling scenario. The simu-

lation results suggest that even though the LOM scenarios during spring conditions result in a higher loading of metal concentrations in the wastes' seepage, the predicted metal concentrations in the surrounding watercourse are lower compared to the average flow conditions (Table 11). Such behaviour is induced from the impact of a higher river flow rate during spring, which leads to a significantly higher dilution factor compared to the scenarios of LOM average. Furthermore, the river water experiences an improvement in quality in the post-closure scenarios because of the reduced infiltration rate, sulphide oxidation rate and the subsequent mobilisation of dissolved metals. The scenarios considering the segregation of PAF material appear to provide better results in terms of elemental loadings and the predicted elemental concentrations in the adjacent river. None of the scenarios explored in this particular study predicted the possible generation of acidic drainage under the assumed boundary and initial conditions, and the seepage pH was in the range of 7.45–7.64.

Table 10. Predicted drainage chemistry from the proposed Aitik waste rock dump (WRD) based on NAG/HCT (from Charles et al. 2016).

	Predicted chemistry based on NAG test results						Predicted chemistry based on HCT test results					
	Segregated WRD			Blended WRD			Segregated WRD			Blended WRD		
	LOM Average	LOM Spring	Closure Average	LOM Spring	Closure Average	LOM Spring	LOM Average	LOM Spring	Closure Average	LOM Average	LOM Spring	Closure Average
Seepage	m <sup>3</sup> /day	1.28e+3	5.95e+3	4.71e+2	1.28e+3	5.95e+3	4.71e+2	1.28e+3	5.95e+3	4.71e+2	1.28e+3	5.95e+3
Cl	g/day	1.25e+3	5.73e+3	4.61e+2	1.26e+3	5.84e+3	4.60e+2	2.64e+5	1.31e+6	2.63e+5	3.97e+5	2.94e+5
F	g/day							2.30e+3	3.75e+3	2.13e+3	1.99e+3	1.45e+3
SO <sub>4</sub>	g/day	1.04e+6	3.75e+6	9.89e+5	1.03e+6	1.04e+6	1.01e+6	6.69e+2	2.03e+6	6.66e+5	7.59e+5	5.52e+5
N as NO <sub>3</sub>	g/day	8.59e+1	3.95e+2	3.13e+1	8.65e+1	4.04e+2	3.13e+1	2.55e+2	6.69e+2	1.97e+2	2.30e+2	5.11e+2
Ca	g/day	1.14e+5	7.38e+5	6.78e+4	1.74e+5	3.45e+5	1.37e+5	1.22e+5	5.31e+5	1.09e+5	1.41e+5	2.91e+5
K	g/day	6.40e+4	6.46e+4	8.08e+4	3.49e+4	3.56e+4	3.46e+4	1.01e+5	2.56e+5	1.01e+5	1.05e+5	7.68e+4
Mg	g/day	1.55e+5	5.38e+5	1.01e+5	1.37e+5	2.79e+5	1.21e+5	3.63e+5	1.21e+6	3.25e+5	4.22e+5	4.23e+5
Na	g/day	2.79e+5	4.01e+5	3.44e+5	1.71e+5	1.75e+5	1.70e+5	9.85e+4	1.06e+5	9.77e+4	7.70e+4	5.87e+4
Al	g/day	3.00e-2	1.28e-1	1.06e-2	2.81e-2	1.37e-1	1.02e-2	2.98e-2	1.35e-1	1.18e-2	2.94e-2	1.34e-1
Fe	g/day	5.03e-1	3.19e+0	2.21e-1	6.55e-1	2.32e+0	3.09e-1	5.68e-1	2.70e+0	2.94e-1	6.15e-1	2.51e+0
Ag	g/day	1.95e+0	1.05e+1	9.19e-1	2.57e+0	6.29e+0	1.28e+0	6.75e+0	1.59e+1	8.15e+0	9.42e+0	6.20e+0
As	g/day	1.48e-3	3.95e+0	5.98e+0	1.68e-3	1.48e-3	1.13e-3	1.29e-2	7.24e-1	5.44e-3	1.16e-2	5.00e-3
Cd	g/day	1.51e+0	3.28e+0	6.33e+0	1.87e+0	1.77e-1	1.58e+0	2.15e+1	1.33e+2	1.84e+1	4.36e+1	4.31e+0
Co	g/day	5.43e+2	2.37e+2	5.60e+2	5.84e+2	1.52e+2	5.08e+2	2.13e+1	3.43e+1	1.84e+1	1.89e+1	4.90e+0
Cr	g/day	6.62e-4	1.67e+0	1.01e-1	9.12e-4	5.85e-5	4.93e-4	8.74e-5	1.41e+0	3.99e-5	2.52e-4	2.55e-5
Cu	g/day	2.30e+1	7.80e+1	9.37e+0	1.90e+1	6.82e+0	7.19e+0	5.40e-1	4.07e+1	1.68e-1	1.22e+0	2.44e-1
Hg	g/day	9.03e-1	2.67e+0	4.29e+0	7.07e-1	4.07e-1	2.81e-1	1.47e+0	2.44e+0	1.50e+0	1.50e+0	6.19e-1
Mn	g/day	1.14e+3	9.12e+2	1.03e+3	1.68e+3	3.97e+2	1.48e+3	6.50e+2	1.56e+3	5.79e+2	6.82e+2	1.65e+2
Mo	g/day	1.38e+3	1.27e+3	2.18e+3	7.31e+2	7.18e+2	5.99e+2	8.75e+2	7.29e+2	7.70e+2	6.14e+2	4.27e+2
Ni	g/day	2.89e+1	2.57e+1	5.42e+1	3.21e+1	4.77e+0	2.33e+1	1.63e+1	5.10e+1	1.08e+1	1.61e+1	2.25e+0
Pb	g/day	3.50e-2	1.18e+1	2.64e+0	3.04e-2	2.48e-3	1.51e-2	3.74e-3	3.27e+0	1.18e-3	2.98e-3	3.40e-4
Sb	g/day	1.85e+1	1.67e+1	2.34e+1	9.97e+0	1.01e+1	9.90e+0	2.79e+1	3.82e+1	2.78e+1	2.30e+1	1.68e+1
Se	g/day	9.74e-1	1.18e+1	1.99e+1	1.55e+0	1.22e+0	7.87e-1	1.89e+0	1.05e+1	6.55e-1	1.35e+0	6.05e-1
U	g/day	8.05e+0	1.33e+1	9.87e+0	5.33e+0	5.37e+0	5.28e+0	4.21e+1	7.88e+1	4.16e+1	3.85e+1	2.80e+1
Zn	g/day	1.13e+2	6.91e+1	1.65e+2	1.09e+2	1.20e+1	8.11e+1	6.03e+0	4.88e+1	3.82e+0	6.38e+0	6.73e-1

Table 11. Predicted water quality in a river adjacent to the proposed Aitiik WRD for different conditions (from Charles et al. 2016).

		Predicted chemistry based on NAG test results						Predicted chemistry based on HCT test results						
		Segregated WRD			Blended WRD			Segregated WRD			Blended WRD			
		LOM Average	Closure Average	LOM Spring Average	LOM Spring	Closure Average	LOM Spring	Closure Average	LOM Average	LOM Spring	Closure Average	LOM Average	LOM Spring	Closure Average
Flow	m <sup>3</sup> /s	7.00e-1	7.00e-1	7.29e+0	7.00e-1	7.29e+0	7.00e-1	7.29e+0	7.00e-1	7.00e-1	7.29e+0	7.00e-1	7.00e-1	7.29e+0
Cl	mg/L	6.23e-1	6.44e-1	6.32e-1	6.31e-1	6.44e-1	6.33e-1	6.31e-1	5.00e+0	2.71e+0	4.97e+0	7.18e+0	1.09e+0	1.09e+0
F	mg/L													
SO <sub>4</sub>	mg/L	1.40e+0	1.86e+1	7.35e+0	1.78e+1	1.84e+1	3.04e+0	1.82e+1	1.25e+1	4.62e+0	1.24e+1	1.39e+1	2.28e+0	2.28e+0
N as NO <sub>3</sub>	mg/L	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0	1.51e+0
Ca	mg/L	4.24e+0	6.13e+0	5.41e+0	5.36e+0	7.12e+0	4.79e+0	6.51e+0	6.25e+0	5.08e+0	6.05e+0	6.57e+0	4.70e+0	4.70e+0
K	mg/L	5.87e-1	1.65e+0	6.90e-1	1.92e+0	1.16e+0	6.44e-1	1.16e+0	2.26e+0	9.93e-1	2.25e+0	2.32e+0	7.09e-1	7.09e-1
Mg	mg/L	1.15e+0	3.71e+0	2.00e+0	2.81e+0	3.42e+0	1.59e+0	3.15e+0	7.16e+0	3.06e+0	6.52e+0	8.12e+0	1.82e+0	1.82e+0
Na	mg/L	1.42e+0	6.03e+0	2.05e+0	7.10e+0	4.24e+0	1.69e+0	4.22e+0	3.04e+0	1.58e+0	3.03e+0	2.69e+0	1.51e+0	1.51e+0
Al	mg/L	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1	2.64e+1
Fe	mg/L	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0	1.78e+0
Ag	µg/L	3.23e-2	1.67e-2	1.52e-2	4.24e-2	9.98e-3	2.12e-2	1.12e-1	2.52e-2	1.35e-1	1.56e-1	9.85e-3	1.20e-1	1.20e-1
As	µg/L	9.70e-2	1.03e-1	1.96e-1	9.70e-2	9.70e-2	9.70e-2	9.72e-2	9.81e-2	9.70e-2	9.71e-2	9.70e-2	9.70e-2	9.70e-2
Cd	µg/L	4.35e-3	2.93e-2	9.55e-3	1.09e-1	3.52e-2	4.63e-3	3.05e-2	3.60e-1	2.16e-1	3.08e-1	7.25e-1	1.12e-2	1.12e-2
Co	µg/L	1.10e-1	9.08e+0	4.86e-1	9.37e+0	9.77e+0	3.51e-1	8.52e+0	4.62e-1	1.64e-1	4.15e-1	4.23e-1	1.18e-1	1.18e-1
Cr	µg/L	2.28e-1	2.28e-1	2.31e-1	2.30e-1	2.28e-1	2.28e-1	2.28e-1	2.30e-1	2.28e-1	2.28e-1	2.28e-1	2.28e-1	2.28e-1
Cu	µg/L	3.46e-1	7.27e-1	4.70e-1	5.01e-1	6.60e-1	3.57e-1	4.65e-1	3.55e-1	4.11e-1	3.49e-1	3.66e-1	3.46e-1	3.46e-1
Hg	µg/L	3.60e-3	1.85e-2	7.84e-3	7.45e-2	1.53e-2	4.25e-3	8.24e-3	2.79e-2	7.47e-3	2.84e-2	2.84e-2	4.58e-3	4.58e-3
Mn	µg/L	2.14e+1	4.03e+1	2.28e+1	3.84e+1	4.92e+1	2.20e+1	4.59e+1	3.21e+1	2.39e+1	3.10e+1	3.27e+1	2.17e+1	2.17e+1
Mo	µg/L	2.62e-1	2.30e+1	2.28e+0	3.63e+1	1.23e+1	1.40e+0	1.02e+1	1.47e+1	1.42e+0	1.30e+1	1.04e+1	9.40e-1	9.40e-1
Ni	µg/L	1.57e-1	6.34e-1	1.97e-1	1.05e+0	6.87e-1	1.64e-1	5.42e-1	4.26e-1	2.37e-1	3.34e-1	4.23e-1	1.60e-1	1.60e-1
Pb	µg/L	3.42e-2	3.48e-2	5.29e-2	7.78e-2	3.47e-2	3.42e-2	3.44e-2	3.43e-2	3.94e-2	3.42e-2	3.42e-2	3.42e-2	3.42e-2
Sb	µg/L	1.16e-2	3.17e-1	3.82e-2	3.99e-1	1.76e-1	2.76e-2	1.75e-1	4.72e-1	7.22e-2	4.70e-1	3.92e-1	3.82e-2	3.82e-2
Se	µg/L	1.61e-2	1.87e-2	3.30e-1	2.57e-2	1.94e-3	1.30e-2	3.13e-2	1.67e-2	1.08e-2	2.23e-2	9.60e-4	2.26e-4	2.26e-4
U	µg/L	2.30e-2	1.56e-1	4.40e-2	1.86e-1	1.11e-1	3.15e-2	1.10e-1	7.19e-1	1.48e-1	7.11e-1	6.60e-1	6.74e-2	6.74e-2
Zn	µg/L	1.26e+0	3.13e+0	1.37e+0	3.98e+0	3.06e+0	1.28e+0	2.60e+0	1.36e+0	1.34e+0	1.32e+0	1.32e+0	1.26e+0	1.26e+0

#### 4.5.2 Modelling in an existing tailings impoundment

This study, performed by Mayer et al. (2002), focused on simulating the release and attenuation of acidic drainage in a decommissioned tailings impoundment at the Nickel Rim mine site, near Sudbury, Canada. By using reactive transport simulations, the authors investigated sulphide mineral oxidation, geochemical evolution and the subsequent transport of dissolved constituents in unsaturated and shallow saturated zones. Simulations were performed along a one-dimensional vertical cross-section, where geochemical data were obtained in a previous study through a multilevel sampling well (Benner et al. 2000). In addition to the geochemical observations, physical parameters such as porosity, hydraulic conductivity, recharge rate, moisture content, and water table were also included in the model. Modelling was performed by using the reactive transport code MIN3P. Initial conditions were also defined from the observations of an earlier study (Bain 1996) and the recharge water was assumed to have the composition of rainwater. The model considered pyrrhotite, pentlandite and chalcopyrite as the main sulphide-bearing miner-

als, whereas the buffering minerals were traces of carbonate and abundant aluminosilicate minerals such as augite, calcic plagioclase and biotite. The mineralogical assemblage was described based on the mineralogical investigations in tailings (Jambor & Owens 1993). Oxidation of the sulphide minerals was modelled using the shrinking-core model (Levenspiel 1972), while laboratory-derived rate laws were used in describing the weathering of aluminosilicates (Mayer et al. 2002). The model considered ferrihydrite, jarosite, gypsum and covellite as secondary mineral phases and simultaneously it allowed the precipitation of siderite, gibbsite and amorphous silica. The simulation was carried out for a period of 39 years, which is representative of the time period between the mine decommissioning and the data collection. Figure 8a shows a schematic diagram of the conceptual model. Detailed information regarding the model setup and input parameters, as well as the definition of boundary and initial conditions can be found in Mayer et al. (2002).

Figures 8b–c illustrate different temporal snapshots of the simulated vertical profiles for the partial pressures of oxygen and carbon dioxide in the tailings. The atmospheric oxygen oxidizes the

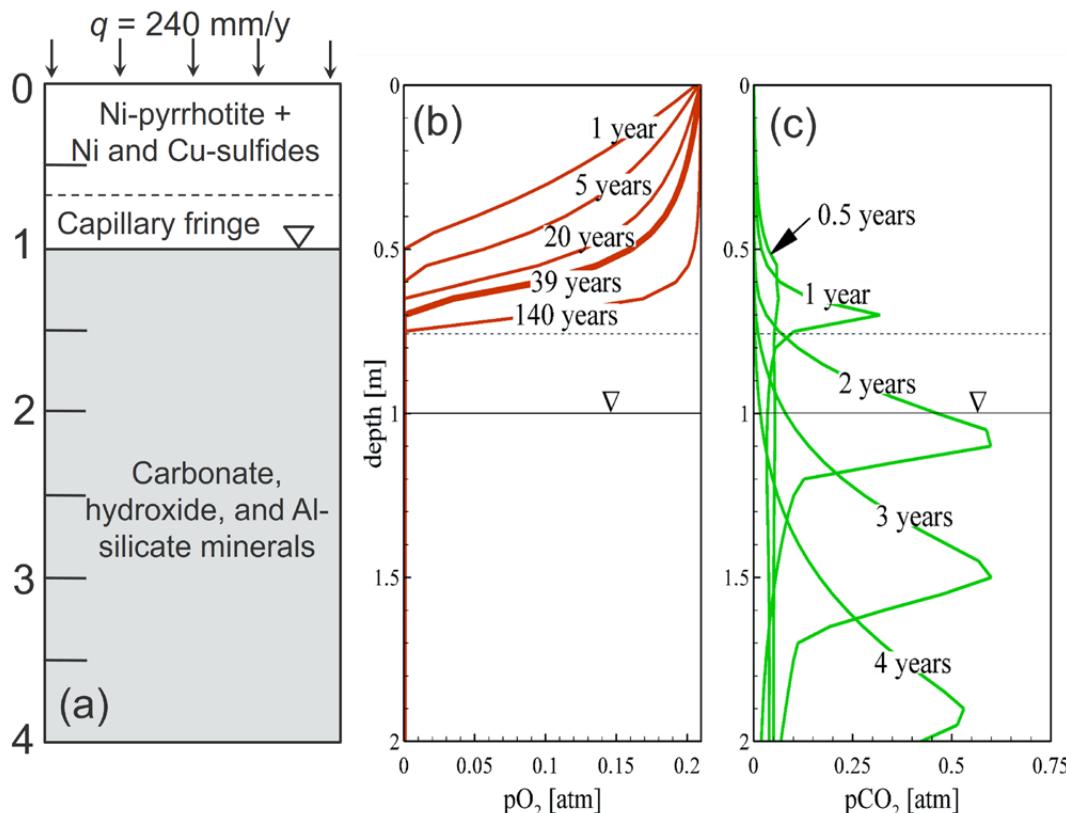


Fig. 8. (a) Vertical cross-section at the Nickel Rim tailings impoundment and simulated partial pressures of (b) oxygen and (c) carbon dioxide concentrations along the depth profile (modified from Mayer et al. 2002).

sulphide minerals and the front of  $P_{O_2}$  successively migrates downward over time as sulphide phases become depleted (Fig. 8b).  $CO_2$  concentrations, resulting from the dissolution of calcite, appear to be depleted in the shallow unsaturated zone due to the possibility of escaping from the tailings (Fig. 8c).

In this modelling exercise, the authors showed that it is possible to consistently reproduce the field observations by the reactive transport simulations if site-specific details are reasonably characterised. Figure 9 presents a comparison of the simulated aqueous concentration profiles with the previously collected field data (Benner et al. 2000). The model appears to capture the overall trends in the meas-

ured concentration profiles reasonably well, and it highlights the potential capabilities to quantitatively estimate the risks related to the acidic drainage.

The acidic front in Figure 9a is directly correlated with the elevated concentrations of dissolved species (Figs. 9b–c). This behaviour is, in fact, the result of the dissolution of the sulphide minerals as presented in Figures 10a–b. The authors mentioned that after approximately 7 years, calcite was completely depleted from the domain, leaving only aluminosilicates as the primary neutralizing minerals (Fig. 10c). The weathering of aluminosilicate minerals is reflected in the gradual increase in the cation concentrations along the depth profile (Figs. 9d–e).

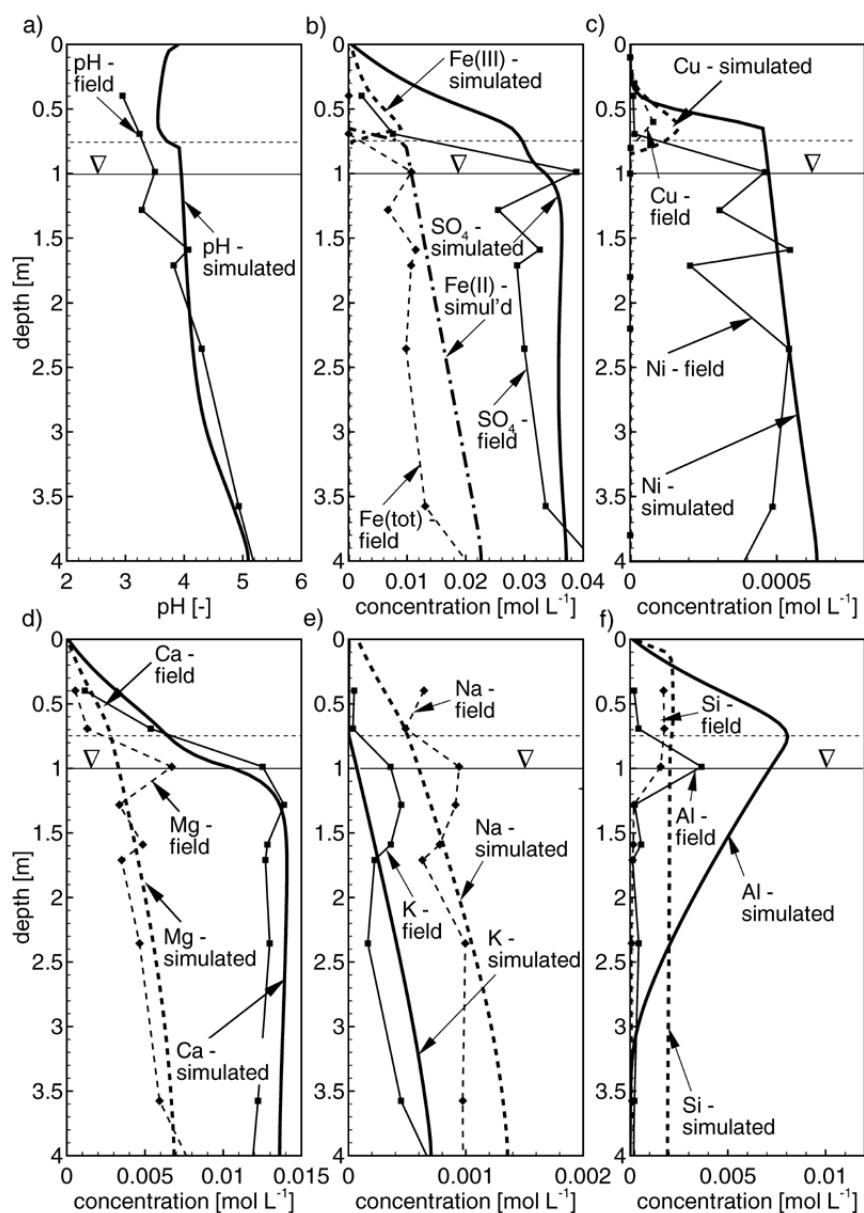


Fig. 9. Simulated and observed aqueous concentration profiles after 39 years at the Nickel Rim tailings impoundment (from Mayer et al. 2002).

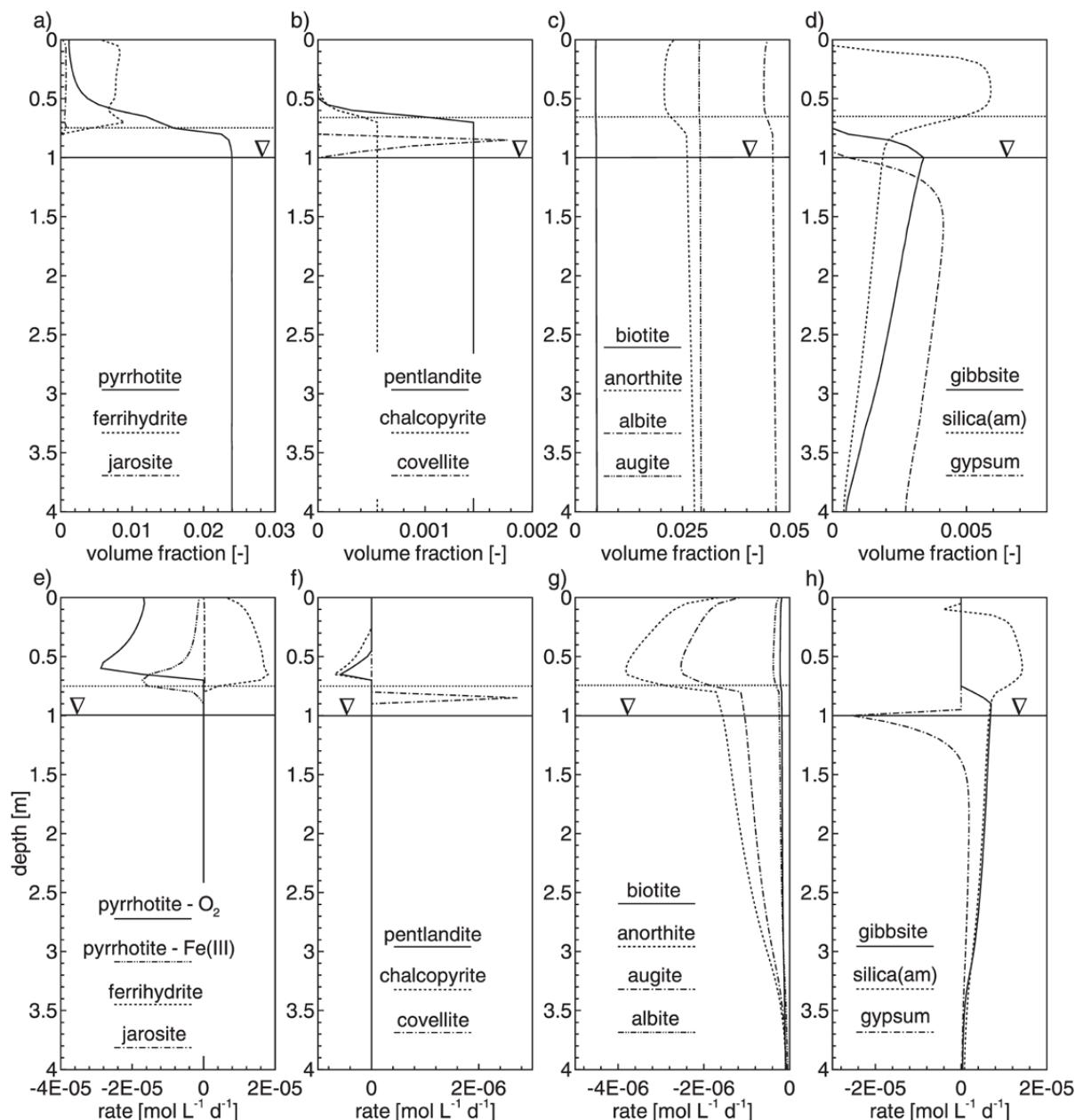


Fig. 10. Simulated mineral fractions and dissolution/precipitation rates after 39 years at the Nickel Rim tailings impoundment (from Mayer et al. 2002).

Concentrations of Al and Si (Fig. 9f) are controlled by the secondary precipitation of gibbsite and amorphous silica (Figs. 10d, h). Additionally, gypsum (Fig. 10d) and covellite (Fig. 10b) profiles tend to be strongly correlated with sulphate (Fig. 10b) and Cu (Fig. 10c) concentrations, respectively, at the oxidation front.

#### 4.5.3 Modelling in an existing waste-rock pile

This example illustrates an application of numerical simulations to estimate sulphide oxidation in the

active Doyon waste rock pile in northern Québec, Canada (da Silva et al. 2009). The simulations were performed in a 2D cross-section of the experimental waste rock pile previously characterised (e.g. Lefebvre 1994, Sracek et al. 2004) and used in other modelling studies (e.g. Lefebvre et al. 2001, Molson et al. 2005). A conceptual model was developed in the previous studies based on the field data collected from the south pile of the Doyon mine site. Modelling was performed by using the 2D finite element pyrite oxidation code THERMOX, which is able to simulate physical and geochemical processes

within waste rocks including variable water saturation and thermal processes. Before its application in a real-scale waste rock pile, the performance of the THERMOX code was verified against another reactive transport code, TOUGHREACT for 1D simple scenarios.

The adopted 2D domain was discretized into 7050 elements and 3685 nodes, and the boundary and initial conditions for both water flow and heat transfer were chosen according to the available data (e.g. Lefebvre 1994, Sracek et al. 2004). Different infiltration rates were applied along the upper and side boundaries (slope) of the pile, whereas the bottom boundary was treated as a free flow boundary having a constant head. Physical parameters of the waste rock were also collected in these previous studies. The model considered pyrite as the only acid-producing mineral and calcite as the neutralizing mineral. As secondary minerals, the model allowed the precipitation of gypsum, siderite, amorphous  $\text{Fe(OH)}_3(a)$  and amorphous  $\text{Al(OH)}_3(a)$ . In particular, simulations were performed for two distinct scenarios representing two end members in that waste rock pile: diffusion-controlled oxygen transport, and convection-controlled transport of oxygen into the waste rock.

Figure 11 presents the simulated distributions of temperature and oxygen concentration within

the waste rock pile. In the Doyon waste rock pile, the transport of oxygen is controlled by convective transport close to the slope and oxygen transport is due to diffusion in the core of the pile. The authors demonstrated that the temperature distribution calculated with the THERMOX code agreed well with the observed field data. Additionally, the simulation results were also found to be consistent with other studies that focused on the modelling of the same site using a different code (e.g. Lefebvre et al. 2001).

Figure 12 depicts the simulated pH and sulphate concentrations in the waste rock pile. The model was able to reproduce the observed pH of the domain reasonably well. However, the sulphate concentration was underestimated compared to the measured field data. The authors argued that the discrepancy might be due to the presence of sericite schist rock, which potentially accelerates the pyrite oxidation process, as well as to the temporal variations in recharge. In order to improve the outcome, they also suggested the inclusion of kinetic dissolution of silicates during the final stages of neutralization. Nevertheless, this modelling exercise provides a good example of how numerical models can be effectively used to estimate acid rock drainage and potential contamination in the surrounding area, and to predict various remediation scenarios.

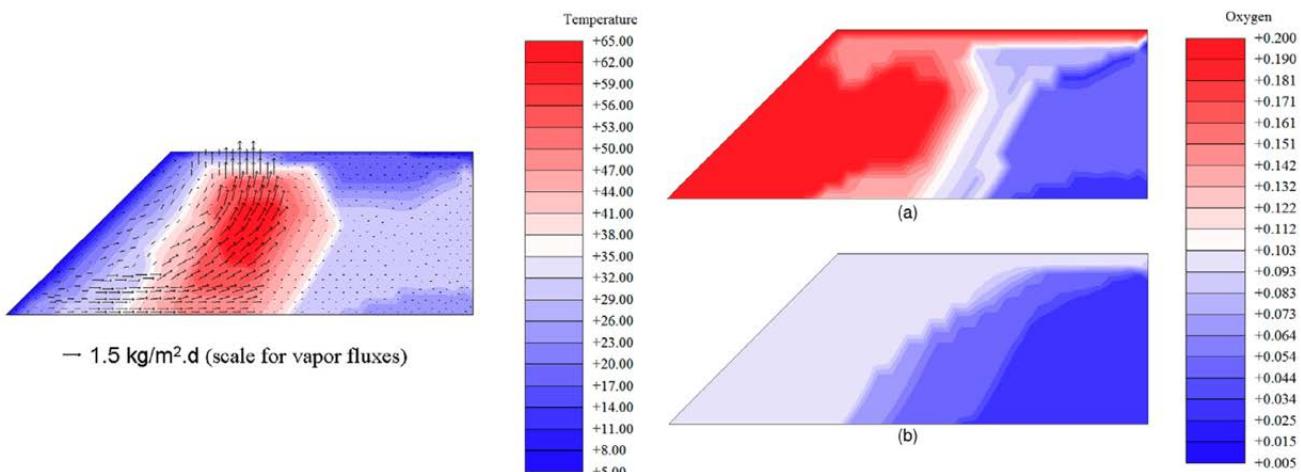


Fig. 11. Simulated distributions of temperature ( $^{\circ}\text{C}$ ) (left) and oxygen concentrations (vol.%) (right) at  $t = 13.5$  years. In the right panel: (a) convective scenario, (b) non-convective scenario (modified from da Silva et al. 2009).

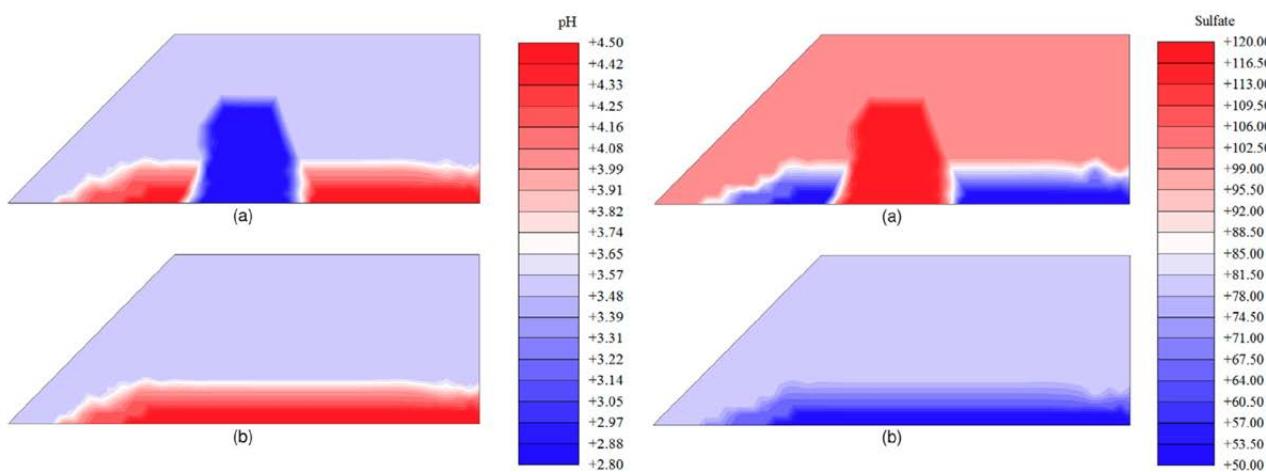


Fig. 12. Simulated pH (left) and dissolved sulphate concentrations (right) at  $t = 13.5$  years: (a) convective case, and (b) non-convective case (modified from da Silva et al. 2009).

#### 4.6 Uncertainties in modelling approaches

Any type of quantitative modelling consists of describing the relevant processes in a particular system of interest using mathematical equations derived from first principles (e.g. mass, momentum, or energy conservation) and from conceptual assumptions made about the system definition. Identifying the correct mathematical relations, by using the right set of parameters and by means of equations, between the quantities of interest and their interactions is at the core of quantitatively predicting the outcome of a system's action. Adequate process understanding is a prerequisite to describe such a system under investigation by means of equations as well as to formulate predictive models.

In the mine waste context, scientific research over the past decades has led to the establishment of fundamental understanding of the key processes governing the rate and extent of sulphide oxidation, the generation of acid mine drainage and the release of metals. Although individual mechanisms in such settings are fairly well known, the relative contribution of these individual processes is the key to developing a predictive model for the overall coupled system (e.g. Amos et al. 2015). Therefore, modelling mine waste drainage in the predictive sense becomes difficult due to the complex interplay between these various processes within mine wastes, and because of the substantial uncertainties and/or errors associated with the conceptual and mathematical formulations and the input data available for the modelling. In fact, uncertainties related to the quantitative models focusing on pre-

dicting mine-waste water quality can result from various sources such as: (i) conceptual uncertainties, (ii) parameter uncertainties and (iii) computational or numerical uncertainties.

Uncertainties associated with the conceptualisation of the system or processes are perhaps the most important source of errors in any quantitative modelling. Specifically, integration of the different dominating processes mechanistically in reactive transport models is extremely challenging due to the variation in scales – which can result in variation by orders of magnitude in both spatial and temporal dimensions – associated with different mechanisms in mined or natural sediment scenarios. For example, processes such as chemical reactions, molecular diffusion or electrochemical processes mainly occur at micro- or molecular scales, but hydrodynamic dispersion, a combined effect of diffusion and pore-scale fluid velocity variations, is usually described at the so-called Darcy scale (e.g. Bear & Bachmat 1967). Additionally, heterogeneities and anisotropies associated with the physical and geochemical properties are usually referred to larger field scales. Furthermore, the time scale of these physicochemical processes can also vary over a wide range spanning from a fraction of a second to years.

In the context of fluid flow in porous media, the smallest relevant scale is the pore scale, which is usually conceptualized by a bundle of capillaries/channels connected through junctions (e.g. Bear 1972). At this scale, the flow of water is described by Navier–Stokes equations and it allows the possibili-

ties of resolving microscopic physical and chemical processes in the porous matrix (e.g. Willingham et al. 2010). Unfortunately, such a formulation is in fact too detailed and computationally impractical for most applications. Therefore, a common solution strategy is to use a volume-averaged description of the pore-scale quantities over a representative elementary volume (REV) (Bear 1972). This step considers these averaged up-scaled properties to be locally constant in a REV, where water flow can be described by Darcy's law. Models that describe processes at this scale are known as continuum models or Darcy scale models. Model parameters at the Darcy scale can possibly be obtained from laboratory experiments. Nevertheless, the domains of interest in real mine waste settings or natural aquifer systems are orders of magnitude larger, and Darcy scale process descriptions can hence be too detailed for field scales. Accurate modelling at this scale would require the assignment of local Darcy scale physical and geochemical characteristics to each naturally present heterogeneous formation. Unfortunately, such information is widely unknown, especially in such detail at typical field sites, and laboratory experiments are not capable of capturing such naturally occurring variabilities and complexities. Therefore, an additional up-scaling step, using effective field-scale parameters, is usually used in order to address reactive transport at larger field scales (e.g. Neuman et al. 1987, Kitanidis 1988, Dagan 1991, Rajaram & Gelhar 1995). These up-scaling approaches and the associated derivations of the effective parameters (e.g. transport and reaction coefficients) are still a matter of current research, and further investigations are required to realistically define these up-scaled parameters, as well as to improve the predictive capabilities of the field-scale models (e.g. Dentz et al. 2011).

In predicting acid-mine drainage release, contaminant transport and their attenuation, the main source of uncertainties is associated with this second upscaling step, as mentioned above (cf. also Chapter 4.2, this review). In fact, it is extremely difficult, by using the up-scaled quantities, to capture all the features of real field-scale scenarios and to correctly predict reactive transport due to the increased complexities of natural systems. The concepts of predictive model formulations commonly rely on continuous process descriptions in both space and time. However, most of the data obtained from the field are extremely sparse; hence, they only provide information on discrete loca-

tions in space or as a few snapshots in time (e.g. Mayer et al. 2003). This low resolution in the collected data and the subsequent inadequate system understanding not only make the development of a conceptual model particularly challenging, but also lead to a poor or oversimplified representation of reality for the whole system. One additional level of uncertainty related to this step is that field data are not usually collected under well-controlled or repeatable conditions, and the conditions may change over time. Consequently, it is often not possible to generalize the outcomes obtained from field sites, and this makes the definition of the realistic boundary and initial conditions required in modelling extremely challenging, if not impossible. Difficulties and/or failures in the long-term predictions of field-scale models basically stem from these aforementioned uncertainties associated with site characterisation, system understanding and conceptualisation. In order to address these issues and as an attempt to fill the gaps concerning the definition and quantification of the parameters to use in large-scale models, stochastic theories and Monte-Carlo simulations are sometimes used (e.g. Gehlar & Axness 1983, Chiogna et al. 2011, Pedretti et al. 2017b). Recently, several investigators have also proposed hybrid-scale models, in which a part of the domain is solved at the pore scale and the rest is solved at the continuum scale described with volume-averaged REVs (e.g. Tang et al. 2015, Karimi & Nakshatrala 2017).

The second degree of uncertainty in a modelling study can be unknowns associated with the model parameters. In fact, parameter uncertainties can also inherently exert control on the conceptual level, as the formulation of a site-specific conceptual model is largely dependent on the input data and measured parameters. Even when a site has been reasonably characterised, major processes have been identified, and conceptual model has been developed, the obtained set of parameters can be insufficient, non-unique or simply wrong to perform predictive modelling. If the available data are inadequate, sensitivity analysis can help not only to identify the most important controlling parameters under a range of possible conditions (i.e. "what-if scenarios"), but also to provide insight regarding further data requirements to enhance the model's predictive capability (e.g. Mayer et al. 2003). Such parameter study can also be useful in testing possible hypotheses, as well as in enhancing understanding of the key processes and their controls.

Another source of error in the predictive capabilities refers to the non-uniqueness of both the parameter sets and the model solutions. Sometimes, identifying the controlling parameters is problematic, because different sets of parameters can possibly produce the same outcome. Alternatively, it is often uncertain whether a particular change in a specific quantity refers to a unique process. For instance, ion-exchange reactions or dissolution–precipitation reactions can lead to similar changes in the concentration of a specific dissolved species (e.g. Mayer et al. 2003). Furthermore, it is extremely difficult to evaluate the relative contributions of the multiple competing processes from a measured set of parameters. In such conditions, additional information is required to constrain the conceptual hypothesis to develop an adequate quantitative model, as well as to tailor its predictive capability.

Besides conceptual and parameter uncertainties, errors can also result from the mathematical formulations, solution procedures or numerical methods used in a quantitative model. Depending on the problem complexity and accuracy of the numerical approaches, such uncertainties can also be tricky in a field-scale simulation capturing complex processes. However, given the current state of knowledge and the recent advances in sophisticated

numerical methods, it can be stated that numerical or computational uncertainties are the least important compared to the conceptual or parameter uncertainties in modelling mine-waste drainage or subsurface processes in general.

Carl Steefel and coworkers performed a series of benchmark studies in order to systematically test the performance of the available reactive transport codes for a range of geochemical problems (Steefel et al. 2015b). In particular, the authors focused on comparing the simulation outcomes from the different codes applied to the same problem. This initiative covered different geochemical topics through a total of 12 reactive transport benchmark examples, including a problem on acid rock drainage (ARD). Each of these benchmark problems has been documented as an individual contribution in a special issue of *Computational Geosciences* (Volume 19, Issue 3, June 2015). The outcome of this series of papers suggest that computational uncertainties were in fact negligible. Furthermore, using the same thermodynamic database and activity equations, different participating reactive transport codes produced practically identical results, irrespective of their numerical formulations (Steefel et al. 2015b). Table 12 lists the specific problems addressed in these benchmark studies.

Table 12. List of the reactive transport benchmark problems performed by Carl Steefel and coworkers (Steefel et al. 2015b).

Benchmark Problems	References
Microbially mediated Cr reduction	Molins et al. (2015)
Cr isotope fractionation	Wanner et al. (2015)
Multicomponent diffusion and electrochemical migration	Rasouli et al. (2015)
Multispecies diffusion and treatment electrostatic effects in a compacted bentonite column	Alt-Epping et al. (2015)
U bioremediation	Yabusaki et al. (2015)
Biogenic uraninite re-oxidation by Fe(III) (hydr)oxides	Şengör et al. (2015)
Surface complexation and dual-domain U(VI) transport	Greskowiak et al. (2015)
Generation and attenuation of ARD	Mayer et al. (2015)
Heavy metal cycling in lake sediments	Arora et al. (2015)
Multicomponent reactive transport across a cement/clay interface	Marty et al. (2015)
Evaluation of permeability-porosity and tortuosity-porosity relationships linked to mineral dissolution-precipitation	Xie et al. (2015)
Decalcification of cracked cement structures	Perko et al. (2015)

## 5 DATA REQUIREMENTS

Given the computer resources available today, the predictive capabilities in modelling mine wastes are mainly limited by the availability of site-specific data rather than the computational power (e.g. Nordstrom 2005, Steefel et al. 2015a). In fact, the detailed characterisation of a site ultimately determines the quality of predictions, as realistic data are a precursor for performing any type of quantitative modelling. Therefore, good quality data are unavoidable in order to develop a realistic conceptual model, as well as to constrain the mathematical model with site-specific information.

As all the different mine waste sites consist of complex geological, hydrological and biological processes, including natural and engineered features, building a perfect model and the exact prediction of long-term behaviour are practically impossible. Therefore, assumptions must be made, together with the use of good quality data and understanding of the deterministic principles of all the processes included (e.g. Mayer et al. 2003, Nordstrom 2017). A model with relevance to a given mine site can be created if sufficient site-specific inputs are collected. These inputs must be as representative as possible of the whole range of conditions at a mine site (Maest et al. 2005).

Essential background information for successful modelling includes data concerning the fields of geology, hydrogeology, geochemistry and microbiology. The specific data needs are related to the objective and scope of each particular model. Besides this information, additional data might also be needed. For example, variables related to the local climate, such as temperature and precipitation, are often essential, as well as infiltration rates through the unsaturated zone and waste dump dimensions (Maest et al. 2005). Moreover, especially when modelling processes in mine waste facilities, particle size is an important parameter, as it affects the reactive geometric surface area. A summary of the information and knowledge requirements of a predictive model for a waste pile is presented in Table 13.

The widely available open databases (e.g. PHREEQC, MINTEQ and PITZER) contain a broad set of thermodynamic equilibrium constants for common minerals. Regrettably, many locally important minerals are often missing, and the datasets need to be complemented manually. Besides equilibrium constants, kinetic rate data for precipitation, co-precipitation and dissolution reactions of important minerals must sometimes be searched for and

inserted into the databases. Selected laboratory and field-scale methods to obtain some of these data are presented in Chapter 3. For more detailed information, see e.g. textbooks by Langmuir (1997), Appelo and Postma (2005) and Nordstrom and Nicholson (2017).

Attempting any form of predictive modelling during the exploration and planning phase of a mine, as suggested in this report, involves additional degrees of difficulty. In such phases, collection of the representative site-specific information is extremely challenging, since the waste facilities (e.g. waste rock piles, tailings) under investigation have not yet been constructed. However, a representative volume of the critical data must be collected, because the formulation of any predictive model (e.g. reactive transport model) relies on process-oriented descriptions. To allow quantitative modelling, the collected data at this stage should particularly provide the most required information, such as

- boundary and initial conditions,
- transport and reaction processes,
- physical and chemical parameters controlling water flow,
- thermodynamic and reaction-progress parameters, and
- relevant primary and secondary mineral phases.

Mayer et al. (2003) pointed out that among all this information, mineralogical composition is the most crucial, because it eventually determines the potential for poor quality drainage.

In addition to the initially collected data to initiate a modelling study (i.e. at the “pre-mining” stage), additional data should be continuously collected as the project progresses in order to compare the model results with the actual evolution at the site. Of primary concern should be mineral evolution (e.g. formation of secondary minerals, depletion of primary minerals), pore-water and pore-gas chemistry, effluent chemistry and changes in water migration pathways. Implementing such a framework of continuous monitoring will allow calibration of the model on a realistic basis and will facilitate the gradual improvement of long-term predictive capabilities. Nevertheless, the available data in many cases may be extremely scarce, especially in the planning phase of a mine, and this must be taken into account when making a particular decision based on this information.

Table 13. Information and knowledge requirements for a predictive model of a waste pile (modified from Maest et al. 2005 and Nordstrom 2017).

Baseline conditions	Waste facility design	Waste characteristics	Knowledge on geochemistry and microbiology
<p><i>Hydrology (surface water &amp; groundwater)</i></p> <ul style="list-style-type: none"> <li>• Water balance</li> <li>• Water cycles</li> <li>• Relationship between geology and groundwater flow</li> </ul> <p><i>Water quality</i></p> <ul style="list-style-type: none"> <li>• Surface water</li> <li>• Groundwater</li> <li>• Rainwater</li> </ul> <p><i>Local geology</i></p> <ul style="list-style-type: none"> <li>• Bedrock (lithology: rock units and their ratio, geological block model; main minerals, formation processes)</li> <li>• Quaternary deposits (units, composition)</li> <li>• Spatial characteristics of geological units (e.g. depth, thickness)</li> <li>• Hydraulic characteristics of geological units (hydraulic conductivity, porosity, storage characteristics)</li> </ul> <p><i>Climate</i></p> <ul style="list-style-type: none"> <li>• Precipitation</li> <li>• Evaporation</li> <li>• Temperature</li> <li>• Annual changes/variation</li> </ul> <p><i>Topography</i></p>	<p><i>Structure (dams, liners, ponds)</i></p> <p><i>Size, height</i></p> <p><i>Disposal type</i></p> <p><i>Water balance (incl. runoff)</i></p> <p><i>Water management (tailings facilities)</i></p> <p><i>Distances to water bodies (surface water, groundwater table)</i></p> <p><i>Mitigation (covers, liners, etc.)</i></p>	<p><i>Masses to be disposed</i></p> <p><i>Compositional variation</i></p> <ul style="list-style-type: none"> <li>• Rock types and their ratios</li> </ul> <p><i>Mineralogical composition</i></p> <ul style="list-style-type: none"> <li>• Mineral identification</li> <li>• Chemical composition of minerals</li> <li>• Relative weathering rates of minerals</li> <li>• Occurrence of sulphides and contaminant sources (liberated vs. non-liberated)</li> </ul> <p><i>Chemical composition</i></p> <ul style="list-style-type: none"> <li>• Totals</li> <li>• Aqua regia leachable</li> </ul> <p><i>Acid generation potential</i></p> <p><i>Element leaching</i></p> <ul style="list-style-type: none"> <li>• Kinetic tests</li> </ul> <p><i>Mineral weathering rates / solute release</i></p> <ul style="list-style-type: none"> <li>• Sulphide oxidation</li> <li>• Chemical release rates</li> <li>• Distribution coefficients</li> </ul> <p><i>Physical and hydraulic properties</i></p> <ul style="list-style-type: none"> <li>• Grain size</li> <li>• Porosity</li> <li>• Infiltration rates</li> <li>• Hydraulic conductivity</li> <li>• Reactive surface area</li> <li>• Oxygen diffusion rates</li> </ul>	<p><i>Mobilisation of solutes</i></p> <ul style="list-style-type: none"> <li>• Sulphide oxidation</li> <li>• Carbonate dissolution and precipitation</li> <li>• Gypsum dissolution and formation</li> <li>• Aqueous oxidation and reduction of trace elements and metalloids</li> <li>• Iron precipitation</li> <li>• Aluminium precipitation</li> <li>• Aluminosilicate dissolution and precipitation</li> <li>• Silica precipitation</li> <li>• Efflorescent salt formation and dissolution</li> <li>• Mixing of waters with reaction</li> <li>• Evaporation of waters with reaction</li> </ul> <p><i>Basic geochemical processes</i></p> <ul style="list-style-type: none"> <li>• Aluminosilicate weathering and clay formation</li> <li>• Carbonate weathering</li> <li>• Dolomitization</li> <li>• Dediolomitization</li> <li>• Evaporation and evaporate mineral formation</li> <li>• Ion exchange</li> <li>• Gas evolution</li> <li>• Geothermal and metasomatic alteration</li> <li>• Mixing of chemically different waters</li> </ul> <p><i>Basic microbiological processes</i></p> <ul style="list-style-type: none"> <li>• Sulphide mineral oxidation</li> <li>• Iron and manganese reduction and oxidation</li> <li>• Nitrate reduction and ammonium oxidation</li> <li>• Sulphate reduction</li> <li>• Methanogenesis</li> <li>• Hydrogenogenesis</li> </ul>

## 6 APPLICABILITY OF EXISTING MODELLING APPROACHES TO NORDIC CONDITIONS

The applicability of modelling approaches, as discussed in Chapter 4, is universal, as they are generally based on the fundamental laws of physics and chemistry. The approach for the construction and application of these models to the various compartments of mining environments is also fundamentally the same and is, in fact, independent of particular environmental conditions. However, depending upon the specific environmental conditions, different sets of key processes can dominate the behaviour of a system. Thus, different conditions in the environment can lead to different dynamics of a system, along with the required input parameters in a model. Therefore, adequate changes in boundary and initial conditions due to the climate conditions should be accurately taken into account during the application of these modelling approaches in a specific condition.

For instance, the weathering rate of sulphide minerals is typically slower in the Nordic climate compared to the tropical or subtropical climate (e.g. Malmström et al. 2000, Amos et al. 2015). Such phenomena involve significantly slower kinetics, a

potentially long-term source of acid rock drainage generation, and long-lasting poor-quality effluents under this condition (e.g. Amos et al. 2015). The cold winter in the Nordic region can often lead to frozen or partially frozen conditions in waste facilities (Linklater et al. 2005, Amos et al. 2015). In addition, seasonality is typical for Nordic conditions, with clear fluctuations in precipitation and temperature, as well as characteristic spring floods as a result of snow melt. All these conditions have the potential to impact on hydrogeology, water and gas influx, preferential fluid migration pathways, weathering rates, leaching of elements and the boundary conditions. These factors can also crucially control the seasonal system behaviour, as the reaction dynamics within waste piles are fundamentally dependent upon the initial distribution of reactants and how other reactants are subsequently introduced into the system. Furthermore, appropriate thermodynamic databases, with customized equilibrium and kinetic reaction constants for Nordic conditions, are required to provide a rigorous predictive analysis.

## 7 SUMMARY AND RECOMMENDATIONS

The predictive modelling of effluents from a planned waste facility is a challenging task, since mineral weathering processes are complex and long term. In addition, the prediction should be made in a phase where data are still limited and the modelling results cannot be calibrated, since the system to be modelled does not yet exist and there are no field observations that the model could be matched with (Alpers & Nordstrom 1999). A predictive model of a waste facility effluents typically combines hydrogeological and geochemical modelling approaches.

The prediction of effluent quality from mine waste facilities in Nordic conditions should basically follow the same principles and fundamentals as in the other climatic conditions. However, the influence of the cold climatic conditions (e.g. lower temperature, spring snow melt) on factors such as slower mineral weathering kinetics should be taken into account, especially when defining the boundary and initial conditions of the predictive model.

The first important step in the development of a predictive model for waste facilities is the construction of a representative conceptual model. This ensures that the appropriate data for numerical modelling are collected and outlines the key processes of a waste facility. Special attention should be paid to the quality of the collected data, as good quality data are the foundation for realistic conceptual modelling. Essentially, the conceptual model should be based on the best available geological, meteorological, hydrogeological, waste facility design, water quality, mineralogical, and waste rock geochemical characterisation data and the identification of the key geochemical/physicochemical processes affecting contaminant transport in the waste pile. It should be remembered that a predictive model can only be as good and accurate as the input data, as well as the conceptual model used and the modeller's understanding of the hydrogeochemical processes (e.g. Alpers & Nordstrom 1999, Bredehoeft 2005, Seppälä & Tuominen 2005).

During the planning and early phases of a mine, data for the modelling are obtained from a baseline study, mine planning and waste characterisation. In general, suitable characterisation methods should be chosen based on the model in demand. To allow quantitative modelling, the data collected in the early phase should particularly provide information regarding the boundary and initial conditions, water balance, physical and chemical parameters controlling water flow, solute transport and reaction processes, thermodynamic and reaction-progress parameters, as well as relevant primary and secondary mineral phases. The mineralogical composition is the most crucial type of information. Thus, a typical waste characterisation scheme needed to predict water quality from waste facilities includes determination of the mineralogical, geochemical, acid production and leaching properties of waste materials. These data are particularly needed to assist in the development of source term leachates to be used as inputs for the geochemical predictive modelling.

For waste characterisation, it is important that the studied waste types represent the geological heterogeneity of the exploited ore. For instance, all the different waste rocks types that will be excavated should be covered in the sampling and characterisation scheme. Therefore, the sampling should be based on block models of the ore deposit to assess the ratios of different rock types in a waste-rock pile. In the early phases of a mine, waste rock samples are typically collected from drill cores and tailings samples from the beneficiation tests.

Mineralogical characterisation is then carried out on the samples. It is necessary to determine the relative abundances of minerals in the wastes for the input data for the predictive modelling, and especially to identify acid-producing and neutralizing minerals, as well as the sources and occurrence of harmful substances. In addition, mineralogical composition is the tool for the first evaluation of the ability of mine wastes to produce acid mine drainage.

The determination of harmful elements and their leaching potential, as well as assessment of the acid production potential of wastes, is carried out using geochemical analyses and short-term static tests. These are used for screening, as input data for modelling, and to plan suitable longer term kinetic tests. Recommended static tests for ARD prediction include the ABA EN 15875 (CEN 2011) and NAG tests (AMIRA 2002). However, their results should be

verified with mineralogical studies. For geochemical characterisation, whole-rock analysis and aqua regia (ISO 11466) extractions are recommended as a minimum for waste characterisation.

Larger scale kinetic tests are used to simulate the long-term behaviour of wastes, and particularly to assess the long-term acid generation of wastes and evaluate the drainage quality. They yield more reliable data than static tests, and the data can be used to verify and enhance models and predictions. However, large-scale tests are highly case dependent and not very standardized, demanding careful consideration of the objectives, implementation, and interpretation and scaling of the results. The humidity cell test (ASMT D5744; ASTM 1996, 2007, 2013) is the only standardized kinetic test and is used to provide data, for example, on mineral oxidation rates, reacting mineral phases, long-term rates of acid generation and metal mobilisation for predictive modelling. However, based on this review, more guidelines are needed for the interpretation of HCT results.

The use of laboratory test data in the prediction of effluent quality requires scaling of the results to match the field conditions of the waste facility. However, scaling is complicated, as it is affected by many parameters and factors, such as the drainage pH, rock type, secondary mineral formation, microbial activity, methods used and reaction environment variables (e.g. temperature, leachate-to-rock ratio, oxygen availability and grain size; Kempton 2012, Eary 2015, Kirchner & Mattson 2015, Lapakko & Olson 2015, Pearce et al. 2015). As a result, several approaches have been developed to scale up, for instance, kinetic tests to field conditions. These include water-to-rock ratios, the water contact time, reaction kinetics for individual minerals comprising rock types, particle size and surface area (Eary 2015). Nevertheless, no single value can be provided for the scaling. Instead, the scaling should always be site-specific. In general, laboratory kinetic tests often overestimate the actual geochemical loads from the waste facilities (Morin & Hutt 1994, Malmström et al. 2000, Kempton 2012), and thus the scaling factor is typically <100%. Scaling is one of the major unsolved problems that also limits the usefulness of HCTs in effluent prediction among other lab-scale tests.

Once the conceptual model is outlined, a numerical model is developed based on it. The numerical prediction of the effluent quality from a planned waste facility is typically carried out using a

forward modelling approach, applying either reaction-path modelling or reactive transport modelling. A variety of codes are available for reactive transport modelling, including PHREEQC, PHAST, PHT3D, MINTEQA2 and/or Geochemist Workbench software. The selection of an appropriate software package/code for use in the modelling should be based on the overall objectives and exact purpose of the modelling task. In addition, factors such as the capabilities and numerical methods included in the code, as well as the availability and user-friendliness, affect the selection. The complexity of the adopted numerical model should be in accordance with the problem at hand.

After the numerical calculations have been completed, it is important to evaluate and report the uncertainties in the prediction and model results. Mine waste water quality prediction involves several sources of uncertainties, especially due to the complexity of the controlling processes. Major sources of uncertainty include the conceptualisation of the waste facility, available input data and computational formulations or numerical methods used. Uncertainties in conceptualisation are probably the most important source of errors in modelling, whereas computational uncertainties are the least problematic. In practice, the predictive capabilities in modelling mine wastes are mainly limited by the availability of site-specific data.

As the mining project progresses, mine waste characterisation, the conceptual model and numerical model should be updated and complemented with new data from field measurements. Additional data should be continuously collected in order to compare the model and other prediction results with the actual water quality evolution at the site and to establish a more interactive examination of key processes, as well as model formulation. It is especially important to investigate mineral evo-

lution (e.g. the formation of secondary minerals, depletion of primary minerals), pore-water and pore-gas chemistry, and changes in water migration pathways. Implementing such a predictive framework of modelling coupled with continuous monitoring is recommended, as it allows calibration of the model on a realistic basis and will enable the systematic improvement of long-term predictive capabilities, which are needed, for instance, for assessing mitigation measures and for mine closure planning.

Nevertheless, it would be practically impossible to build a perfect model for a mine site or to precisely forecast the evolution of long-term behaviour, because each real-scale site consists of unique natural and engineering features and their heterogeneity, as well as complex geological, hydrological and biological processes. Accurately resolving all these features, their local heterogeneous properties, and the coupled multi-scale mechanisms in great detail is simply unachievable. Hence, a simplified system description in real systems is inevitable, and assumptions must be made in order to reduce unnecessary or irresolvable details. However, the whole modelling framework must rely on the deterministic principles of the key processes and it should be based on adequate, good quality data.

To improve the reliability of the predictive calculations, further research should be conducted to compare laboratory, pilot and field-scale tests, and to assess the usability of generalized scaling equations and suitable scaling factors. In Finland, humidity cell tests should be conducted more often, and more data should be collected to increase the available information concerning the scaling of laboratory results to field conditions in the Finnish climate. This research would be supported if HC testing facilities were also established in Finland.

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