

TOOLS FOR ASSISTING WITH THE ASSESSMENT OF ACID AND METALLIFEROUS DRAINAGE (AMD)

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ABSTRACT

Management of Acid and Metalliferous Drainage (AMD) is one of the most environmentally challenging issues facing the mining industry. Early prediction of AMD reduces risk by facilitating intervention and management. An acid-base accounting, spreadsheet-based toolkit has been developed to assist mine planners, geologists and environmental staff with initial characterisation of AMD and management of mine site water quality.

The three main applications in this toolkit permit: a) desktop analysis of the Net Acid Producing Potential (NAPP) of mine materials (Acid Base Accounting tools); b) assessment of the quality of laboratory water chemistry data (Charge Balance tool); and c) identification of water treatment requirements, reagent choice and costs (Acidity tool).

The NAPP tools estimate the potential for acidity generation from geologic materials utilising mineralogical data obtained visually from geological logs (volume % mineralogy) or from X-Ray analysis (weight % mineralogy). This tool can rapidly screen geologic materials for their potential to generate AMD prior to conducting any acid base accounting testwork. In this way it can assist with the selection of the most appropriate samples for acid-base accounting testwork.

The Charge Balance tool enables rapid and rigorous identification of problematic analytical data, thus assisting with quality assurance and quality control on water quality data.

The Acidity tool utilises pH and metal concentration data to estimate acidity values for water samples. The acidity calculation is combined with relevant site water volumes or flow rates to evaluate the Total Acidity Load for a water body or water flow. The Total Acidity Load is indicative of the severity of an AMD issue and can be used to predict treatment reagent requirements (quantities and costs) for a range of potential reagent types. Acidity calculations can also be used to compare laboratory measured values to provide another QA/QC check on laboratory data.

A detailed description of calculations and assumptions inherent in each tool are provided in this paper. The toolkit is provided as shareware at no cost to users, and is regularly reviewed, updated and expanded. Feedback and improvement advice is sought from users. The current version is ABATES v1.4 (Acid-Base Accounting Tool) and is available from the GARD Guide website.

1.0 INTRODUCTION

Management of Acid and Metalliferous Drainage (AMD) is one of the most environmentally challenging issues facing the mining industry. AMD arises when sulfidic materials located below the natural groundwater table become exposed to oxidising conditions as a result of mining and mine dewatering processes. Oxidisation of sulfidic materials can lead to the release of low pH water with elevated concentrations of metals and sulfate into receiving surface waters and groundwater, with impacts that may extend well beyond the operational

life of a mine if not well managed. The complexity and cost of AMD management can be significantly lowered, however, if the potential for AMD is identified and quantified during the early stages of mine planning.

At present, static geochemical characterisation tests (e.g. Acid Base Accounting and Net Acid Generation Tests), combined with AMD block modeling, kinetic geochemical testwork (e.g. column leach and oxygen consumption methods) and water chemistry analysis, are the main tools available to predict and monitor the extent and rate of AMD generation from various mine materials.

Static geochemical characterisation tests rely on specific sample preparation and laboratory-based analytical procedures that are time consuming, with a typical delay of days to weeks between sample collection and analysis. This can limit the value of geochemical data as a tool for day-to-day management decisions (e.g. waste rock segregation and handling). Water chemistry data from mine sites often fails to include Total Acidity analysis. An understanding of Total Acidity concentrations is vital for quantifying the total load of pollutants in a water body or stream. Such data informs the most appropriate treatment method (e.g. passive or active treatment) and can be used to determine the amount of reagent required to fulfil water quality objectives.

An Excel-based program called ABATES has been developed to address some of these issues and assist mine planners, geologists, geochemists and environmental personnel with AMD and water quality assessments. The program includes a series of tools as follows:

- **Acid Base Accounting tools** can be used to estimate Net Acid Producing Potential (NAPP) of geological materials using mineralogical data from geological logs or X-Ray Diffraction (XRD) data.
- **Charge Balance Estimator tool** is designed to provide a quality assurance / quality control (QA/QC) check on analytical chemistry data for any water sample, by estimating the Charge Balance Error (CBE) to verify that anionic and cationic species are correctly balanced.
- **Acidity Estimator tool** enables quantitative determination of the Total Acidity and Total Acidity Load of a water body or stream, based on water chemistry data, in order to assess AMD treatment reagent requirements.

The flexibility of ABATES allows it to be used routinely for estimating AMD potential, assessing water chemistry data and providing a basis for AMD management and treatment at all stages of mine development, as illustrated in Figure 1.

While the program is not a substitute for detailed geochemical testing, it is particularly useful for initial screening of AMD issues and to objectively identify existing issues with the accuracy of geochemical and water chemistry analytical data.

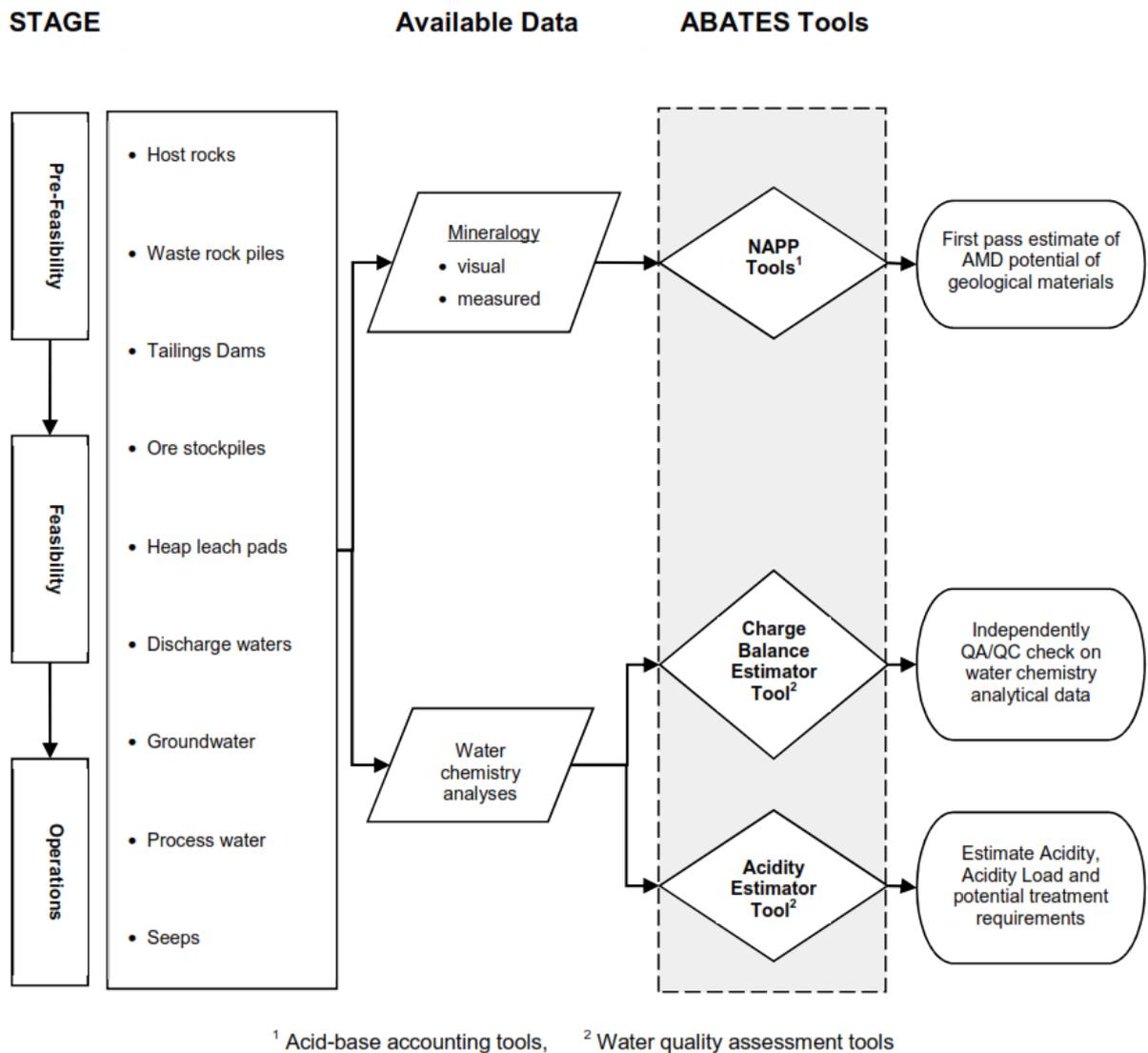


Fig. 1: Simplified flow chart indicating the various stages of mine planning and operation where ABATES can be applied to site geochemical characterisation, AMD monitoring and management programs.

This paper is organised into two main sections: the first section deals with Acid Base Accounting (NAPP tools), while the second deals with water quality assessment (Charge Balance and Acidity tools). Each section contains a brief description of the conventional laboratory-based tests, followed by an explanation of the corresponding theoretical methods used in ABATES. In addition, the section on water chemistry tools describes how the program evaluates the quality of water chemistry data.

2.0 GEOCHEMICAL CHARACTERISATION BASED ON NET ACID PRODUCING POTENTIAL

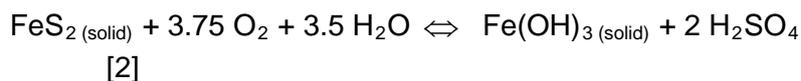
Net Acid Producing Potential (NAPP) is a measure of the difference between the capacity of a sample to generate acid (Acid Producing Potential or APP¹) and its capacity to neutralise acid (Acid Neutralising Potential or ANC). Acid generating reactions are promoted by the oxidation of key sulfide minerals once exposed to atmospheric oxygen, while acid neutralising reactions result from the dissolution of alkaline minerals, mainly carbonates. NAPP is calculated as follows:

$$\text{NAPP} = \text{APP} - \text{ANC} \quad [1]$$

In Australia NAPP, APP and ANC are generally expressed in units of kg H₂SO₄ / tonne of material.

2.1 Analytical Evaluation of NAPP

Laboratory evaluation of NAPP requires two separate analytical procedures to quantify the APP and the ANC of a sample, respectively. These methods are summarised briefly below². APP is determined by analysing the Total Sulfur content (wt.% S) of a sample. All sulfur is assumed to occur as pyrite (FeS₂), which is completely oxidised to produce sulfuric acid (H₂SO₄), as shown in Eqn. [2].



According to the stoichiometry of Eqn. [2], for each mole of pyrite, two moles of H₂SO₄ are generated. Thus, a sample containing 1 wt.% S can generate 30.6 kg H₂SO₄ per tonne. APP is therefore computed as follows:

$$\text{APP (kg H}_2\text{SO}_4\text{/tonne)} = \text{Total Sulfur (wt.\% S)} \times 30.6 \text{ (conversion factor)} \quad [3]$$

APP may be overestimated if a sample contains forms of sulfur other than pyrite, such as commonly occurring sulfate minerals (e.g. anhydrite - CaSO₄, gypsum - CaSO₄.2H₂O, and barite - BaSO₄), native sulfur, non acid forming sulfides (e.g. sphalerite - ZnS, covellite – CuS; Stewart et al., 2003) or weakly acid generating organic sulfur-bearing compounds.

ANC is determined by adding hydrochloric acid (HCl) to a sample and titrating the resulting solution to a pH of 7.0 with sodium hydroxide (NaOH). The amount of acid consumed by the initial reaction between the sample and HCl represents the ANC.

Surface passivation effects on carbonate minerals (ie. precipitate coatings), mineral acidity, incomplete reactions (i.e. oxidation of Fe²⁺; precipitation of Fe, Al and other metals) and the presence of soluble acid salts may influence the “effective” ANC of a sample³.

The main drawback of laboratory-based APP and ANC measurement, and hence NAPP determination, is that sample mineralogy is not taken into account (Jambor, 2003).

¹ APP is commonly also referred to as Maximum Potential Acidity or MPA.

² Detailed descriptions of NAPP analytical methods are provided in Sobek et al (1978), US EPA (1994), MEND (2000), Skousen et al. (2002), AMIRA (2002) and Jambor (2003).

³ These issues are described further in Weber et al. (2004a, 2004b, 2005) and Jambor (2003).

2.2 Mineralogical Evaluation of NAPP Using ABATES

To overcome the some of the limitations of laboratory-derived NAPP data as described above, NAPP can be estimated in ABATES when mineralogical data are available. This:

- Avoids the issues associated with using Total Sulfur to compute APP.
- Removes the influences of carbonate passivation and mineral acidity in the ANC test.
- Overcomes the problems of incomplete oxidation and slow reaction kinetics during laboratory testwork.

NAPP values are estimated in ABATES by using mineral abundance data for acid generating and acid neutralising minerals (in wt.% or vol.% units) as a basis for calculating APP and ANC, respectively.

Specifically, the APP is computed based on the theoretical potential of FeS₂ and other sulfide minerals to generate sulfuric acid under oxidising conditions. The calculation draws on a comprehensive reference list (Table 1) which contains the most commonly occurring sulfide minerals and details the stoichiometry of each potential sulfide oxidation reaction. For each reaction, the stoichiometry is used to determine the moles of sulfuric acid produced by complete oxidation of each mole of sulfide mineral. This approach takes into account the fact that not all sulfide minerals react with atmospheric oxygen to generate sulfuric acid.

Similarly, estimation of ANC in ABATES is based on the individual contributions of a range of commonly occurring carbonate minerals and the stoichiometry of their reactions with acid (Table 2). The program accounts for the fact that not all carbonate minerals have equivalent neutralising capacity to CaCO₃, and some even exhibit zero net neutralising capacity. This point is illustrated by the dissolution of siderite (FeCO₃) in the presence of acid (Eqns. [4] and [5]) in which the net effect is neither consumption nor production of acid:



Depending on the mineralogical data available, two options are available to compute NAPP values in ABATES:

- The first option uses visual estimates of mineral abundances (vol.%) from geological logs and/or field observations. The advantage of this option is that geological data are commonly available at any stage of mine development, enabling a rapid first pass NAPP estimate for both in-situ materials and waste rock piles.
- The second option uses laboratory measurements of mineral abundances (wt.%). These can be obtained by X-Ray Diffraction (XRD) and are therefore more accurate, but also more time-consuming and costly than visual estimates.

Key assumptions used in the NAPP calculations are summarised below:

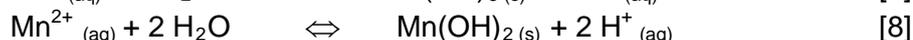
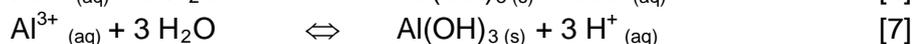
- Mineralogical data are fully representative of the geological materials being assessed.
- Minerals are present as their pure-end member compositions and polymetallic sulfide minerals have fixed molar ratios of metals.
- Only reactive sulfide minerals (i.e. not all sulfides) completely oxidise in the presence of atmospheric oxygen in accordance with the stoichiometric relationships shown in Table 1.
- Each carbonate mineral undergoes complete reaction with acid in the presence of atmospheric oxygen (i.e. no surface passivation of carbonate minerals takes place) in accordance with the stoichiometric relationships shown in Table 2.

- Oxides, sulfates and silicates have negligible effect on acid generation or neutralisation.

3.0 WATER CHEMISTRY ASSESSMENT TOOLS

The assessment of mine site water chemistry begins in the early stages of mine planning (pre-feasibility) and continues through mine development and post-closure. Water chemistry is often routinely monitored to fulfill regulatory requirements, assess options for water reuse or discharge, assess the effectiveness of AMD management, and in some cases assess treatment requirements. The Total Acidity of a water body or stream is probably the best single indicator of the severity of AMD and likely treatment requirements.

Total Acidity, reported as milligrams of CaCO₃ equivalent per litre (mg CaCO₃ / L), provides an indication of how much CaCO₃ would be required to neutralise an acidic solution, commonly to a pH of 8.3. Total Acidity takes into account both existing H⁺ ions (determined from pH) and latent H⁺ ions that may be produced by metal hydrolysis and precipitation. Hydrolysis and precipitation reactions for Fe, Al and Mn are shown in Eqms. [6]-[8]:

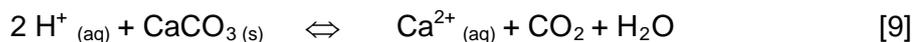


The Acidity tool in ABATES can be used to estimate Total Acidity, Total Acidity Load and likely treatment reagent requirements from routine water chemistry data, providing a quick and low cost method of quantifying an existing AMD issue. A comparison of methods for analytical evaluation of Total Acidity, and the method used in ABATES, is provided below.

This is followed by an explanation of how ABATES can be used to estimate charge balance errors, providing an independent means for evaluating the quality of water chemistry data.

3.1 Analytical Evaluation of Total Acidity

Total Acidity is determined in the laboratory by titrating a fully oxidised water sample with a strong base (e.g. APHA et al, 2005). The sample is oxidised with hydrogen peroxide (H₂O₂) and then titrated to a pH of 8.3 with sodium hydroxide (NaOH) (Eqn. [9]). Results are then equated to an equivalent amount of CaCO₃, and reported as mg CaCO₃ / L.



Total Acidity may also be underestimated during laboratory tests as:

- The titration to pH 8.3 may remove the majority of dissolved metal species via precipitation as metal hydroxides, but not all metals (e.g. manganese).
- In some cases, insufficient addition of H₂O₂ may lead to incomplete oxidation and hydrolysis of dissolved metal species.

3.2 Estimating Total Acidity and Total Acidity Load Using ABATES

Within the Acidity tool of ABATES, Total Acidity can be calculated from standard water chemistry analyses using pH and dissolved metal concentration data. This avoids the need to perform additional laboratory test work. Calculation of Total Acidity in ABATES can also be used as a QA/QC check on laboratory-derived acidity measurements.

In ABATES, dissolved metal concentrations are converted to H⁺ equivalent concentration, or Latent Acidity, using Eqn. [10], and then Eqn. [11] is used to estimate Total Acidity, in mg/L CaCO₃ equivalent, from Latent Acidity and pH.

$$\text{Latent Acidity} = \sum \left[\text{charge on metal ion} \times \frac{\text{metal concentration (mg/L)}}{\text{metal atomic weight (g/mol)}} \right] \quad [10]$$

$$\text{Total Acidity} = \frac{M(\text{CaCO}_3)}{2} \times (\text{Latent Acidity} + 1000 \times (10^{-\text{pH}})) \quad [11]$$

The calculation of Total Acidity assumes complete oxidation and hydrolysis of all metal species in the sample and is therefore comparable to a theoretical titration with pH endpoint of roughly 9.5, rather than 8.3 as used in laboratory-based acidity measurement. As a result, calculated Total Acidity values are often greater than those obtained using the standard laboratory method, and provide a better (more conservative) estimate of AMD treatment reagent requirements¹.

When entering pH and dissolved metal concentration data, the user should be mindful that:

- Metal concentrations should represent the dissolved (ie. 0.45 µm filtered water analysis) rather than total concentrations to avoid overestimating the Total Acidity.
- Oxidation, hydrolysis and precipitation of dissolved metal species between the time of field sampling and laboratory analysis may alter both pH and dissolved metal concentrations. Use of field pH data provides a better estimate of Total Acidity.
- There are two options for entering Iron (Fe) and Copper (Cu) concentrations, depending on redox state. If this is unknown, all Fe can be assumed to be present as Fe(III), and Cu as Cu(II), to provide a conservative estimate of Total Acidity².

The Total Acidity Load of a water stream can also be calculated in ABATES, using Eqn. [12], and is essentially equivalent to ongoing AMD treatment reagent requirements.

$$\text{Total Acidity Load} = \text{Total Acidity} \times \text{Flow Rate} \quad [12]$$

Total Acidity Load is expressed in tonnes CaCO₃ equivalent per unit time (e.g. 1.0 tonne CaCO₃ per day). Eqn. [12] utilises the Total Acidity value obtained via Eqn. [11] and the estimated stream flow rate in megalitres per unit time (ML / unit time). In the case of a fixed water body (e.g. pit lake), Flow Rate may be substituted for Volume of the water body in Eqn. [12], in which case the Total Acidity Load is expressed in tonnes CaCO₃ equivalent.

Once the Total Acidity Load is known, ABATES can convert its value, on a molar basis, to any neutralisation reagent of choice (e.g. 1.0 tonne CaCO₃ per day = 740 kg Ca(OH)₂ per day) to provide an estimate of AMD treatment reagent requirements and costs.

3.3 Analytical Evaluation of Water Chemistry Data Accuracy

Charge balance calculations are a useful means of evaluating the accuracy of water chemistry data. In natural waters, there is a balance between cations (positively charged species) and anions (negatively charged species). In any water chemistry analysis, calculating the difference between all measured cationic and anionic species, or the Charge Balance Error (CBE), can provide an indication of the quality of the analytical data.

The most accurate way of calculating the charge balance of a solution is by calculating the

¹ Calculation of Total Acidity may also be more accurate than laboratory-derived acidity measurements, as metal concentrations are often measured to a much greater accuracy (e.g. ± 0.001 mg/L) than Total Acidity (e.g. ± 5 mg/L).

² Other redox sensitive metals such as Arsenic (As), Manganese (Mn) and Chromium (Cr) are assumed to be present as As(V), Mn(II) and Cr(VI), respectively.

aqueous speciation of the solution from a water analysis. These aqueous speciation calculations “match” cations with anions to form likely aqueous complexes based on a number of variables including ionic strengths, valence states and activity coefficients. CBE indicates if there are residual cations or anions left unmatched.

Aqueous speciation calculations are performed by complex computer programs, which commonly result in the identification of hundreds of aqueous complexes in a sample. These programs provide a more detailed assessment than is often required for a preliminary evaluation of water chemistry data, as the charge balance of a sample is generally dominated by a relatively small number of major cation and anion species.

3.4 Estimation of Water Chemistry Data Accuracy Using ABATES

ABATES provides a simple alternative to conducting complex aqueous speciation calculations for the estimation of CBE, by focusing on the major cations and anions that tend to be the dominant aqueous species in water samples. While the complexity of true aqueous speciation of any sample is acknowledged, the method used in ABATES (described below) is generally considered to be sufficiently accurate for first pass identification of significant CBE's.

ABATES estimates the CBE by summing cation (including H⁺) and anion (including OH⁻) concentrations on a milli-equivalent basis. In particular, the analyte concentrations are converted from mg/L to mEq/L (milli-equivalents per litre). For each anion and cation present in solution, its mEq/L value is computed as follows:

$$mEq/L = \frac{mg/L}{molecular\ weight} \times charge \quad [13a]$$

The contribution of H⁺ and OH⁻ to charge balance is computed as follows:

$$\begin{aligned} H^+ \quad mEq/L &= 10^{-pH} \\ OH^- \quad mEq/L &= 10^{-(14-pH)} \end{aligned} \quad [13b]$$

In the above equation, the absolute value of the charge is used so that the milli-equivalent amount is always positive. Milli-equivalents for anionic and cationic species are summed separately and the charge balance error is calculated using Eqn. [14]:

$$CBE = \left[\frac{\sum(mEq) \text{ cations} - \sum(mEq) \text{ anions}}{\sum(mEq) \text{ cations} + \sum(mEq) \text{ anions}} \right] \times 100\% \quad [14]$$

The following assumptions are made in ABATES to estimate CBE:

- Metals are assumed to be present in dissolved form (i.e. 0.45 µm filtered water analysis). Use of total concentrations may lead to overestimation of the CBE.
- Fe, Mn, Cu, Zn and Pb are assumed to carry a 2⁺ charge.
- Arsenic¹ is assumed to be present as H₂AsO₄⁻ at a pH of less than 6.5, or HAsO₄²⁻ at a pH greater than 6.5.
- Chromium¹ is assumed to be present as H₂CrO₄⁻ at a pH of less than 6.5, or HCrO₄²⁻ at a pH greater than 6.5.
- All ammonia is assumed to be present as NH₄⁺.
- Volatile acids, reported as acetic acid, are assumed to be present as CH₃CO₂⁻.

¹ The charge of arsenic and chromium, which contribute to the anionic charge balance, is pH dependent.

- Phosphorus is assumed to be present as orthophosphate PO_4^{3-} .

There is no industry, regulatory or academic consensus on what constitutes an acceptable CBE. ABATES considers an error of $\pm 10\%$ acceptable for total anion sums of between 10 and 100 mEq/L. For samples with total anion sums less than 10 mEq/L, an error of $\pm 5\%$ is considered acceptable, however low cation and anion totals decrease the reliability of these calculations for evaluating analytical data. For total anion sums greater than 100 mEq/L, an error of $\pm 15\%$ is considered acceptable in ABATES.

Large errors in charge balance (i.e. excess of positively or negatively charged species) may be attributed to problems with the analytical procedure, exclusion of one or more charged species from the analysis and/or data entry or transcription errors.

4.0 CONCLUSIONS

While ABATES is not intended to replace the need for detailed geochemical testwork, it does provide a quick and low cost method for estimating the AMD potential of geological materials, Total Acidity of mine waters and likely AMD treatment reagent requirements using routinely collected data. It also offers a useful method for QA/QC checks on water chemistry data.

ABATES can be used at any stage of mine development, from pre-feasibility through to post-closure. Estimates provided by ABATES for NAPP and Total Acidity have a number of benefits over more detailed laboratory-based geochemical/AMD test procedures.

NAPP values can be estimated for any sample or geological log for which mineralogical data are available. NAPP estimates based on mineralogical data account for the variable acid producing potential of sulfide minerals (and the fact that not all sulfides are acid producing) as well as the variable acid neutralising capacity of carbonate minerals, unlike laboratory-based NAPP tests. NAPP estimates can also be used to inform sample selection and analytical procedure selection for more detailed static or kinetic geochemical testwork.

Total Acidity values can be readily determined in ABATES for historic and new water chemistry analyses, for which no laboratory measurement of acidity is available. By combining Total Acidity values with field estimates of stream flow rate (or water volume), ABATES can also rapidly assess AMD treatment reagent requirements (quantities and costs). Estimates of Total Acidity are comparable to a laboratory titration to pH 9.5, rather than the standard method for acidity determination (titration to pH 8.3). This leads to slightly higher estimates of Total Acidity than the standard method, but is a more conservative approach to assessing treatment reagent requirements for the purpose of maximising metal removal efficiency.

Identifying the potential for AMD at the early stages of mine planning can dramatically reduce the associated risks and enable more informed design and implementation of specific test work and monitoring programs to assist with AMD assessment and management.

4.1 A note on the availability of the current version

The current version is ABATES v1.4 (Acid-Base Accounting Tool) and is available from the Earth Systems website (<http://www.earthsystems.com.au/resources/acid-drainage>) and can also be accessed via the GARD Guide website (http://www.gardguide.com/index.php/Chapter_7). The toolkit is provided as shareware at no cost to users, and is regularly reviewed, updated and expanded. The current version can be freely distributed, provided the tools are used only as intended and are not modified in any way. Feedback and improvement advice is sought from users, via the contact details provided within the toolkit.

5.0 REFERENCES

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Table 1: Summary of sulfide mineralogical data used by ABATES for estimating NAPP values. The reactions do not necessarily represent actual or likely reactions in natural systems, but are useful for accurately calculating the potential for acid production and neutralisation for systems in equilibrium with atmospheric oxygen. The final metal oxidation states apply to the first and second metals as they appear in each Equation.

Sulfide Mineral Name	Sulfide Formula	Mineral	Molar Mass of sulfide mineral (g/mol)	Sulfide Mineral Density (g/cm ³)	Equation	Mol of sulfuric acid (H ₂ SO ₄) produced per Mol of mineral oxidised	Final Metal Oxidation state
Orpiment	As ₂ S ₃		246.04	3.52	As ₂ S ₃ + 6 H ₂ O + 7 O ₂ = 2 HAsO ₄ ⁻² + 10 H ⁺ + 3 SO ₄ ⁻²	Oxidises	3
Realgar	AsS		106.99	3.56	AsS + 5/2 H ₂ O + 11/4 O ₂ = HAsO ₄ ⁻² + 4 H ⁺ + SO ₄ ⁻²	Oxidises	1
Bismuthinite	Bi ₂ S ₃		514.16	7.00	Bi ₂ S ₃ + 3 H ₂ O + 6 O ₂ = Bi ₂ O ₃ + 6 H ⁺ + 3 SO ₄ ⁻²	Oxidises	3
Greenockite	CdS		144.48	4.49	CdS	Unknown	0
Cobaltite	CoAsS		165.92	6.33	CoAsS + 7/2 H ₂ O + 13/4 O ₂ = HAsO ₄ ⁻² + Co(OH) ₂ + SO ₄ ⁻² + 4 H ⁺	Oxidises	1
Chalcocite	Cu ₂ S		159.16	5.65	Cu ₂ S + 5/2 O ₂ + H ₂ O = 2 CuO + 2 H ⁺ + SO ₄ ⁻²	Oxidises	1
Digenite	Cu ₉ S ₅		146.45	5.71	Cu ₉ S ₅	Unknown	0
Bornite	Cu ₅ FeS ₄		501.84	5.09	Cu ₅ FeS ₄ + 11/2 H ₂ O + 37/4 O ₂ = 5 CuO + Fe(OH) ₃ + 8 H ⁺ + 4 SO ₄ ⁻²	Oxidises	4
Cubanite	CuFe ₂ S ₃		271.43	4.70	CuFe ₂ S ₃ + 6 H ₂ O + 13/2 O ₂ = CuO + 2 Fe(OH) ₃ + 6 H ⁺ + 3 SO ₄ ⁻²	Oxidises	3
Chalcopyrite	CuFeS ₂		183.52	4.19	CuFeS ₂ + 17/4 O ₂ + 7/2 H ₂ O = CuO + Fe(OH) ₃ + 4 H ⁺ + 2 SO ₄ ⁻²	Oxidises	2
Covellite	CuS		95.61	4.68	CuS	Unknown	0
Tennantite	Cu ₁₂ As ₄ S ₁₃		1479.08	4.65	Cu ₁₂ As ₄ S ₁₃ + 61/2 O ₂ + 19 H ₂ O = 12 CuO + 4 HAsO ₄ ⁻² + 34 H ⁺ + 13 SO ₄ ⁻²	Oxidises	13
Tetrahedrite	Cu ₁₂ Sb ₄ S ₁₃		1666.44	4.95	Cu ₁₂ Sb ₄ S ₁₃ + 57/2 O ₂ + 15 H ₂ O = 12 CuO + 4 HSbO ₂ + 26 H ⁺ + 13 SO ₄ ⁻²	Oxidises	13
Enargite	Cu ₃ AsS ₄		393.82	4.47	Cu ₃ AsS ₄ + 35/4 O ₂ + 11/2 H ₂ O = 3 CuO + HAsO ₄ ⁻² + 10 H ⁺ + 4 SO ₄ ⁻²	Oxidises	4
Greigite	Fe ₃ S ₄		295.80	4.05	Fe ₃ S ₄ + 17/2 H ₂ O + 33/4 O ₂ = 3 Fe(OH) ₃ + 8 H ⁺ + 4 SO ₄ ⁻²	Oxidises	4
Arsenopyrite	FeAsS		162.83	6.07	FeAsS + 4 H ₂ O + 7/2 O ₂ = Fe(OH) ₃ + HAsO ₄ ⁻² + 4 H ⁺ + SO ₄ ⁻²	Oxidises	1
Violarite	FeNi ₂ S ₄		301.49	4.65	FeNi ₂ S ₄ + 11/2 H ₂ O + 31/4 O ₂ = Fe(OH) ₃ + 2 NiO + 8 H ⁺ + 4 SO ₄ ⁻²	Oxidises	4
Pyrrhotite	Fe _(1-x) S _x		85.12	4.61	FeS + 5/2 H ₂ O + 9/4 O ₂ = Fe(OH) ₃ + 2 H ⁺ + SO ₄ ⁻²	Oxidises	1
Troilite	FeS		87.91	4.61	FeS + 5/2 H ₂ O + 9/4 O ₂ = Fe(OH) ₃ + 2 H ⁺ + SO ₄ ⁻²	Oxidises	1
Marcasite	FeS ₂		119.98	4.89	FeS ₂ + 7/2 H ₂ O + 15/4 O ₂ = Fe(OH) ₃ + 4 H ⁺ + 2 SO ₄ ⁻²	Oxidises	2
Pyrite	FeS ₂		119.98	5.00	FeS ₂ + 7/2 H ₂ O + 15/4 O ₂ = Fe(OH) ₃ + 4 H ⁺ + 2 SO ₄ ⁻²	Oxidises	2
Cinnabar	HgS		232.66	8.10	HgS	Stable	0
Molybdenite	MoS ₂		160.09	5.50	MoS ₂	Stable	0

Sulfide Mineral Name	Sulfide Mineral Formula	Molar Mass of sulfide mineral (g/mol)	Sulfide Mineral Density (g/cm ³)	Equation	Mol of sulfuric acid (H ₂ SO ₄) produced per Mol of mineral oxidised	Final Metal Oxidation state
Millerite	NiS	90.76	5.50	NiS	Unknown	0
Pentlandite	(Ni,Fe) ₉ S ₈	771.94	4.96	(Fe,Ni) ₉ S ₈	Unknown	0
Galena	PbS	239.27	7.40	PbS	Stable	0
Stibnite	Sb ₂ S ₃	339.72	4.63	Sb ₂ S ₃ + 4 H ₂ O + 6 O ₂ = 2 HSB ₂ O ₂ (aq) + 6 H ⁺ + 3 SO ₄ ⁻²	Oxidises	3
Native Sulfur	S ₈	256.52	2.08	S ₈	Stable	0
Sphalerite	ZnS	97.45	4.05	ZnS	Stable	0

Table 2: Summary of carbonate mineralogical data used by ABATES in estimating NAPP values. The reactions may not necessarily represent actual or likely reactions in natural systems, but are useful for accurately calculating the potential for acid production and neutralisation for systems in equilibrium with atmospheric oxygen. Where two or more reactions are shown, the first is the neutralisation step and subsequent reactions show the hydrolysis of the aqueous metal ion and resultant Latent Acidity produced. In most cases, the number of moles of H⁺ consumed by the neutralisation step is offset by the number of moles of H⁺ produced by hydrolysis of the metal ion. The number of moles of sulfuric acid produced is equal to half the number of moles of H⁺ ions produced. The final metal oxidation states apply to the first and second metals as they appear in each Equation.

Carbonate Mineral Name	Carbonate Mineral Formula	Molar Mass of carbonate mineral (g/mol)	Carbonate Mineral Density (g/cm ³)	Equation	Mol of sulfuric acid (H ₂ SO ₄) consumed per Mol of mineral neutralised	Final Metal Oxidation state
Mangansiderite	(Fe,Mn)CO ₃	115.40	3.80	i. (Fe,Mn)CO ₃ + 3/8 O ₂ + 7/2 H ⁺ = 1/2 Fe ³⁺ + 1/2 Mn ⁴⁺ + 7/4 H ₂ O + CO ₂ (3 1/2 mole H ⁺ consumed) ii. 1/2 Fe ³⁺ + 3/2 H ₂ O = 1/2 Fe(OH) ₃ + 3/2 H ⁺ (3/2 mole H ⁺ produced) ii. 1/2 Mn ⁴⁺ + 2 H ₂ O = 1/2 Mn(OH) ₄ + 2 H ⁺ (2 mole H ⁺ produced)	0	3,4
Witherite	BaCO ₃	197.34	4.30	BaCO ₃ + 2 H ⁺ = H ₂ O + CO ₂ + Ba ²⁺	1	2
Ankerite	Ca(Fe, Mg, Mn)(CO ₃) ₂	206.39	3.05	Ca(Fe,Mg,Mn)(CO ₃) ₂ + 8/3 H ⁺ + 1/4 O ₂ = Ca ²⁺ + 2 CO ₂ + 1/3 Mg ²⁺ + 1/3 Fe(OH) ₃ + 1/3 Mn(OH) ₄ + 1/6 H ₂ O	1.33	3,4
Aragonite	CaCO ₃	100.09	2.93	CaCO ₃ + 2 H ⁺ = H ₂ O + CO ₂ + Ca ²⁺	1	2
Calcite	CaCO ₃	100.09	2.71	CaCO ₃ + 2 H ⁺ = H ₂ O + CO ₂ + Ca ²⁺	1	2
Dolomite	CaMg(CO ₃) ₂	184.40	2.84	CaMg(CO ₃) ₂ + 4 H ⁺ = 2 H ₂ O + 2 CO ₂ + Ca ²⁺ + Mg ²⁺	2	2,2

Tools for Assisting with the Assessment of AMD

Carbonate Mineral Name	Carbonate Mineral Formula	Molar Mass of carbonate mineral (g/mol)	Carbonate Mineral Density (g/cm ³)	Equation	Mol of sulfuric acid (H ₂ SO ₄) consumed per Mol of mineral neutralised	Final Metal Oxidation state
Huntite	CaMg ₃ (CO ₃) ₄	353.03	2.70	$\text{CaMg}_3(\text{CO}_3)_4 + 8 \text{H}^+ = \text{Ca}^{2+} + 3 \text{Mg}^{2+} + 4 \text{H}_2\text{O} + 4 \text{CO}_2$	4	2,2
Otavite	CdCO ₃	172.42	5.03	i. $\text{CdCO}_3 + 2 \text{H}^+ = \text{Cd}^{2+} + \text{CO}_2 + \text{H}_2\text{O}$ (2 mole H ⁺ consumed) ii. $\text{Cd}^{2+} + 2 \text{H}_2\text{O} = \text{Cd}(\text{OH})_2 + 2 \text{H}^+$ (2 mole H ⁺ produced)	0	2
Sphaerocobaltite	CoCO ₃	118.94	4.10	i. $\text{CoCO}_3 + 3 \text{H}^+ + 1/4 \text{O}_2 = \text{Co}^{3+} + \text{CO}_2 + 3/2 \text{H}_2\text{O}$ (3 mole H ⁺ consumed) ii. $\text{Co}^{3+} + 3 \text{H}_2\text{O} = \text{Co}(\text{OH})_3 + 3 \text{H}^+$ (3 mole H ⁺ produced)	0	3
Malachite	Cu ₂ CO ₃ (OH) ₂	221.12	3.80	i. $\text{Cu}_2\text{CO}_3(\text{OH})_2 + 4 \text{H}^+ = 2 \text{Cu}^{2+} + \text{CO}_2 + 3 \text{H}_2\text{O}$ (4 mole H ⁺ consumed) ii. $2 \text{Cu}^{2+} + 4 \text{H}_2\text{O} = 2 \text{Cu}(\text{OH})_2 + 4 \text{H}^+$ (4 mole H ⁺ produced)	0	2
Azurite	Cu ₃ (CO ₃) ₂ (OH) ₂	344.67	3.83	i. $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2 + 6 \text{H}^+ = 3 \text{Cu}^{2+} + 2 \text{CO}_2 + 4 \text{H}_2\text{O}$ (6 mole H ⁺ consumed) ii. $3 \text{Cu}^{2+} + 6 \text{H}_2\text{O} = 3 \text{Cu}(\text{OH})_2 + 6 \text{H}^+$ (6 mole H ⁺ produced)	0	2
Siderite	FeCO ₃	115.85	3.96	i. $\text{FeCO}_3 + 3 \text{H}^+ + 1/4 \text{O}_2 = \text{Fe}^{3+} + \text{CO}_2 + 3/2 \text{H}_2\text{O}$ (3 mole H ⁺ consumed) ii. $\text{Fe}^{3+} + 3 \text{H}_2\text{O} = \text{Fe}(\text{OH})_3 + 3 \text{H}^+$ (3 mole H ⁺ produced)	0	3
Magnesite	MgCO ₃	84.31	3.00	$\text{MgCO}_3 + 2 \text{H}^+ = \text{H}_2\text{O} + \text{CO}_2 + \text{Mg}^{2+}$	1	2
Rhodochrosite	MnCO ₃	114.95	3.69	i. $\text{MnCO}_3 + 4 \text{H}^+ + 1/2 \text{O}_2 = \text{Mn}^{4+} + \text{CO}_2 + 2 \text{H}_2\text{O}$ (4 mole H ⁺ consumed) ii. $\text{Mn}^{4+} + 4 \text{H}_2\text{O} = \text{Mn}(\text{OH})_4 + 4 \text{H}^+$ (4 mole H ⁺ produced)	0	4
Nahcolite	NaHCO ₃	84.01	2.20	$\text{NaHCO}_3 + \text{H}^+ = \text{Na}^+ + \text{CO}_2 + \text{H}_2\text{O}$	0.5	1
Hellyerite	NiCO ₃ ·6(H ₂ O)	226.79	1.97	i. $\text{NiCO}_3 \cdot 6\text{H}_2\text{O} + 2 \text{H}^+ = \text{Ni}^{2+} + \text{CO}_2 + 7 \text{H}_2\text{O}$ (2 mole H ⁺ consumed) ii. $\text{Ni}^{2+} + 2 \text{H}_2\text{O} = \text{Ni}(\text{OH})_2 + 2 \text{H}^+$ (2 mole H ⁺ produced)	0	2
Gaspeite	(Ni _{0.6} , Mg _{0.3} , Fe _{0.1}) CO ₃	108.10	3.70	$(\text{Ni}_{0.6}, \text{Mg}_{0.3}, \text{Fe}_{0.1}) \text{CO}_3 + 18/10 \text{H}^+ + 1/40 \text{O}_2 = 3/10 \text{Mg}^{2+} + 6/10 \text{Ni}^{2+} + 1/10 \text{Fe}(\text{OH})_3 + 15/20 \text{H}_2\text{O} + \text{CO}_2$	0.9	2,2,3
Cerussite	PbCO ₃	267.21	6.58	i. $\text{PbCO}_3 + 2 \text{H}^+ = \text{Pb}^{2+} + \text{CO}_2 + \text{H}_2\text{O}$ (2 mole H ⁺ consumed) ii. $\text{Pb}^{2+} + 2 \text{H}_2\text{O} = \text{Pb}(\text{OH})_2 + 2 \text{H}^+$ (2 mole H ⁺ produced)	0	2
Strontianite	SrCO ₃	147.63	3.78	i. $\text{SrCO}_3 + 2 \text{H}^+ = \text{Sr}^{2+} + \text{CO}_2 + \text{H}_2\text{O}$ (2 mole H ⁺ consumed) ii. $\text{Sr}^{2+} + 2 \text{H}_2\text{O} = \text{Sr}(\text{OH})_2 + 2 \text{H}^+$ (2 mole H ⁺ produced)	0	2
Smithsonite	ZnCO ₂	125.39	4.45	i. $\text{ZnCO}_3 + 2 \text{H}^+ = \text{Zn}^{2+} + \text{CO}_2 + \text{H}_2\text{O}$ (2 mole H ⁺ consumed) ii. $\text{Zn}^{2+} + 2 \text{H}_2\text{O} = \text{Zn}(\text{OH})_2 + 2 \text{H}^+$ (2 mole H ⁺ produced)	0	2
Hydrozincite	Zn ₅ (CO ₃) ₂ (OH) ₆	548.96	3.50	i. $\text{Zn}_5(\text{CO}_3)_2(\text{OH})_6 + 10 \text{H}^+ = 5 \text{Zn}^{2+} + 2 \text{CO}_2 + 8 \text{H}_2\text{O}$ (10 mole H ⁺ consumed) ii. $5 \text{Zn}^{2+} + 10 \text{H}_2\text{O} = 5 \text{Zn}(\text{OH})_2 + 10 \text{H}^+$ (10 mole H ⁺ produced)	0	2