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Scaling Factors of Humidity-Cell Kinetic Rates for Larger-Scale Predictions

by K.A. Morin

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Abstract

In the prediction of minesite-drainage chemistry, an important aspect is reasonably upscaling the results of smaller-scale testwork to larger scales. However, this goal remains elusive. Case studies show that the underestimation (underprediction) of full-scale drainage chemistry and water contamination is the preferred objective of upscaled prediction.

A major reason for the predictive errors and underpredictions in upscaling is the scaling factors for small-scale kinetic testwork. In many cases, small-scale kinetic testwork should not be upscaled into equilibrium conditions typical of full-scale minesite components. However, such upscaling is becoming more common and popular, so a closer look at kinetic scaling factors is warranted.

Small-scale kinetic rates can be upscaled using hundreds or thousands of scaling factors, reflecting each physical, chemical, biological, and engineering aspect. For simplicity, most authors choose a small subset of factors.

Interestingly, the literature shows that nearly all scaling factors in regular usage are less than 1.0. Because the Cumulative Scaling Factor (CSF) applied to small-scale kinetic rates is a multiplicative product of each individual scaling factor, the CSF decreases with each additional factor considered. This is one cause of the common underprediction of drainage chemistry and water contamination. Another is the usage of a long-term average, or late-stage stable, rate for upscaling, rather than a maximum measured rate.

Examples of measured CSF values can be found in the literature, where measured smaller-scale kinetic rates were upscaled to measured larger-scale testwork and to monitored full-scale minesite components. These CSF values were mostly between 0.05 and 0.60, or in other words the larger-scale rate was typically 5% to 60% of the small-scale rate.

Surprisingly, typical values of common individual scaling factors (see below) are often within this CSF range. As a result, in many cases, a single scaling factor can accurately predict the CSF used for upscaling. In other words, the inclusion of additional factors can lead to the commonly observed underprediction of drainage chemistry.

In this MDAG Internet Case Study, the individual scaling factors discussed in detail, and with reported values, include: particle size, temperature, contact by drainage water, level of pore-gas oxygen, and solid-phase level of elements. The importance of unique scaling factors for each

aqueous element is also discussed. This highlights the error in the common application of the scaling factor for sulphate-production rate (sulphide-oxidation rate) to every element of concern.

As an example of an individual scaling factor, the Arrhenius Equation is often used to estimate the scaling factor for temperature differences between small-scale testwork and the larger-scale component being predicted. This is usually simplified to: the oxidation rate of sulphide, the production of sulphate, and the leaching of all other elements will decrease by a factor of 2-3 for each 10°C decrease in temperature. There is often no justification for such a factor; data show that such a factor could be incorrect; and applications of this factor have been based on misunderstandings. Nevertheless, for temperature differences of 10-20°C, the resulting scaling factors of 0.17-0.50 encompass measured Cumulative Scaling Factors. Thus, no additional scaling factors can be used if this one for temperature is used. Alternatively, the combination of this scaling factor with others, which is common, can account for the typical underestimation of full-scale minesite-drainage chemistry and water contamination during operation.

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1. INTRODUCTION

An important aspect in the prediction of minesite-drainage chemistry is reasonably upscaling the results of smaller-scale testwork to larger scales (e.g., Price, 2009). However, this goal remains elusive. Case studies show that the underestimation (underprediction) of full-scale drainage chemistry and water contamination is the preferred objective of upscaled prediction (Morin, 2011 and 2010; Morin and Hutt, 1997b).

An important facet of upscaling lies in the differentiation of kinetics and equilibrium (Morin and Hutt, 2007a). Figure 1 shows that smaller-scale testwork often (but not always) lies in the kinetic range. In contrast, full-scale drainage chemistry is often (but not always) in the equilibrium range, displaying emergent trends and properties not seen in smaller-scale testwork (Morin et al., 2012; Morin and Hutt, 1997a and 2001a). Nevertheless, there are some cases where small-scale testwork, involving abundant rinsing of 1 kg samples unlike field conditions, has produced about the same aqueous concentrations (mg/L) as larger-scale testwork and full-scale minesite components (e.g., Morin and Hutt, 2007a).

Therefore, reasonable upscaling from smaller scales requires careful differentiation of scales falling within the kinetic range and within the equilibrium range. Where two scales are within the kinetic range, various “scaling factors” can be applied to reconcile them. Where two scales are within the equilibrium range, no significant scaling factors are needed. Where one scale is within the kinetic range and another in the equilibrium range, scaling factors are not constant or relevant due to the “apples-and-oranges” comparison.

This MDAG Internet Case Study focusses on scaling factors used between two kinetic-range scales. To be clear, scaling factors are typically not appropriate when upscaling from small-scale testwork to full-scale minesite components, because equilibrium conditions often apply at full scale.

Interestingly, the inappropriate approach to scaling, from a kinetic to an equilibrium scale, is indeed common in published literature and environmental impact assessments. Without scaling factors, kinetic-based predictions should be higher under equilibrium conditions (see the two fine lines in Figure 1 that cross at the “Scale Transition” point). Therefore, scaling factors provide the opportunity to lower kinetic-based predictions below equilibrium predictions within the equilibrium range! This is commonplace in environmental assessments I have read.

Scaling factors in minesite-drainage literature are nearly always less than 1.0 (always lessening the upscaled predictions). This is a major reason for the documented preference for underpredicting full-scale drainage chemistry and water contamination discussed in the first paragraph. In other words, scaling factors from small-scale kinetic testwork to larger scales are a major source of error in the prediction of minesite-drainage chemistry. Because of this, taking a closer look at these factors is worthwhile.

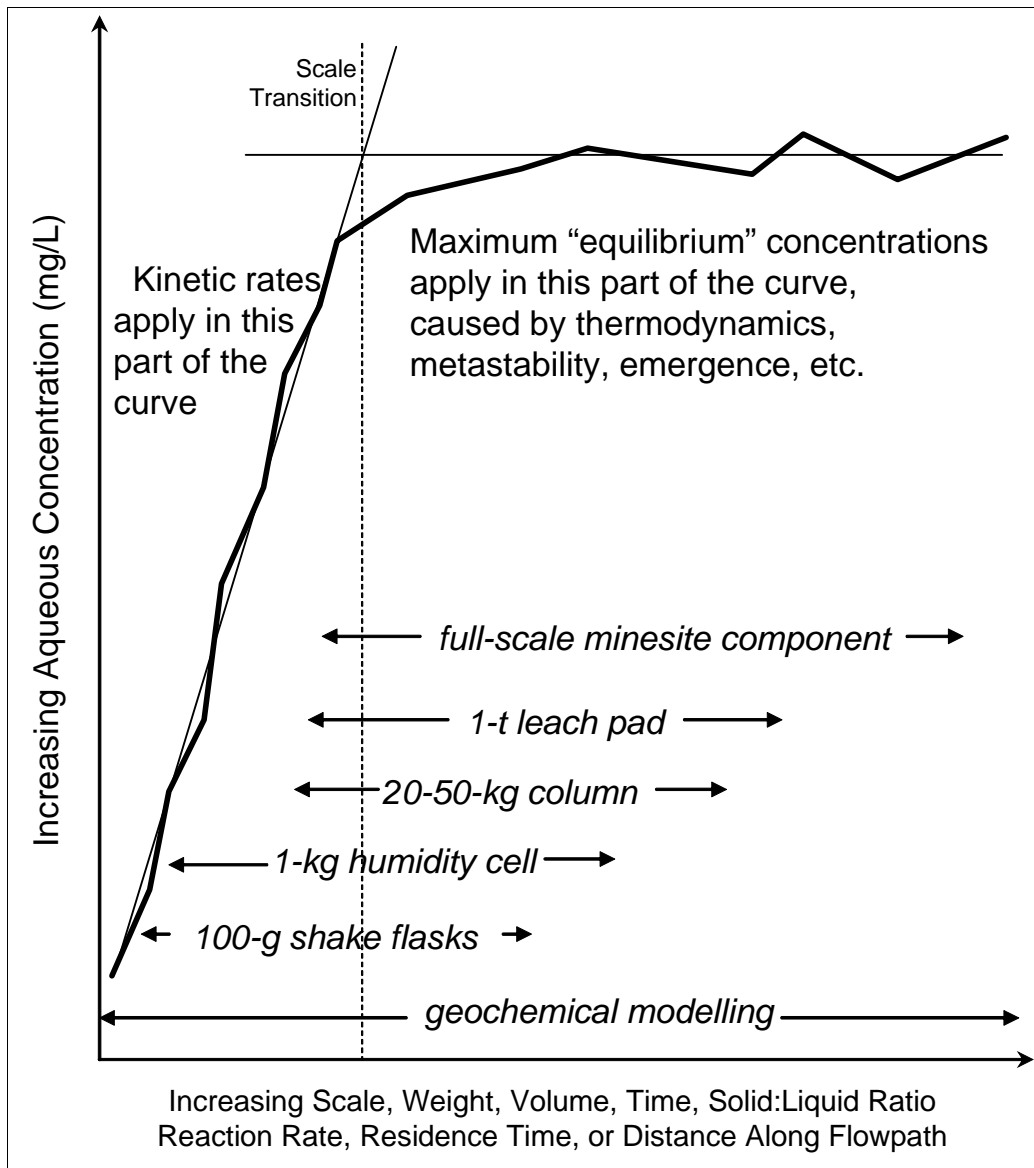


Figure 1. The Conceptual Model for Scaling Minesite-Drainage Chemistry, with General Ranges of Scale for Various Types of Geochemical Testwork and Models (from Morin and Hutt, 2007a).

2. SCALING FACTORS FOR MINESITE-DRAINAGE CHEMISTRY AND THE CUMULATIVE SCALING FACTOR (CSF)

There is no rigid definition for a scaling factor. There could be hundreds or thousands that can be invoked when adjusting drainage-chemistry predictions from one scale to another, reflecting each physical, chemical, biological, and engineering aspect. Consequently, many authors have simply selected the individual scaling factors they thought would be most important. Because of the typical underestimation of drainage chemistry, it is helpful to review the literature on individual kinetic-based scaling factors.

The most recent International Conference on Acid Rock Drainage (ICARD) was held in 2012. This conference showed an increasing international interest in scaling factors and their quantification (e.g., Hanna and Lapakko, 2012; Shaw and Samuels, 2012; Kempton, 2012; Andrina et al, 2012). Nevertheless, the search for these scaling factors has been ongoing for decades (e.g., ElBoushi, 1975; Morin and Hutt, 1994).

One lesson learned from the literature on scaling factors is: provide a precise and clear delineation of the units of the smaller-scale information and the larger-scale predictions. For example, some authors upscale a smaller-scale rate (mg/kg/wk) to a larger-scale rate (mg/kg/wk), or to a larger-scale concentration (mg/L). Some authors upscale based on unit weight (kg of sample), whereas others upscale based on a single element or mineral (kg of pyrite or sulphur). Another way to explain this ambiguity is that some authors implicitly include more scaling factors than others. Upscaling from mg/kg/wk to mg/L requires more individual scaling factors, including flow rates of water, than upscaling to mg/kg/wk. Upscaling to mg/(kg of sulphur)/wk requires a factor for variation in sulphur levels among scales. Thus, the units highlight some scaling factors being used. This MDAG Case Study will focus on kinetic units of mg/kg/wk.

While Section 3 of this Case Study discusses various individual scaling factors and their values, it is important to understand that all scaling factors (SF) come together as one final value for predictions. This final value can be called the Cumulative Scaling Factor (CSF), defined through multiplication as:

$$\text{Cumulative Scaling Factor (CSF)} = \text{SF1} * \text{SF2} * \text{SF3} * \text{SF4} * \text{SF5} * \text{SF6} * \dots \quad (\text{Eq. 1a})$$

and

$$\text{Larger-scale Kinetic Rate (mg/kg/wk)} = \text{CSF} * \text{Measured Small-scale Kinetic Rate (mg/kg/wk)} \quad (\text{Eq. 1b})$$

and

$$\text{Larger-scale Aqueous Concentration (mg/L)} = \text{Larger-scale Kinetic Rate (mg/kg/wk)} * \text{Larger-scale Mass (kg)} * \text{Larger-scale Water Flow (L/wk)} \quad (\text{Eq. 1c})$$

Because scaling factors are typically less than 1.0 for minesite drainage (Sections 1 and 3), the CSF decreases in value as more individual scaling factors are considered (Equation 1a). For

example, if each factor were 0.5 in value, the CSF for only four individual factors would be 0.06 ($0.5 \times 0.5 \times 0.5 \times 0.5$), whereas the CSF would be 0.015 for six individual factors. Thus, measured CSF values of 0.05 to 0.60 (5-60% of small-scale rates, illustrated below), compared to lower, predicted CSF values, imply some individual scaling factors are not as low as currently thought or too many factors are included for predictions (Section 3).

To help focus this issue, examples of measured CSF values are available based on comparing measured small-scale kinetic rates to measured larger-scale chemistry. These following examples will prove useful for discussions of individual scaling factors in Section 3.

2.1 Cumulative Scaling Factor Example 1

At a closed taconite mine (1954-2000) in Minnesota, USA, 160 million tonnes of net-neutralizing waste rock contribute sulphate, hardness, and alkalinity to mined pits and local drainages (Hanna and Lapakko, 2012). Solid-phase analyses were conducted of both weathered (8 to 42 years) and unweathered rock, with samples of this rock also tested in humidity cells. These small-scale kinetic rates, normalized to % pyrite, were compared to full-scale rates, normalized to % pyrite and based on on-site field monitoring of drainage chemistry in streams (“in-stream rates”) and in mined pits (“in-pit rates”).

The average laboratory rate had to be multiplied by a scaling factor of 0.4 (a CSF of 0.4 or 40%) to match the average in-stream rate, and by 1.2 (a CSF greater than 1.0) to match the average in-pit rate. Again, these rates and scaling factors are relative to the mass of pyrite (based on sulphide values) and not to mass of rock (see Section 3.7). If the mass of rock were used instead of pyrite, scaling factors would be around 0.1-0.2 (10-20%).

Hanna and Lapakko (2012) noted that the maximum particle size for their small-scale humidity-cell samples was 2 mm, rather than the more typical 6 mm. The authors argued this should have resulted in higher small-scale higher rates and lower scaling factors (see Section 3.2), but it did not. Overall, the authors pointed out that scaling factors should have been lower, but were relatively not affected by particle size (Section 3.2), degree of particle-surface flushing or rinsing (Section 3.4), submergence of pit walls, or temperature (Section 3.3). In particular, the authors pointed out that temperature correction by the Arrhenius Equation (defined in Section 3.3) should have yielded scaling factors below 0.1, but that was not measured.

Hanna and Lapakko (2012) observed that the humidity-cell rates for fresh unweathered bedrock were about 10 times lower than cell rates of decades-old-weathered rock. This “temporal evolution of sulfide oxidation” was apparently related to increasing exposure of sulphide minerals during weathering. It highlights the issue of selecting the optimum small-scale rate to be upscaled, discussed further in Section 3.1.

This example showed that weight-based CSF values were 0.1 to 0.2 (10-20%). Such a high CSF value based on measured two-scale information generally exceeds CSF values calculated with Equation 1 using individual factors (Section 3).

2.2 Cumulative Scaling Factor Example 2

Shaw and Samuels (2012) provided an informative comparison of kinetic results from laboratory-based humidity cells to monitoring results for larger-scale in-field barrels (not a full-scale minesite component) over a roughly one-year period. This testwork used four relatively fresh samples, three of intrusive rock and one of meta-sedimentary rock, with all four having roughly similar geochemistry, mineralogy, and ABA characteristics.

For sulphate, aqueous concentrations (mg/L) from the in-field barrels were roughly 10 times higher than from cells, whereas unit-weight production rates (mg/kg/wk) from these barrels were roughly 10 times lower. Release rates of some elements were often, but not always, higher from the cells than corresponding barrels, highlighting the importance of unique scaling factors for each element (Section 3.8).

Particle size distributions for the two scales were not given. However, a simple comparison suggested the two scales contained a similar amount of material finer than 0.6 cm. Therefore, the small-scale results were upscaled simply by adjusting for the differences in mass (1 kg vs. 280 kg) and water:solid ratio (0.5 L/kg for cells and 0.01 L/kg for barrels), which is basically Equation 1c in this Case Study. Scaling factors for temperature and flushing of particle surfaces (Sections 3.3 and 3.4) were not invoked, and in the terminology of Equation 1 would have further distorted Cumulative Scaling Factors.

Based on average cell rates (not including the early weeks with higher rates more typical of active mining, see Section 3.1), upscaled aqueous concentrations of the relatively conservative elements of potassium and sodium were less than measured barrel predictions by roughly factors of 2 to 4. The inclusion of early weeks of cell testing might reconcile this, but data were not included to evaluate this potential.

This simplified upscaling also predicted aqueous calcium concentrations up to a factor of roughly 50 times higher than measured for the barrels. Also, predicted sulphate was lower than measured for the barrels by less than a factor of 20. For testwork with acidic pH at both scales, upscaled copper and zinc were lower than barrel-measured concentrations (underpredicted) by factors of 13 and 20, respectively. Similarly, at near-neutral pH, upscaled predictions for copper and zinc were closer to barrel-measured concentrations, differing by factors less than 10 and 2, respectively.

For the elements where upscaled predictions underpredicted barrel-measured concentrations, the differences were attributed to various aspects of humidity cells. These were minimization of acidic micro-environments, minimal precipitation of secondary minerals, and enhanced water flushing. In contrast, such enhanced flushing in cells is often argued by others to cause accelerated rates, not depressed rates, requiring a scaling factor less than 1.0 (Section 3.4).

Although not literally a kinetic rate, the lag time until a near-neutral sample becomes acidic can be dependent on kinetic rates. Shaw and Samuels (2012) reported that calculations of Neutralization Potential (NP) depleted from cells indicated several years of lag time before net acidity. However, some samples became acidic earlier, showing cells “may overestimate lag time in the field”. However, one potential error by the authors was assuming all measured NP was reactive, and other studies suggest most of their measured NP could have been “unavailable” and

unreactive under field conditions (e.g., Morin and Hutt, 2008a and 2008b).

2.3 Cumulative Scaling Factor Example 3

Kinetic testing for the Grasberg Minesite in Indonesia involved several scales: laboratory columns containing 2 and 35 kg, meso-scale “panel” (thin, sloping, tabular samples otherwise similar to vertical columns) with 1 tonne, meso-scale in-field test pads with 500 t, and in-field trial dumps with 50,000 t (Andina et al, 2012). The tests contained either “low potential acid forming (PAF)” or “high PAF” rock. Average sulphur was 2-5%S, mostly as pyrite and chalcopyrite, and lag times to net acidity were short.

Overall, the variations among scales were “not quantitatively equivalent”, precluding reliable scaling factors under Equation 1. Nevertheless, the variations showed a consistent pattern of generally decreasing rate with increasing scale. Infiltration, oxygen transfer, and particle size “could have a major role”. However, leach columns with particles finer than 3.9 cm and the in-field test pad with up to 30 cm particles produced similar oxidation rates, suggesting particle-size scaling was not a major scaling factor.

Intrinsic oxidation rates (IOR) were calculated from cumulative sulphate over yearly periods. However, there was no recognition that larger-scale tests were not likely fully rinsed like smaller scales. As a result, larger-scale IOR’s would likely not be oxidation rates (see Section 3.1), but other processes such flushing rates (see Sections 3.2 to 3.10). Nevertheless, the authors concluded, “the IOR at a larger scale experiment such as the trial dump can be considered as the oxidation rate of the entire waste rock dump”.

Based on comparisons of selected scales and samples, IOR scaling factors (now called “release rates” by the authors, suggesting the approach of Equation 1b) varied between 11% and 58% for oxidation and between 4% and 50% for copper.

2.4 Cumulative Scaling Factor Example 4

A full-scale waste-rock pile at a cold, wet polymetallic minesite contained approximately 100,000 tonnes of rock (Morin et al, 1997; Morin and Hutt, 2000 and 2001b). This pile had been releasing ARD for a few years, and the drainage was being treated by neutralization. The company decided to excavate the waste rock and place it underwater, allowing a detailed investigation of the geochemical evolution of the pile during excavation. As well, several small-scale humidity cells had been operated on this waste rock, allowing the calculation of a CSF based on both small-scale and full-scale data.

For the cells, the simple upscaling of sulphate-production rates from non-ore rock indicated 530 tonnes of CaCO₃ equivalent acidity /100,000 tonnes/year was generated by the relatively fine, fully oxygenated, and full flushed small samples. This was based on the average cell rate of 97 mg SO₄/kg/wk multiplied by 100,000,000 kg and 52 weeks, and thus no individual scaling factor was involved in this value.

The monitoring data of full-scale ARD, using measured acidity, plus measured calcium to

represent internally neutralized acidity, indicated the 100,000 t of waste rock released about 190 t CaCO_3 acidity/year. Also, the disassembly of the pile indicated about 30 t CaCO_3 acidity/year had been retained and accumulated in the pile. Thus, the dump:

- produced about 220 t CaCO_3 /year (190 + 30) of acidity,
- retained about 14% (30/220) of annual acidity,
- released ARD after only two years when only 10-20% of its Neutralization Potential had been consumed, and
- would no longer experience active oxidation after roughly 26 years (a total potential acidity of 5760 t based on sulphur levels divided by 220 t/yr), which would be followed by release of retained acidity.

Based on this information, the CSF for this example is 0.42 (or 42% or 220/530). As with Example 1 (Section 2.1), such a high CSF value based on measured two-scale information generally exceeds CSF values calculated with Equation 1 using individual factors (Section 3). However, the individual scaling factor(s) accounting for this CSF value of 0.42 was not explored.

2.5 Cumulative Scaling Factor Example 5

Morin and Hutt (1994) compared measured results from small-scale humidity cells to measured results of full-scale acidic and near-neutral drainage from waste rock. The small-scale kinetic rates for sulphate, acidity, and various metals were converted from mg/kg/wk to mg/L using precipitation at the minesite (Equation 1c).

The comparison of these small-scale predicted mg/L to the measured full-scale mg/L in drainage showed that a CSF of 0.05 (5%) was needed to match full-scale waste-rock drainage under acidic and near-neutral conditions. This did not apply to elements whose aqueous concentrations were controlled by equilibrium conditions (see Figure 1).

The authors attributed this entire CSF of 0.05 to the degree of flushed rock-particle surfaces (see Section 3.4). Based on this, calculations indicated roughly 5-10% of rock surfaces were flushed regularly within most of the measured flow rate. However, at the highest levels of measured flows, up to 40% of rock surfaces could be flushed.

In summary, the CSF for this example is 0.05 (or 5%). As with the previous examples, these relatively high, measured CSF values generally between 0.05 and 0.60 generally exceed CSF values calculated with Equation 1 using individual factors (Section 3).

3. SOME SCALING FACTORS FOR MINESITE-DRAINAGE CHEMISTRY

As discussed in Section 2, there can be hundreds or thousands of scaling factors. However, authors select those they consider most important, which can lead to a mathematically arbitrary CSF (Equation 1a). This section discusses the factors often selected by authors and the details behind them. However, the CSF examples, typically ranging between 0.05 and 0.60 in Section 2, show that including more than two to three individual scaling factors from below can lead to the common underprediction of drainage chemistry and water contamination.

3.1 Small-Scale Kinetic Rate for Upscaling

Although literally not a scaling factor, this is important. What kinetic rate should be used from small-scale testwork for upscaling? Should the long-term average be used, or the initial rate that is often the maximum, or a later-period stabilized rate, or another statistical value?

For a small-scale test, the differences among these rates from a single test can reach factors of 100 or more, so the choice of a rate is the first, critical step in upscaling. Even small-scale tests analyzed every second week can be in error by a factor of 10 or more compared to analyses every week (Morin and Hutt, 2007b). Thus, just the sampling schedule can add significant error to the selected rate for upscaling.

The common choice for a kinetic rate is a long-term average. However, authors sometimes choose to exclude from this average the early weeks of testing when values can be highest. For predictions such as the long-term depletion of sulphide, this may be reasonable. Conversely, it is not reasonable for predictions of aqueous chemistry during active mining and operations.

During active mining, rock in the mine is blasted frequently, with the elevated pressure and heat of the blast resulting in rapid, “flash” weathering and oxidation of freshly exposed rock surfaces. Thus, not only are fresh surfaces exposed, they are quickly weathered and accumulate weathering products. The percentage of finer particles (Section 3.2) is also increased by the blasting. This flash-weathered rock is then removed from the mine by equipment like shovels, which cause grinding-upon-grinding of the rock particles during loading. This creates even more freshly exposed surfaces and even more finer particles. The rock is dumped into transport vehicles, again increasing freshly exposed surfaces and finer particles. The loaded rock is hauled and dumped in a waste-rock pile or ore stockpile, increasing even more the fresh surfaces and finer particles. Any further movement of the rock, such as by dozer for resloping, again creates more fresh surfaces and finer particles. This rock lays over other rock beneath that has gone through the same processes.

Because the preceding paragraph represents ongoing processes day after day, month after month, year after year, with rock placed on top of rock, until the minesite closes, which rate from the small-scale kinetic testwork should be used for upscaled predictions? To repeat, the common rate is the long-term average, sometimes excluding the early weeks with the highest value. However, the previous paragraph shows that the reasonable rate is based on the highest values, often from the early weeks. After active mining and for long times into closure, a lower kinetic rate, reflecting the decline in weathering, may become appropriate if no geochemical retention and accumulation (see Section 3.4) have occurred.

In contrast to the preceding points, Hanna and Lapakko (2012) reported humidity-cell rates for fresh unweathered bedrock about 10 times lower than cell rates of decades-old-weathered rock. This “temporal evolution of sulfide oxidation” was apparently related to increasing exposure of sulphide minerals during weathering. In this case, long-term predictions such as through closure should be based on a higher rate.

In summary, one of the largest errors, a factor of 10 or more, in upscaling for active mining can be found in the choice of a kinetic rate from small-scale testwork. Typically, some lower, long-term average rate is used, whereas recognition of ongoing mining of rock highlights the importance of maximum rates during operation. This can account for underestimation of full-scale minesite-drainage chemistry and water contamination during operation (Section 1). This also emphasizes that any upscaled prediction based on a long-term average may be too low to be on the reasonable side.

3.2 Particle Size

The most common individual scaling factor for minesite-drainage chemistry reflects differences in particle size with changing scale. Smaller-scale testwork is typically conducted on particles (e.g., silt and sand) whose maximum size can be less than full-scale conditions (e.g., silt, sand, gravel, and boulders). This may also change the weight-percentage of any size range (e.g., between 0.1 and 0.2 cm).

How does this affect the upscaling of a kinetic rate (mg/kg/wk)? Opinions abound, with little empirical data for confirmation.

Some basic approaches often used for this scaling factor are as follows.

Approach 1) All particle sizes up to the maximum particle size of the small-scale testwork (e.g., 0.6 cm) are assumed to represent most or all of the significantly reactive particles at the larger scale. The particle-size distribution of the larger scale is predicted (assumed), or measured when possible. The percentage of the larger scale that is less than the small-scale maximum is then given the kinetic rate of the small-scale testwork. For example, a full-scale waste-rock dump is assumed to have only 5% of its particles finer than 0.6 cm, which is also the maximum particle size of the small scale. As a result, one kg of full-scale waste rock on average will have 5% of the small-scale kinetic rate. Thus, Full-Scale Rate (mg/kg/wk) = 0.05 * Small-Scale Rate. An old “rule of thumb” in this matter used to say that, on the full scale, 5-20% of dumped rock could be expected to be finer than 0.6 cm.

Approach 2) Kinetic rates are derived for each particle-size interval in the small-scale test, often by assuming rate is proportional to particle diameter. These rates are then applied to the size intervals at the larger scale, with coarser particles often considered unreactive.

Approach 3) A cumulative particle-surface area is estimated for the small-scale testwork from the particle-size distribution (e.g., 21 m² of particle surfaces per kg). A cumulative particle-surface area is assumed for the larger scale (e.g., 3 m² of particle surfaces per kg). Thus, one kg of full-scale waste rock on average will have 15% (3/21) of the small-scale kinetic rate from the small scale. Thus, Full-Scale Rate (mg/kg/wk) = 0.15 * Small-Scale Rate.

The first approach is apparently used most often. Sometimes, the second or third approach is used with an assumed (not measured) particle-size distribution for the small scale, with no explanation of why the distribution was not simply measured. In other cases, these approaches are mixed together in bewildering ways. The following gives some examples.

Kempton (2012), and many others, simplify the relationship of reaction rate to particle size by assuming most to all reaction is attributable to particles smaller than a certain size, independent of the particle-size distribution below this criterion (Approach 1 above). For example, a shrinking-core model (which is known not to apply to minesite wastes) showed that fragments greater than 20 cm contributed very little to oxidation.

A case study in Kempton (2012) reported that waste-rock fragments less than roughly 2-3 cm were flushed by infiltration (see also Section 3.4). Kempton incorrectly concluded that this “reduc[ed] the oxidation focus to this small size” flushed by water. In reality, coarser rock will (1) still react and accumulate reaction products even in the presence of humidity (Section 3.6), (2) eventually release its accumulated reaction products as the rock pile settles differentially through time, and (3) weather through time into the smaller “reactive” particle sizes on which Kempton focusses.

Furthermore, Kempton (2012) presented cases of widely varying particle-size distributions within waste rock:

- 90% of particles were finer than 20 cm based on a modelling study;
- 30% were finer than 0.6 cm and 50% finer than 2 cm based on large-scale columns holding more than one tonne (roughly similar to the third case in Kempton’s Figure 1);
- 17-60% finer than 7 mm from a full-scale waste-rock sieve, highlighting the real difficulty of characterizing the amount of fines at the scale of a full minesite component;
- 23-40% finer than 0.6 cm and 58% finer than 2 cm from a full-scale waste-rock sieve;
- 23% finer than 0.6 cm and 45% finer than 2 cm from a relatively small sample removed from a full-scale waste-rock pile;
- 20-100% less than 0.6 cm and 30-100% less than 2 cm from a large-scale sieve analysis;
- 3-9% finer than 0.6 cm and 12-20% finer than 2 cm from a large-scale sieve analysis;
- roughly 10% of particles were finer than 0.6 cm and 20-35% finer than 2 cm in two large-scale sieve samples; at only a slightly larger size of 3 cm much more, 40-60%, of particles were finer, highlighting the error involved in selecting a particle-size criterion above which no reaction is included in the predictions;
- roughly 40% was finer than 0.6 cm and 57% finer at 2 cm in a large-scale sieve sample.

Considering the preceding paragraphs, the percentage of rock particles at smaller sizes could be 3-100% based on particle-size criteria of 0.6 cm (used in small-scale testwork) and 2 cm (based on one of many options) defining maximum size contributing to drainage chemistry. This encompasses the old “rule of thumb” of 5-20% finer than 0.6 cm, but is too variable to be useful.

Interestingly, much of this work considers coarser rock to be stable and unreactive, although mined waste is known to crack, break, and/or settle differentially through time, leading to the ongoing creation of fresh finer particles. For example, Kempton (2012) incorrectly concluded that particle size did not “result in extending the duration of pollutant release” despite considering time periods of “decades to centuries”. In other words, Kempton considered currently coarser particles to remain permanently coarse and unreactive. Part of the justification for this was the impression

that the larger particles were not “flushed by water”. This aspect of water flushing is discussed later in Section 3.4.

Mardones et al (2009) “fine-tuned” the blasting pattern and procedure based on full-scale calibration of blasted production rock at the Andina Minesite in Chile. Production blasts produced ~5-15% of particles finer than 0.6 cm, and ~10-25% finer than 2 cm, depending on details of the blast like inter-hole time delays. The particle-size distributions were fitted with the Swebrec function (discussed below) and these percentages fall into the old rule-of-thumb of 5-20%.

To continue this bewildering situation, Hanna and Lapakko (2012) pointed out that their measured Cumulative Scaling Factor (CSF, Section 2.1) was relatively not affected by particle size. Andina et al (2012) found that leach columns with particles finer than 3.9 cm and the in-field test pad with up to 30 cm particles produced similar oxidation rates, suggesting particle-size scaling was not a major scaling factor.

Despite the general belief that upscaled reaction rates are directly proportional to particle-surface area and thus diameter (Approach 2 above), a case study showed that (1) as diameter decreased by a factor of 13 (from 1.3 cm to 0.1 cm) reaction rate increased only by a factor of roughly 3 and (2) as diameter decreased by a factor of 25 (from 2.5 cm to 0.1 cm) reaction rate increased only by a factor of roughly 5 (Kempton, 2012). Thus, the relationship of reaction rate, and to be clear only sulphide oxidation was addressed in this matter (discussed below in Sections 3.3 and 3.7), showed an inverse relationship not directly proportional to diameter.

To look at this particle-size issue in a more organized and scientific manner, we can turn to work carried out in Europe.

In Europe, aggregate and mining processes produce around 1.35 billion tons of blasted rock annually, out of which, 20% consists of material ranging between 1 and 2 cm (consistent with the old rule-of-thumb of 5-20%). This finer material cannot be efficiently processed, requires increasing land space for disposal, is not very stable, and may potentially become hazardous for public safety and the environment. Thus, there has been some good, detailed work on fragmentation in rock particles upon blasting (Ouchterlony, 2005 and 2010; Sanchidrián et al., 2012 and 2013; Johansson and Ouchterlony, 2011).

Johansson and Ouchterlony (2011) focussed on magnetite ore and how it fragmented upon blasting in small-scale tests. This work showed that typically 5-20% was finer than 0.6 cm (the old rule-of-thumb), and ~20-70% finer than 2 cm, under unconfined “free face” conditions. Under confined conditions, ~4-9% was finer than 0.6 cm, and ~15-40% was finer than 2 cm.

In more general studies of hundreds of small-scale and full-scale blasts, Sanchidrián et al. (2012 and 2013) divided 448 particle-size distributions into six groups (Figure 2):

- Group 1 Full-scale mine blasts (78 data sets)
- Group 2 Smaller-scale blast “specimens” (197 data sets)
- Group 3 Primary crusher (42 data sets)
- Group 4 Secondary and tertiary crusher (50 data sets)
- Group 5 Rod/ball mills (43 data sets)
- Group 6 Multiple-stage crushers and mills (38 data sets)

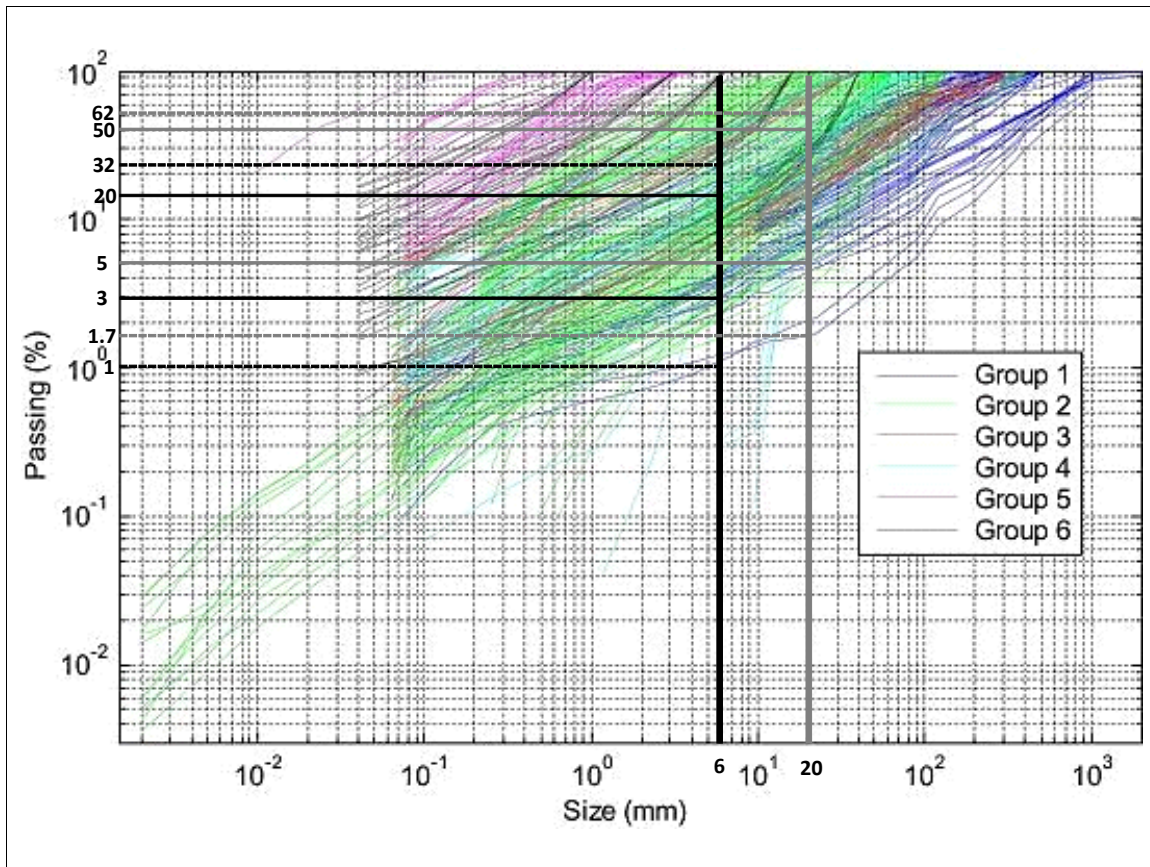


Figure 2. Rock-particle size distributions after blasting, from Sanchidrián et al. (2012) (see text for explanations of the Groups; vertical lines represent commonly discussed particle sizes of 0.6 and 2.0 cm).

Of most interest in this MDAG Case Study is the full-scale Group 1. These 78 distributions show that, except for a few extremes (Table 1), rock particles finer than 0.6 cm were 3-20% of the total mass, consistent with the old rule-of-thumb. Only in the most extreme cases did particles finer than 0.6 cm make up as little as 1% or as much as 32% of the total mass. Interestingly, some minesite-drainage predictions are now using 1% finer, obviously the most extreme condition, based on no supporting data or justification.

Table 1. Percentage of full-scale rock masses finer than various particle sizes after blasting (from Figure 2)			
	<u>0.01 cm</u>	<u>0.6 cm</u>	<u>2 cm</u>
Extreme Minimum % Finer	0.15%	1%	1.7%
Common Minimum % Finer	0.4%	3%	5%
Common Maximum % Finer	2.0%	20%	50%
Extreme Maximum % Finer	3.5%	32%	62%

A comparison of various equations that represent particle-size distributions in blasted and crushed rock was conducted by Ouchterlony (2005 and 2010), Sanchidrián et al. (2012 and 2013), and Johansson and Ouchterlony (2011). These studies identified the “Swebrec function” as the best statistical fit to the hundreds of particle-size distributions across orders of magnitude.

The basic Swebrec function is a three-parameter fragment size distribution, which ties together rock fragmentation by blasting and crushing. It gave excellent fits to more than 400 sets of sieved fragmentation data with correlation coefficients of usually $r^2 = 0.995$ or better over a range of fragment sizes spanning 2 to 3 orders of magnitude. This applied to hundreds of sieved blasting, crushing, and grinding data, from full-scale and model blasts, from sites around the world, including rock types like gneiss, limestone, dolomite, dolerite, magnetite, and andesite. This included fully sieved 500-tonne blasts down to 9 cm particles, with subsequent sieving on quartered samples down to roughly 0.008 cm. The particle-size distribution from sieving was considered more reliable than that from image analysis.

The basic Swebrec function (Equation 2) uses the median or 50% passing value, X_{50} , as the central parameter. It also includes an upper limit to fragment size, X_{max} . The third parameter, b , is a curve-undulation parameter. These three factors are interdependent to some extent. The Swebrec function removes two drawbacks from other related equations: the poor predictive capacity in the finer range and the upper limit cut-off of block size.

$$P(x) = 1 / \{ 1 + [\ln(x_{max}/x) / \ln(x_{max}/x_{50})]^b \} \quad (\text{Eq. 2})$$

where $P(x)$ = proportion of mass finer than particle size x (relative to 1.0 as 100% of mass)

x = selected particle size

x_{50} = central particle size

x_{max} = maximum particle size

b = curve-undulation fitting parameter

Two examples from Johansson and Ouchterlony (2011) were:

“crushed granite, 0-16 mm”: $x_{50} = 4$ mm, $x_{\max} = 16$ mm, and $b = 1.3$ (porosity = 20%);

“crushed granite UCS = 240 MPa”: $x_{50} = 8$ mm, $x_{\max} = 16$ mm, and $b = 2.2$ (porosity = 36%)

A five-parameter version (Equation 3) reproduces sieved fragmentation curves to the 100-micron range and also handles ball mill grinding data.

$$P(x) = 1/\{1+(a[\ln(x_{\max}/x)/\ln(x_{\max}/x_{50})]^b+(1-a)[(x_{\max}/(x-1))/(x_{\max}/(x_{50}-1))]^c)\} \quad (\text{Eq. 3})$$

For example, parameters for a granitic gneiss were: $x_{50} = 459$ mm, $x_{\max} = 1480$ mm, $b = 2.224$, $a=0.99999812$, and $c=2.0$.

The usage of extra explosives tended to produce lower values of x_{50} and x_{\max} , and higher values of b . The authors provided additional equations for estimating x_{50} and b from other factors, like explosive weight per hole, blasthole diameter, blasthole spacing, and bench height.

Still, the Swebrec function could have an error of roughly a factor of two or more in estimating cumulative amounts of finer particles, with much greater potential errors for individual finer intervals (Sanchidrián et al., 2012 and 2013; Ouchterlony, 2010). Where ultra-fine sieve data were available, the three-parameter Swebrec function fit the particle-size distribution well down to 66 μm , or five orders of magnitude (Ouchterlony, 2010).

In summary, small-scale kinetic reaction rates can be upscaled through the assumption that larger scales may have larger particles, or fewer finer particles, that are proportionally less reactive. While not consistently true, a common approach is worse: assume coarser particles are unreactive and only particles below a particular size react like small-scale testwork. No matter how this is handled, this scaling factor can range from less than 1% (<0.01) to 100% (1.0). However, the old rule-of-thumb of 5-20% (0.05-0.20) would be typical and most common based on case studies and examples. This range encompasses the measured Cumulative Scaling Factors of Section 2, and thus no additional scaling factors can often be used (Equation 1) if this one is chosen. Alternatively, the combination of this scaling factor with others, which is common, can account for the typical underestimation of full-scale minesite-drainage chemistry and water contamination during operation (Section 1). This observation is also made below for other individual scaling factors.

3.3 Temperature

Another common scaling factor for minesite-drainage chemistry is temperature. The rationale is that a larger-scale temperature different from the temperature in the smaller-scale testwork will produce different kinetic rates. While this makes some sense, the implementation of this scaling factor in the literature is woefully misleading.

Most authors adjusting for temperature invoke the simplified empirical Arrhenius Equation:

$$k = Ae^{[-E_a/RT]} \quad (\text{Eq. 4})$$

where k = reaction rate, often given the units of 1/s, which indicates the reaction can only be first degree or that A is complex

A = an empirical constant at temperature T , which can deviate significantly from values based on chemistry and physics; A varies with temperature, mass or chemical activity of molecules, and collision of molecules

E_a = activation energy of the reaction (kJ/mole), which is the minimum energy input to a chemical system, containing potential reactants, to initiate a chemical reaction

R = universal gas constant (0.008314 kJ/mole/K)

T = temperature (Kelvin)

This empirical Arrhenius Equation, applied to the oxidation of specific samples of pyrite and pyrrhotite, indicates the oxidation rate will decrease by a factor of 2 to 3 for each temperature decrease of 10°C. This decrease is invoked by many authors, but there are many reasons why this can lead to significant errors.

- 1) The most obvious weakness is that pyrite (or another sulphide mineral) is not one worldwide constant. Factors E_a and A in Equation 4, and thus the oxidation rate, are site dependent for reasons such as: pyrite comes in n and p forms, its crystallinity can be distorted by metamorphism, impurities distort the pyrite crystal structure and reaction stoichiometry, water flow rates affect the mass or chemical activity of reaction products, etc. For any particular minesite, there is no *a priori* reason to expect a rate decrease by 2 to 3 times for a temperature decrease of 10°C, yet this is often used.
- 2) Further to the preceding point, experimental testwork has been conducted on samples at 20°C and 4°C for the Canadian federal government (SRK Consulting, 2006). This is a 16°C decrease that should theoretically lower the sulphide oxidation rate to about 25%-30% (0.25-0.30) of the 20°C rate. The test results showed this reduction was rarely encountered: in some cases no reduction in rate was measured, and rarely even greater reductions were encountered (Figure 3). This often unreasonable, predicted decrease in reaction rate alone can account for the typical erroneous underestimation of full-scale minesite-drainage chemistry and water contamination (Section 1). Furthermore, Hanna and Lapakko (2012) pointed out that their measured Cumulative Scaling Factor was relatively not affected by temperature (Section 2.1). Shaw and Samuels (2012) also could not justify temperature corrections (Section 2.2).
- 3) What temperature should be used in Equation 4 for the larger scale, or used to calculate kinetic-rate reductions for every 10°C decrease? In Canada, recent environmental assessments that I have reviewed used average annual air temperature at the sites! This is unfathomable. Most people in Canada know that, under snow cover in winter, ground temperatures are often warmer than winter air temperatures. Thus, the usage of average annual air temperature in Canada, instead of ground temperature, must be a deliberate attempt to underestimate the severity of full-scale drainage chemistry. This is consistent with the common predictive errors discussed in Section 1 of this Case Study

Also, the usage of average annual air temperature (which includes frozen winter air temperatures) underestimates aqueous contaminant concentrations in the warmer months of spring, summer, and fall when water is actively draining from minesite components. Finally, the usage of any air or background ground temperatures ignores the well documented, abundant heat produced by the exothermic reaction of sulphide oxidation (the very issue to which the Arrhenius Equation is applied). For example, Kempton (2012) and Morin et al (2012), among many others, highlight how sulphidic minesite components can be warmer than ambient air, up to 70°C.

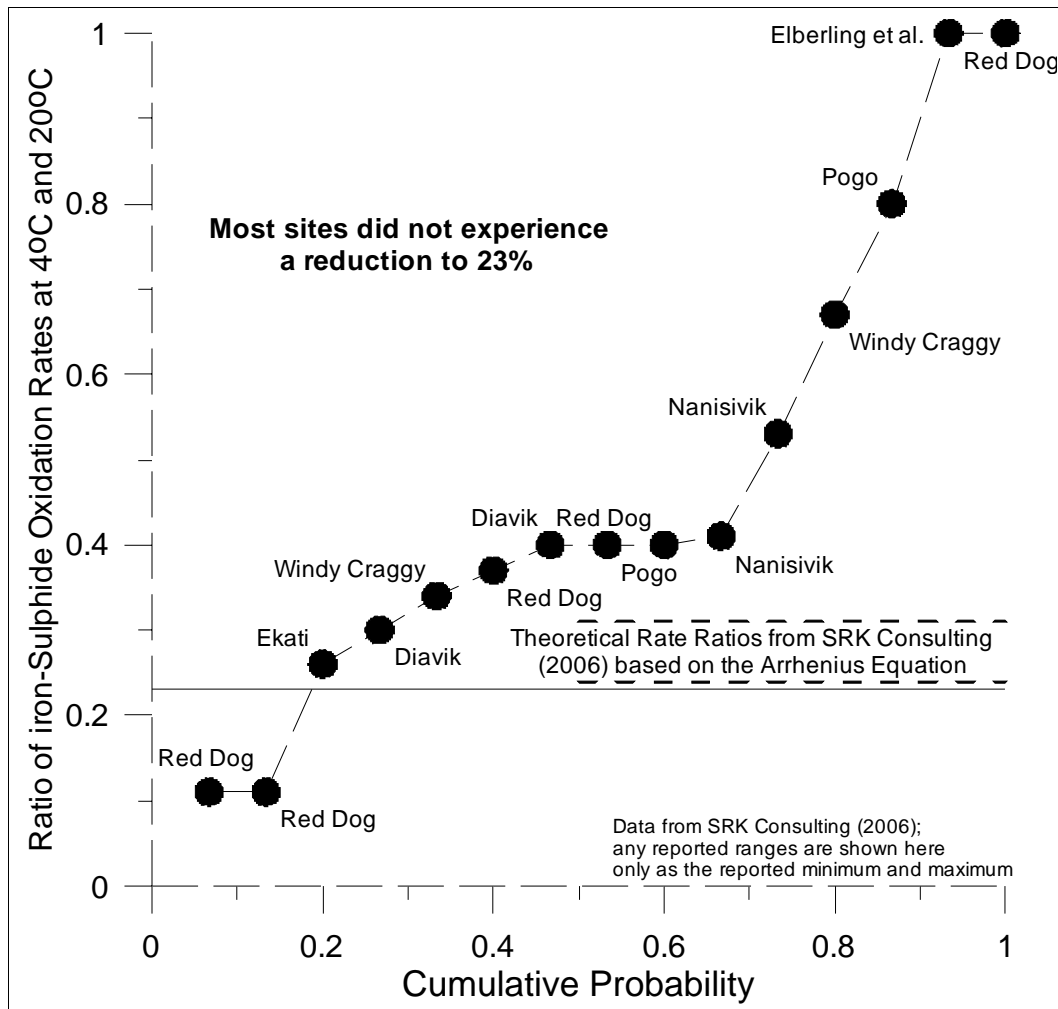


Figure 3. Reductions in the oxidation rates of iron-sulphide minerals based on laboratory testwork, showing the Arrhenius Equation does not accurately reflect the reductions (from data in SRK Consulting, 2006).

Full-scale mine wastes with temperatures above those of small-scale testwork (say, around 20°C) should be predicted to have higher rates, but often a cooler temperature (T) is used in Equation 4. Again, this is consistent with the common underprediction of water contamination at minesites.

- 4) All discussion in this section to this point has carried a hidden, but major, implication: every single other aqueous and solid-liquid reaction, and leaching of every element, has the same temperature scaling factor (including same E_a and A) as calculated for sulphide oxidation! I have read environmental assessments where the predictions for every element were adjusted by the same factor used for sulphide oxidation. This might be a valid assumption if all the following conditions were met: (1) every other element is contained 100% within sulphide (which is rarely the case), (2) sulphide oxidation completely and fully solubilizes each element in direct proportion to sulphide oxidation (no justification for this), and (3) all subsequent aqueous complexing and solid-liquid interactions are exothermic to the same extent as sulphide oxidation (which is wrong). There was no evidence all these would be met in the assessments.

For example, Kempton (2012) assumed all aqueous elements were released by the oxidation of sulphide, despite a case study showing this resulted in errors of factors of 5 to 10. In contrast, Shaw and Samuels (2012) documented a unique factor for each element (Sections 2.2 and 3.8). Kempton's error can be traced to the reasoning that "many regulated metals are bound as sulfides and thus dissolve in proportion to sulphate". Such a misconception does not recognize that portions of many elements are also bound simultaneously to silicates, oxides, carbonates, etc., and do not dissolve in proportion to sulphate production.

Thus, there is no reason that a temperature scaling factor for sulphide oxidation (typically unreasonably low based on the abuse of the Arrhenius Equation) should be applied to the leaching of all other elements of concern (in turn, unreasonably lowering all these other predicted larger-scale rates). This approach can be in substantial error for reactions such as reductive dissolution of oxide minerals, leaching of some aluminosilicate minerals, attainment of equilibrium, and dissolution of carbonate minerals into dilute infiltrating waters.

In summary, the scaling factor for temperature differences between small-scale testwork and the larger-scale component being predicted is often based on the Arrhenius Equation. More specifically, the oxidation of sulphide, the production of sulphate, and the leaching of all other elements will decrease by a factor of 2-3 for each 10°C decrease in temperature. There is often no justification for such a factor, data show that such a factor could be erroneous, and implementations of this factor have been based on misunderstandings. In any case, the scaling factor for every 10°C decrease is reportedly 0.33-0.50. For temperature differences of 10-20°C, the resulting scaling factors of 0.17-0.50 encompass the measured Cumulative Scaling Factors of Section 2, and thus no additional scaling factors can be used (Equation 1) if this one is used. Alternatively, the combination of this scaling factor with others, which is common, can account for the typical underestimation of full-scale minesite-drainage chemistry and water contamination during operation (Section 1). This observation is also made for other individual scaling factors.

3.4 Contact by Drainage Water

Minesite materials have pore spaces filled with water, with pore gases such as nitrogen, oxygen, carbon dioxide, and water vapour, or with some combination. If concern is limited to a reaction such as sulphide oxidation, the pore-gas levels of oxygen and water vapour can be important and can be included as scaling factors, which is discussed in Sections 3.5 and 3.6. This subsection focusses on the common scaling factor that addresses the proportion of reactive minesite materials rinsed and flushed of their reaction products by moving water within the pore spaces.

Under unsaturated conditions, some proportion of full-scale minesite materials will not be thoroughly and regularly flushed of their reaction products by drainage waters. Instead, the unflushed reaction products accumulate through time, like a geochemical “battery” being charged. Under saturated conditions, a higher proportion may be regularly flushed, but aspects like secondary-mineral precipitation and capillary fringes can still lead to some retention and accumulation. As a result, the kinetic rate from a well-rinsed, small-scale kinetic test can be divided into two basic portions for upscaling: the portion of the rate released regularly, and the portion retained and accumulated on a larger scale.

To be clear, if the small-scale test is not well rinsed, then it already experiences some retention and accumulation, as expected in trickle-leach humidity cells and leach columns. This small-scale retention has to be accounted for in a complicated manner. If the small-scale flushing is close to 100% on a regular basis, then the following scaling factors can apply. If the small-scale flushing is significantly less than 100%, then the following scaling factors will not apply, and applicable factors can be less than or greater than 1.0 depending on the small-scale procedure.

With diluted white paint sprayed onto small rock piles and rock-filled columns, ElBoushi (1975) found that less than 20% of rock surfaces were coated with paint below depths of 1 m. Based on a similar approach, Morin et al (1997) and Morin and Hutt (2000 and 2001b) found the percentage of surfaces coated with paint in a full-scale waste-rock pile varied widely (from roughly 25-100%) over short distances. This reflected mining- and dumping-induced variations and stratifications in particle size (discussed in Section 3.2).

Morin and Hutt (1994) used a kinetic-rate scaling factor of 0.05 (5%) for rock-surface flushing by water to match full-scale waste-rock drainage under acidic and near-neutral conditions. This did not apply to elements whose aqueous concentrations were controlled by equilibrium conditions (Figure 1). Kempton (2012) concluded that this scaling factor could range from roughly 0.10 to 0.65 or higher.

In contrast, Hanna and Lapakko (2012) pointed out that their measured Cumulative Scaling Factor was relatively not affected by the degree of particle-surface flushing (Section 2.1). Shaw and Samuels (2012) presented similar evidence in their work (Section 2.2). Thus, there is some contradictory measured information that shows the extent of particle-surface flushing is not an important scaling factor.

While the preceding examples did consider the extent of flushing, the effect of time-variable flowrates of water (or white paint) was often not considered. In reality, flowrates can be highly variable seasonally, annually, and over longer periods. As a result, the amount of flushed rock surfaces, or more precisely the amount of reaction products flushed from rock surfaces, depends to

some extent on flow (discussed further in Section 3.9). One full-scale case study showed that rock-surface flushing was generally steady around 5% of surfaces as flow increased, until a high flow threshold was exceeded and then up to 40% of surfaces were flushed (Morin and Hutt, 1994). Also, based on a mass-balance approach, reaction products not flushed one year during lower flows could be flushed in later years by higher flows (Morin et al., 2012).

An empirical way to express a flow dependency was developed by field work in the 1960's at underground mines (Morth et al., 1972), and carried over to open pits in the 1990's (Morin, 1990; MEND, 1995; Morin and Hutt, 1995, 2001c, and 2004). This approach classified rock surfaces empirically as (1) flushed regularly, (2) flushed occasionally, and (3) flushed only after long periods or upon submergence. Studies of open pits have shown that only a few percent of annual reaction products is removed regularly from the walls, roughly 10-30% is removed occasionally, and 70-90% is retained throughout operation until submergence. In contrast to pits, underground mines typically have lower percentages retained (5-50%) during operation. In any case, this complicates the desire for a single scaling factor characterizing the degree of flushed rock surfaces.

In addition to water flow, condensation within rock piles and mine walls has been documented. While condensation may not result in an effluent, it can (1) mobilize reaction products from poorly flushed zones to better flushed zones and (2) maintain reactions that require water or water vapour (Section 3.6). This greatly complicates a scaling factor for the percentage of flushed rock surfaces.

In my experience reviewing environmental assessments for proposed minesites, all this is handled by assuming a set proportion of surfaces is flushed annually, such as 20%. That's it. There was no further consideration of accumulation or occasional peak releases or condensation.

Kempton (2012) provided an interesting discussion on how this scaling factor for drainage contact and the factor for particle size (Section 3.2) could be synonymous, due to water moving only through finer particles. "Unsaturated-flow models and [small laboratory scale] column studies of waste rock structures demonstrate that unsaturated flow is conveyed preferentially through fine materials at low water flux typical of capped waste rock facilities". Unfortunately, Kempton does not explain that such models are Darcian-capillary-based and thus by definition have to inevitably show preferential unsaturated flow in finer particles. Further, there was no explanation how all finer materials on a full scale turn out to be all hydraulically connected. Also, laboratory testwork does not include coarser rock, which in reality would carry more water faster, under non-Darcian conditions. Non-experts have no problem understanding this, when asked whether a pile of silt or a similar-sized pile of boulders would release water first if buckets of water were poured on top.

It is remarkable that published discussions of particle size (Section 3.2) emphasize how few finer, reactive particles are typically present among abundant coarse rock and boulders, leading to reduced overall geochemical reactivity. Then, when water movement is considered, finer particles become sufficiently abundant to be continuously connected and control flow.

In summary, the scaling factor for rock-surface contact and flushing by moving water can be complex, and vary with time and flow rate. This is usually simplified to a factor representing regularly flushing, with no consideration of reaction-product accumulation and peak releases. Such simplified scaling factors are in the general range of 1-20% (0.01 to 0.20), although values above 65% are possible. This range is less than (too low) or consistent with the measured Cumulative

Scaling Factors of Section 2, and thus no additional scaling factors can be used (Equation 1) if this one is used. Alternatively, the combination of this scaling factor with others, which is common, can account for the typical underestimation of full-scale minesite-drainage chemistry and water contamination during operation (Section 1). This observation is also made for other individual scaling factors.

3.5 Level of Oxygen

For reactions that require oxygen as a reactant (note again the focus on sulphide oxidation; see Sections 3.3, 3.7, and 3.8), the pore-gas level of oxygen can affect the kinetic rate. However, the way in which the kinetic rate is affected is not well defined. Past work has shown that sulphide oxidation does not necessarily decrease linearly with decreasing oxygen levels (e.g., Morin and Hutt, 2001d; Jerz and Rimstidt, 2004), and levels of oxygen can be very low and not significantly retard the rate of sulphide oxidation. Moreover, a full-scale case study showed no relationship of temperature (representing oxidation rate and heat production) with pore-gas oxygen (Morin et al., 2012). One potential reason for this is that pore-gas oxygen is not required for oxidation, as other oxidants exist such as ferric iron, nitrate, and sulphate.

Kempton (2012) discussed case studies of non-reactive sulphide-oxidation zones defined by low pore-gas oxygen or “completely depleted in oxygen”. Complete depletion in oxygen cannot be measured, as analytical technology is subject to detection limits. In any case, low levels of pore-gas oxygen could simply mean that the sulphide minerals are consuming pore-gas oxygen as quickly as it is transported to the minerals, which is definitely not non-reactive. Also, oxidants other than pore-gas oxygen may be present. So, caution is needed in any kinetic-rate scaling factor based on pore-gas oxygen, and for many reactions no pore-gas oxygen is needed anyway.

Kempton (2012) estimated the pore-gas-oxygen scaling factor at roughly 0.2 to 0.5 (20-50%) for rock with roughly 1-5% sulphide. However, the inhibition of convective air flow could reportedly result in lower scaling factors.

In summary, this scaling factor applies to kinetic rates that require pore-gas oxygen and that vary significantly with variations in gaseous oxygen. However, testwork has been generally contradictory on the quantitative relationship of pore-gas oxygen to such oxygen-dependent reactions. Furthermore, some full-scale monitoring data have shown oxygen levels to be unimportant, and the presence of other oxidants may minimize the importance of this scaling factor. Nevertheless, the rare estimates of this scaling factor are around 0.2 to 0.5 for rock with 1-5% sulphide. This range lies in the measured range of Cumulative Scaling Factors of Section 2, and thus no additional scaling factors can be used (Equation 1) if this one is used. Alternatively, the combination of this scaling factor with others, which is common, can account for the typical underestimation of full-scale minesite-drainage chemistry and water contamination during operation (Section 1). This observation is also made for other individual scaling factors.

3.6 Moisture Content (Water Vapour)

This less common scaling factor has some synergy with the scaling factor for water contact (Section 3.4). However, whereas water contact addressed the removal and transport of reaction

products from rock-particle surfaces, this scaling factor reflects whether water-dependent reactions even occur on rock-particle surfaces.

Kempton (2012) pointed out that this scaling factor was generally considered unimportant due to the common presence of some moisture (or humidity). Thus, Kempton reasoned that this factor should be set at 1.0 unless good evidence indicates gravimetric moisture is below roughly 2%. However, due to processes like water-vapour transport in pore gases and daily condensation from warming and cooling, even rock with lower moisture contents would likely have sufficient moisture for chemical reactions. In spite of an average rainfall below 1 mm/year in the Atacama Desert of Chile, condensation has been documented as sufficient to form dew. Also, frozen soils and rock often contain some liquid water even well below zero (e.g., literature review in Dawson and Morin, 1996). As a result, even in these extreme climates, there is sufficient water to permit aqueous reactions, even if the volume of water is insufficient to result in active drainage. This situation would result in reaction-product retention and accumulation, producing a charging geochemical “battery”, as discussed in Section 3.4.

In summary, this less common scaling factor considers conditions in which water or water vapour is so limited that water-dependent reactions cease. Even in extreme climates, this is unlikely. Therefore, this scaling factor can mostly be ignored, or in other words set to a value of 1.0.

3.7 Solid-Phase Level of Elements

As with some other scaling factors, this one often reflects the single-minded and unjustified focus on sulphide oxidation as the cause and strict control on all aqueous elements in minesite-drainage chemistry. Unlike other scaling factors, this one can have values much greater than 1.0 if the larger-scale minesite materials contain much more solid-phase sulphide than the small-scale testwork.

The usage of this scaling factor requires that kinetic rates at various scales are directly proportional, or proportional in a well-defined manner, to the percentage of solid-phase sulphide. This is not always the case. Thus, this scaling factor should be used only if the correlation is well defined. Hanna and Lapakko (2012) resolved the issue by normalizing their sulphate kinetic rates to kg of pyrite, rather than kg of rock, at both scales.

This scaling factor, while often limited to solid-phase sulphide, can be extended to other elements for robust predictions. For example, the leaching rates of copper and cadmium may reflect the amount of solid-phase copper, or the leaching rate of manganese may reflect the amount of solid-phase Neutralization Potential. However, this requires scaling factors for each element, rather than only sulphide, which is currently not standard practice (Section 3.8).

In summary, correlations of kinetic rates with a solid-phase element, combined with differences in the solid-phase levels between scales, results in this scaling factor. The factor typically considers only sulphide, and the sulphide factor is often unreasonably applied to all predicted elements. However, this factor can be more flexible, with applications to all solid-phase and aqueous elements of concern, as discussed further in the next subsection.

3.8 Scaling Factor for Each Element

As discussed in several previous subsections, current practice often calculates scaling factors for sulphide oxidation using the sulphate-production kinetic rate. A Cumulative Scaling Factor (CSF) is then calculated for sulphate (Equation 1). This value is then typically applied to all other elements of concern, based on the arguments that sulphide oxidation is the only source of all these other elements and that all these other elements leach in the same exact proportion as sulphate (e.g., Kempton, 2012). Detailed work and monitoring have shown this is not so and that each element can have its own scaling factor (e.g., Shaw and Samuels, 2012).

Discussions and case studies in the preceding subsections should be sufficient to expect each element of concern to have separate individual scaling factors and CSF. An alternative approach is to multiply the sulphate-based CSR (Equation 1) by values greater than or less than 1.0 to reflect each element's unique behaviour.

3.9 Water Flow

Although the rate of water flow can differ among scales and may affect the degree of particle-surface flushing (Section 3.4), it is often not considered a scaling factor that appears explicitly in Equation 1a. This is because the kinetic rate itself is often considered independent of flow. However, water flow and its variability are more often applied later to an upscaled kinetic rate to obtain aqueous concentrations (Equation 1c).

Some studies have upscaled small-scale rates (mg/kg/wk) to larger-scale aqueous concentrations (mg/L) in one step, and reported a Cumulative Scaling Factor (Equation 1b) that implicitly included flow as an individual scaling factor (Equation 1c). This is why Section 2 of this MDAG Case Study emphasized care when reporting units used in upscaling. Also, where equilibrium conditions apply, flow is often not a major factor (e.g., Morin et al., 2012), and kinetic rates should not be upscaled into the equilibrium range in any case (Figure 1).

Some authors prefer to use the ratio of solid mass (or particle surfaces, Section 3.2) to water, rather than flow (e.g., Shaw and Samuels, 2012). This ratio is effectively the combination of two factors in Equation 1c, mass and flow rate. Thus, this ratio does not require separate consideration from water flow.

3.10 Other Individual Scaling Factors

As explained earlier in this section and in Section 2, there can be hundreds or thousands of scaling factors. This Case Study was not intended to be exhaustive, but to discuss common or misleading scaling factors in common usage.

Nevertheless, scaling factors can be included to consider differences in processes at different scales, like microbial activity, electrical ground charges, and barometric effects. However, as explained in Section 2 and by Equation 1a, the more scaling factors less than 1.0 considered, the lower the Cumulative Scaling Factor. This can account for the common underestimation of larger-scale drainage chemistry and water contamination, so care is needed in selecting the number and

types of scaling factors.

4. SUMMARY

An important aspect in the prediction of minesite-drainage chemistry is reasonably upscaling the results of smaller-scale testwork to larger scales. However, this goal remains elusive. Case studies show that the underestimation (underprediction) of full-scale drainage chemistry and water contamination is the preferred objective of upscaled prediction.

A major reason for the predictive errors and underpredictions in upscaling is the scaling factors for small-scale kinetic testwork. In many cases, small-scale kinetic testwork should not be upscaled into equilibrium conditions typical of full-scale minesite components. However, such upscaling is becoming more common and popular, so a closer look at kinetic scaling factors warranted.

The literature shows that nearly all scaling factors in regular usage are less than 1.0. Because the Cumulative Scaling Factor (CSF) applied to small-scale kinetic rates is a multiplicative product of each individual scaling factor (Equation 1a), the CSF decreases with each additional factor considered. This is one cause of the common underprediction of drainage chemistry and water contamination. Another is the usage of a long-term average, or late-stage stable, rate for upscaling, rather than a maximum measured rate.

Examples of measured CSF values in the literature are mostly between 0.05 and 0.60 (Section 2), or in other words the larger-scale rate is typically 5% to 60% of the small-scale rate. In comparison, typical values of common individual scaling factors were often within this CSF range. This means that, in many cases, one individual scaling factor can accurately predict the CSF used for upscaling. In turn, the inclusion of additional factors can lead to the commonly observed underprediction.

In Section 3, several individual scaling factors were discussed in detail, including reported values. These scaling factors included: particle size, temperature, contact by drainage water, level of pore-gas oxygen, solid-phase level of elements, moisture content, and flow rate of water. The importance of unique scaling factors for each aqueous element was also discussed. This highlighted the error in the common usage of the scaling factor for sulphate-production rate (sulphide-oxidation rate) applied to every element of concern.

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