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Applicability of scaling factors to humidity-cell kinetic rates for larger-scale predictions



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What Do I Mean by “Scaling Factor”?

- “Scaling factor” is used in this presentation as a general term to represent all factors that differ between a small-scale kinetic test and a full-size minesite component.
- Factors like temperature differences between laboratory and field are not usually real scaling factors gradually changing with scale, but are called that here. Thus, scaling factors in this presentation = correction factors + adjustment factors + translation factors + conversion factors + true scaling factors + etc.
- Such factors have become common in the prediction of minesite-drainage chemistry. Laboratory tests containing ~ few kgs of sample are scaled up to predict chemistry from minesite components containing millions of tonnes (a weight-based scale difference of 10^9 !) to billions of tonnes (a scale difference of 10^{12} !). Can such predictions be valid when they span such vast differences in scale?

Implications of Increasing Scale – Emergent Conditions

- Emergence can generally be defined as the appearance of distinct patterns or properties as scale increases, due to self-organization in complex systems, or “the whole becomes not merely more, but very different from the sum of its parts”
 - Anderson, P.W. 1972. More is different: Broken symmetry and the nature of the hierarchical structure of science. *Science* 177, p. 393-396.
- “Deep analysis of the underlying explanation of scale is missing. One of the intriguing propositions of complex systems theory is the emergence of new structures at a high level of scale that are difficult if not impossible to predict from constituent parts. Emergent properties are not the mysterious creation of ‘new material’ in the system, but rather the placement of the components of the system into their logical contexts (scales) so that the observer/modeler can see structures arise from them for the first time.”
 - Easterling and Kok, 2002, *Integrated Assessment*, 3, p. 233-246.

Implications of Increasing Scale – Emergent Conditions

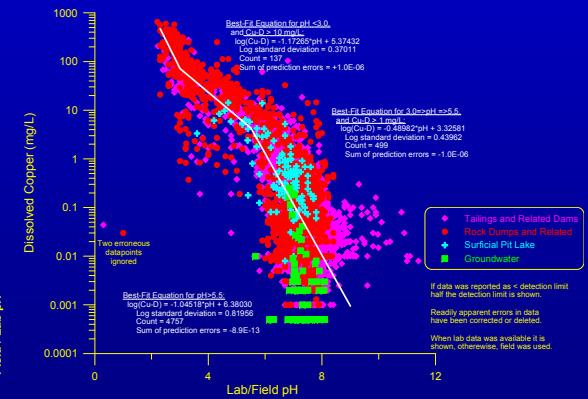
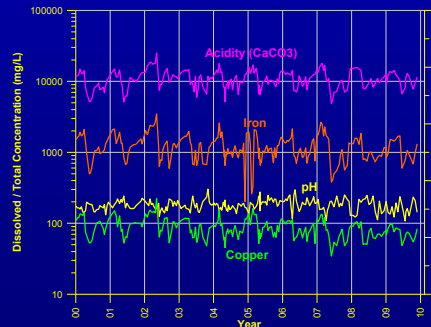
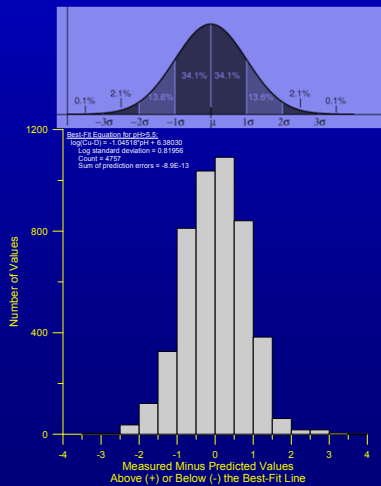
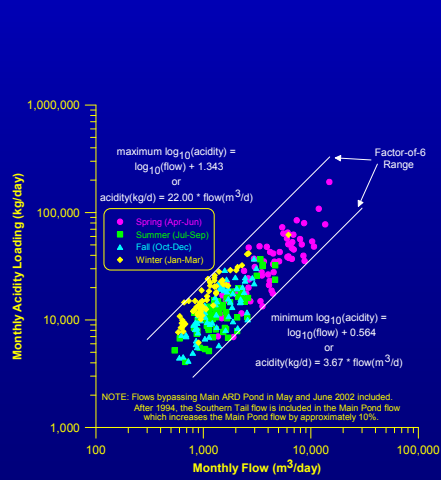
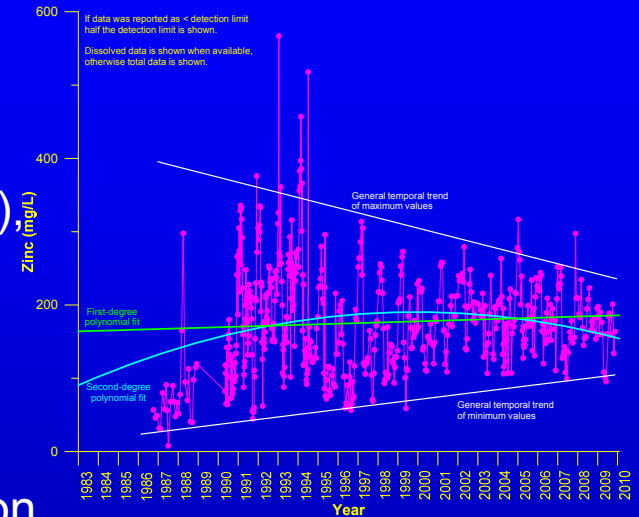
- “[There is] the emergence of new structures at a high level of scale that are difficult if not impossible to predict from constituent parts.” “[T]he whole becomes ... different from the sum of its parts”.



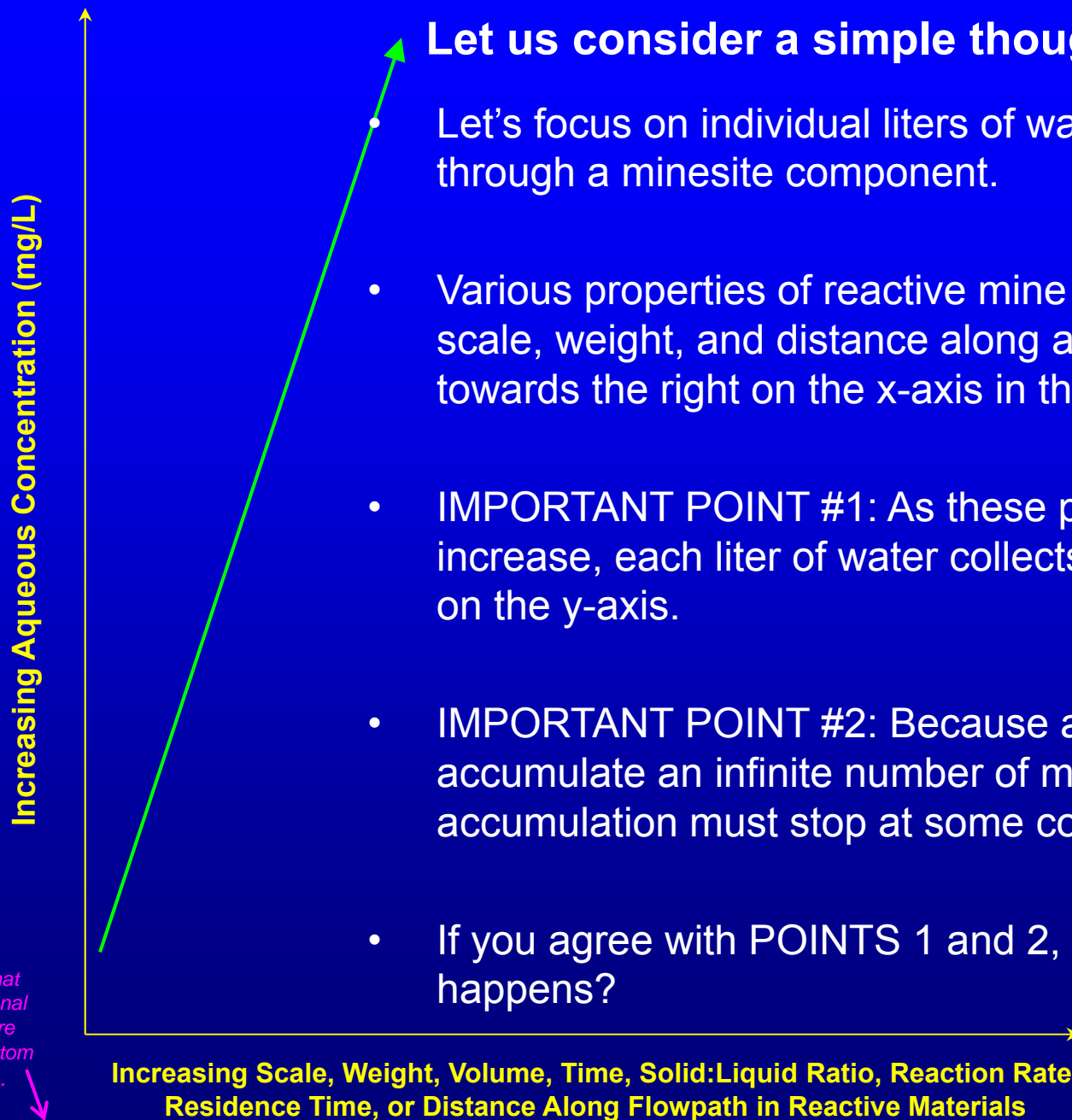
- Does a small-scale kinetic test like a humidity cell contain all the geochemical information needed to “scale it up” to a full-scale minesite component for prediction of drainage chemistry (by $\sim 10^9 - 10^{12}$ times)? Is such a test a complete geochemical “microcosm” of the enormously larger component?

Implications of Increasing Scale – Emergent Conditions

- I have evaluated minesite-drainage databases containing thousands of analyses, collected over decades or collected ~ every hour.
- The temporal full-scale patterns and trends in these databases are not readily explainable, cannot be fully detected by routine full-scale monitoring (e.g., monthly) and are certainly not predictable from a small-scale kinetic rate. Thus, unidentified emergent processes do come into play with increasing scale of minesite-drainage chemistry.
- So I agree: “Deep analysis of the underlying explanation of scale is missing” for minesite-drainage chemistry.



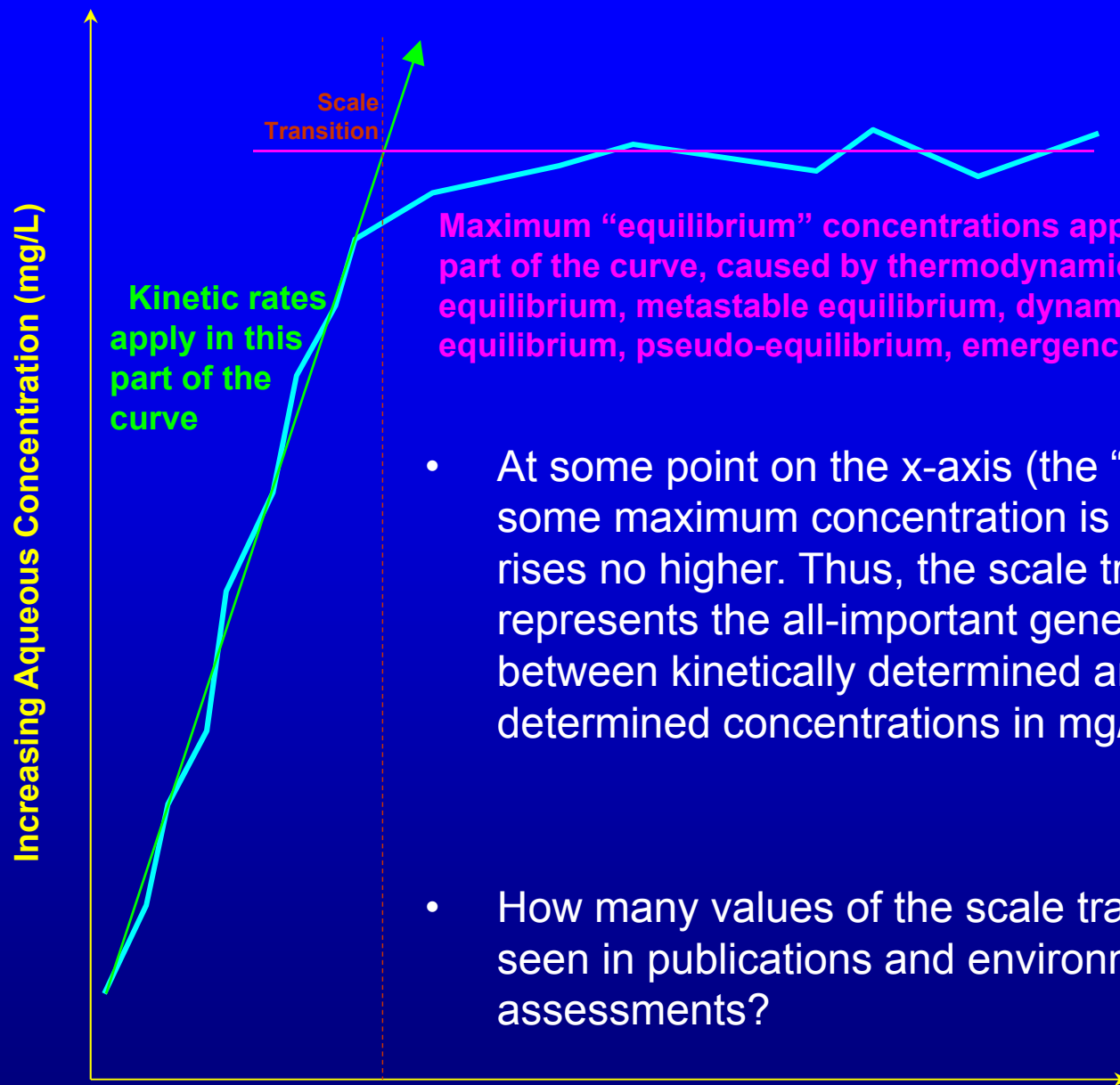
References that provide additional information are listed at the bottom of the pages.



Let us consider a simple thought experiment

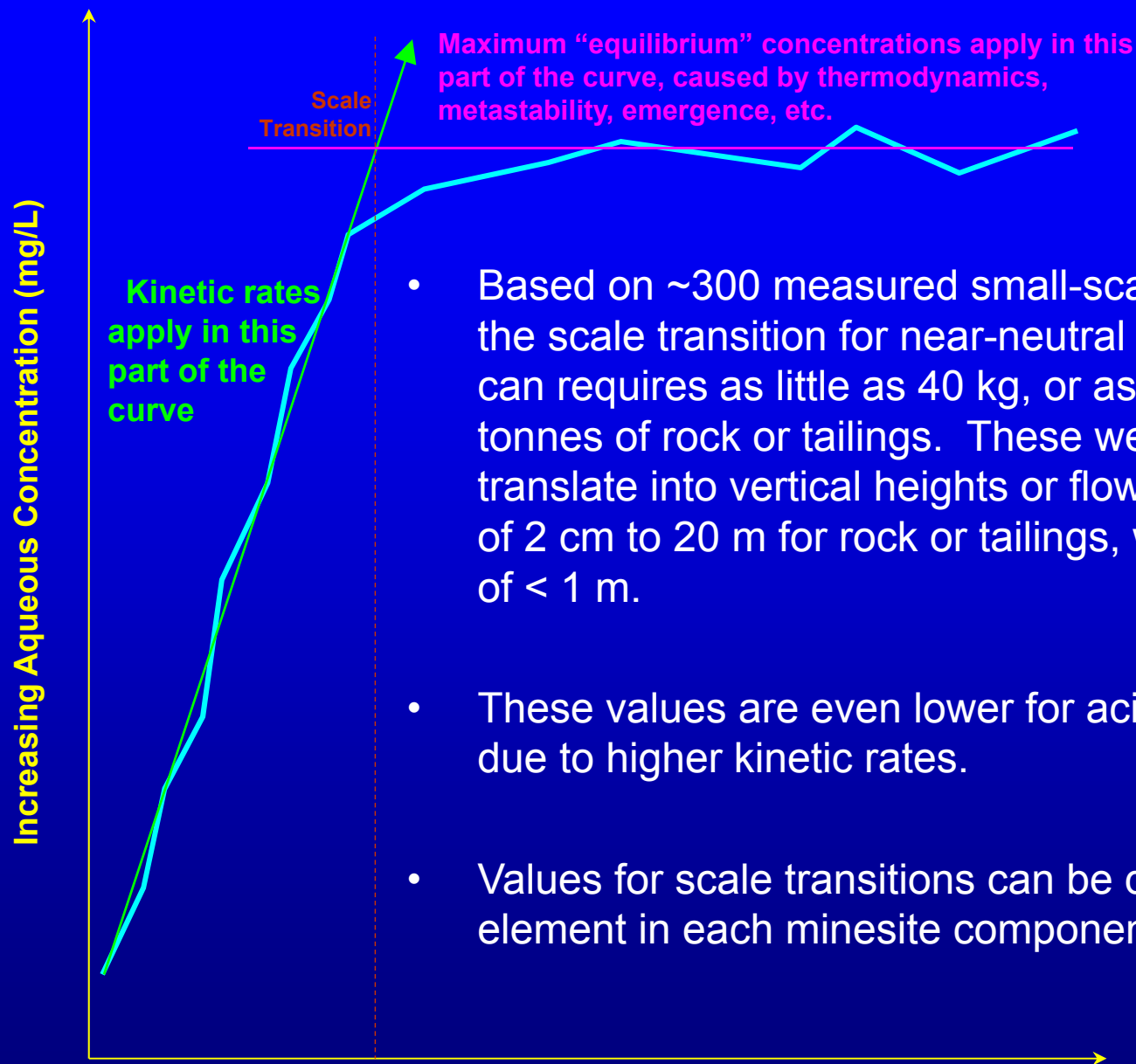
- Let's focus on individual liters of water passing through a minesite component.
- Various properties of reactive mine materials such as scale, weight, and distance along a flowpath increase towards the right on the x-axis in this diagram.
- **IMPORTANT POINT #1:** As these properties generally increase, each liter of water collects additional mg/L on the y-axis.
- **IMPORTANT POINT #2:** Because a liter will not accumulate an infinite number of mg/L, the accumulation must stop at some concentration.
- If you agree with POINTS 1 and 2, then what happens?

References that provide additional information are listed at the bottom of the pages.



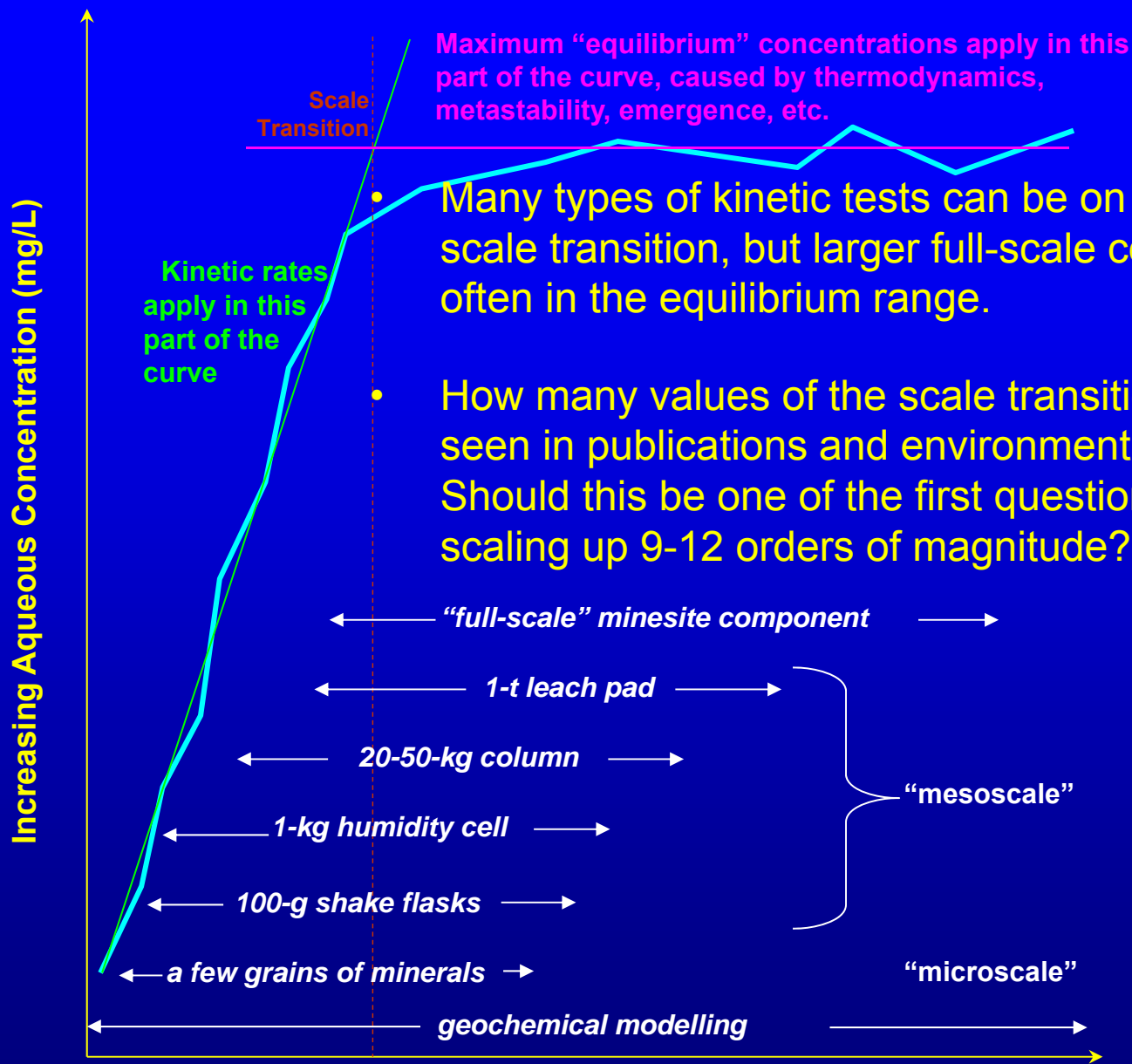
- At some point on the x-axis (the “scale transition”), some maximum concentration is achieved and rises no higher. Thus, the scale transition represents the all-important general break between kinetically determined and equilibrium determined concentrations in mg/L.
- How many values of the scale transition have you seen in publications and environmental assessments?

Increasing Scale, Weight, Volume, Time, Solid:Liquid Ratio, Reaction Rate, Residence Time, or Distance Along Flowpath in Reactive Materials

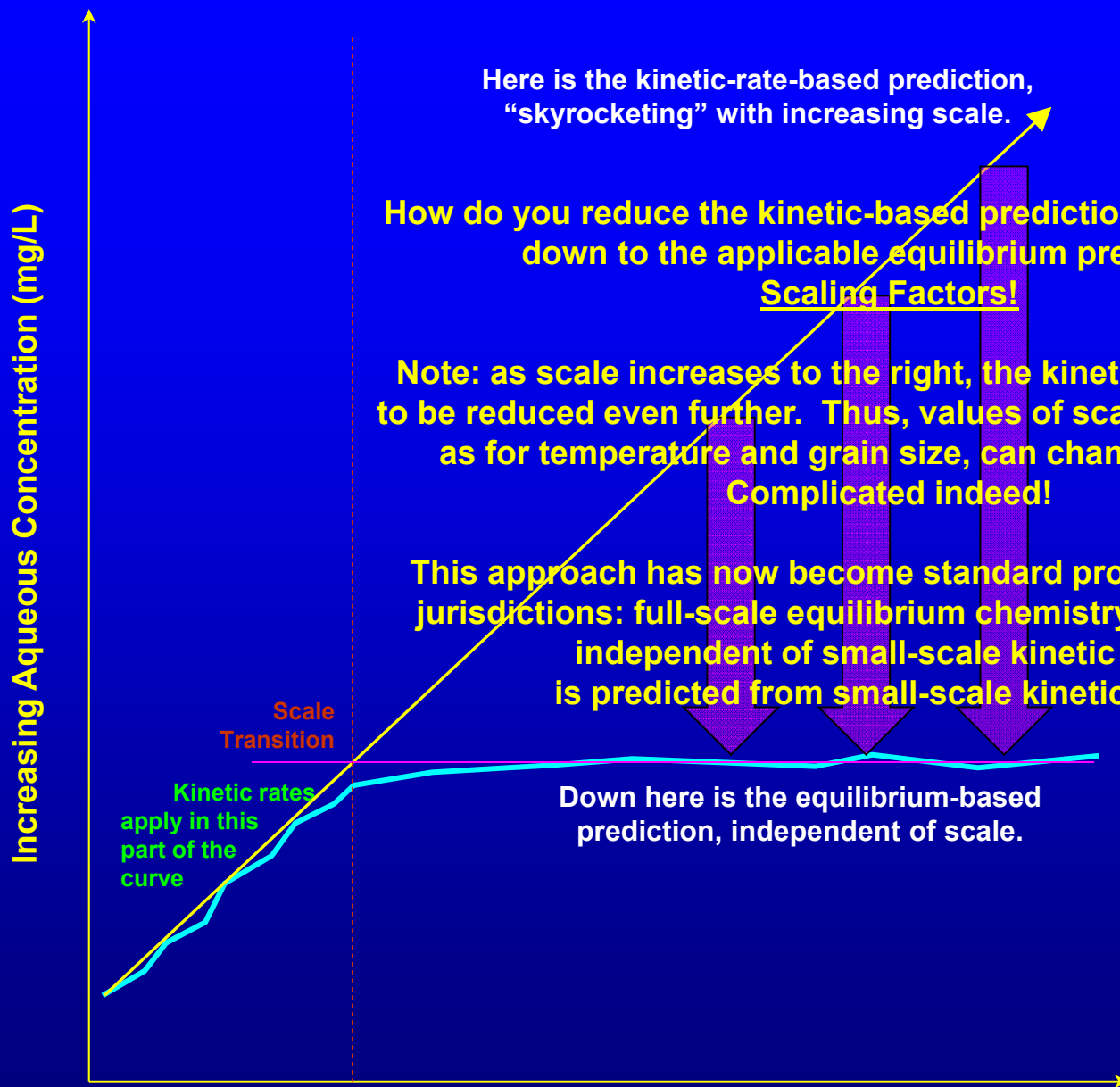


- Based on ~300 measured small-scale kinetic rates, the scale transition for near-neutral copper leaching can require as little as 40 kg, or as much as 40 tonnes of rock or tailings. These weights can translate into vertical heights or flowpath distances of 2 cm to 20 m for rock or tailings, with an average of < 1 m.
- These values are even lower for acidic conditions due to higher kinetic rates.
- Values for scale transitions can be different for each element in each minesite component.

Increasing Scale, Weight, Volume, Time, Solid:Liquid Ratio, Reaction Rate, Residence Time, or Distance Along Flowpath in Reactive Materials



Increasing Scale, Weight, Volume, Time, Solid:Liquid Ratio, Reaction Rate, Residence Time, or Distance Along Flowpath in Reactive Materials



Increasing Scale, Weight, Volume, Time, Solid:Liquid Ratio, Reaction Rate, Residence Time, or Distance Along Flowpath in Reactive Materials

Basic Equation (Forward and Backward Directions)

- Calculation of Kinetic Rate based on Aqueous Concentrations from Small-Scale Well-Rinsed Kinetic Tests

- Kinetic Rate (mg/kg/wk) =
Effluent Concentration (mg/L) /
Amount of Rinse Water (L) /
Period of Time Between Rinses (wks)

- Prediction of Larger-Scale Aqueous Concentrations

- Larger-scale Effluent Concentration (mg/L) =
Kinetic Rate (mg/kg/wk) *
Weight of Reactive Mine Material (kg) /
Flow Through the Reactive Mine Material (L/wk)

This small-scale rate is often adjusted downward through multiplication by one or more individual "scaling factors" less than 1.0.

For most full-size minesite components, measured concentration (mg/L) rarely shows a 1:1 inverse correlation with flow, so this division by flow is rarely justified and correct.

Cumulative Scaling Factors (CSF)

- Cumulative Scaling Factor (CSF) = SF1 * SF2 * SF3 * SF4 * SF5 * SF6 * . . .
 - Because scaling factors are typically less than 1.0 for minesite drainage, the CSF decreases in value as more individual scaling factors are considered. For example, if each factor were 0.5 in value, the CSF for only three individual factors would be 0.13 (0.5*0.5*0.5), whereas the CSF would be 0.016 for six individual factors.
- Larger-scale Aqueous Concentration (mg/L) =
CSF * Measured Small-scale Kinetic Rate (mg/kg/wk)*
Larger-scale Mass (kg) /
Larger-scale Water Flow (L/wk)

Cumulative Scaling Factors (CSF)

- Small-scale kinetic rates can be adjusted using dozens or hundreds or thousands of scaling factors, reflecting each physical, chemical, biological, and engineering aspect.
- For simplicity, most authors choose a small subset of factors.
- Does nature re-adjust itself to use only the factors chosen by the authors for that particular site?
- Furthermore, have we quantified all possible scaling factors? How about microbial activity (especially for microbes that RNA studies show we have not yet identified), or changes in electrostatic charges due to weather variations (after all, mineral surfaces are electrostatic surfaces)?
- The choice by a human does not block other factors from being important; it just means the human failed to consider them.

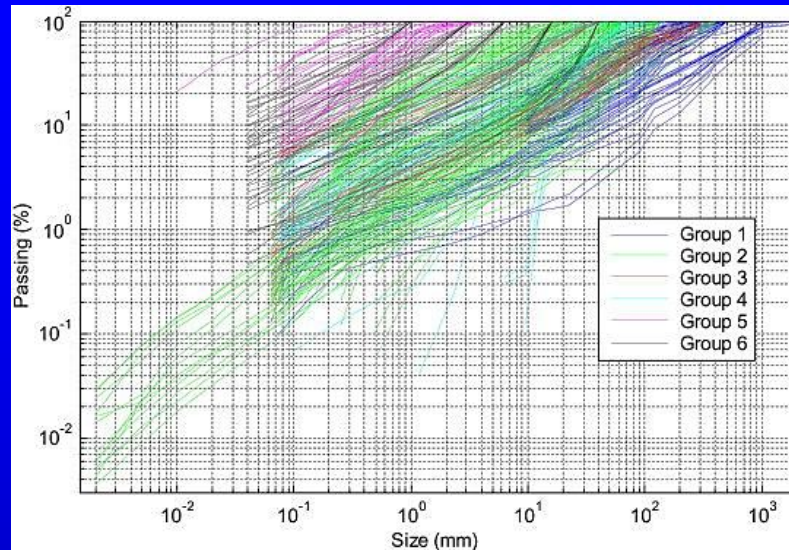
Cumulative Scaling Factors (CSF)

- CSF values are very important for proper prediction of minesite-drainage chemistry. So one would expect dozens or hundreds of measured CSF values have been documented and published. This would confirm or refine this approach of scaling up measured smaller-scale kinetic rates to full-scale minesite components. Remarkably, there are very few measured CSF values in the literature!
- The few examples of CSF values that I located were between 0.05 and 0.60. In other words the larger-scale rate was typically 5% to 60% of the small-scale rate. Therefore, the multiplication of all individual factors operative under real on-site conditions (in addition to authors' preferred factors) should often yield a value around 0.05 to 0.60.

Examples of Individual Scaling Factors

- *Watch out for mathematical units in the factors and rates!*
- Selection of Small-Scale Kinetic Rate for Upscaling
- Particle Size
- Temperature
- Contact by Drainage Water
- Level of Oxygen
- Moisture Content (Water Vapour)
- Solid-Phase Level of Elements
- Scaling Factor for Each Element
- Water Flow
- Other Individual Scaling Factors

A Scaling Factor: Particle Size



The typical, but not correct, assumption here is that only finer particles react. The old “rule-of-thumb” said waste rock would often contain 5-20% fines.

In studies of hundreds of small-scale and full-scale blasts, Sanchidrián et al. (2012 and 2013) divided 448 particle-size distributions into six groups (see figure). Of most interest to us is Group 1 (78 data sets; see table).

This showed that the old “rule-of-thumb” of 5-20% was reasonable. However, recently used values of 1% fines are extreme and rarely justified, but they result in lower predicted concentrations.

Percentage of full-scale rock masses finer than various particle sizes after blasting (% content of fines)

	<u><0.6 cm</u>	<u><2 cm</u>
Extreme Minimum % Finer	1%	1.7%
Common Minimum % Finer	3%	5%
Common Maximum % Finer	20%	50%
Extreme Maximum % Finer	32%	62%

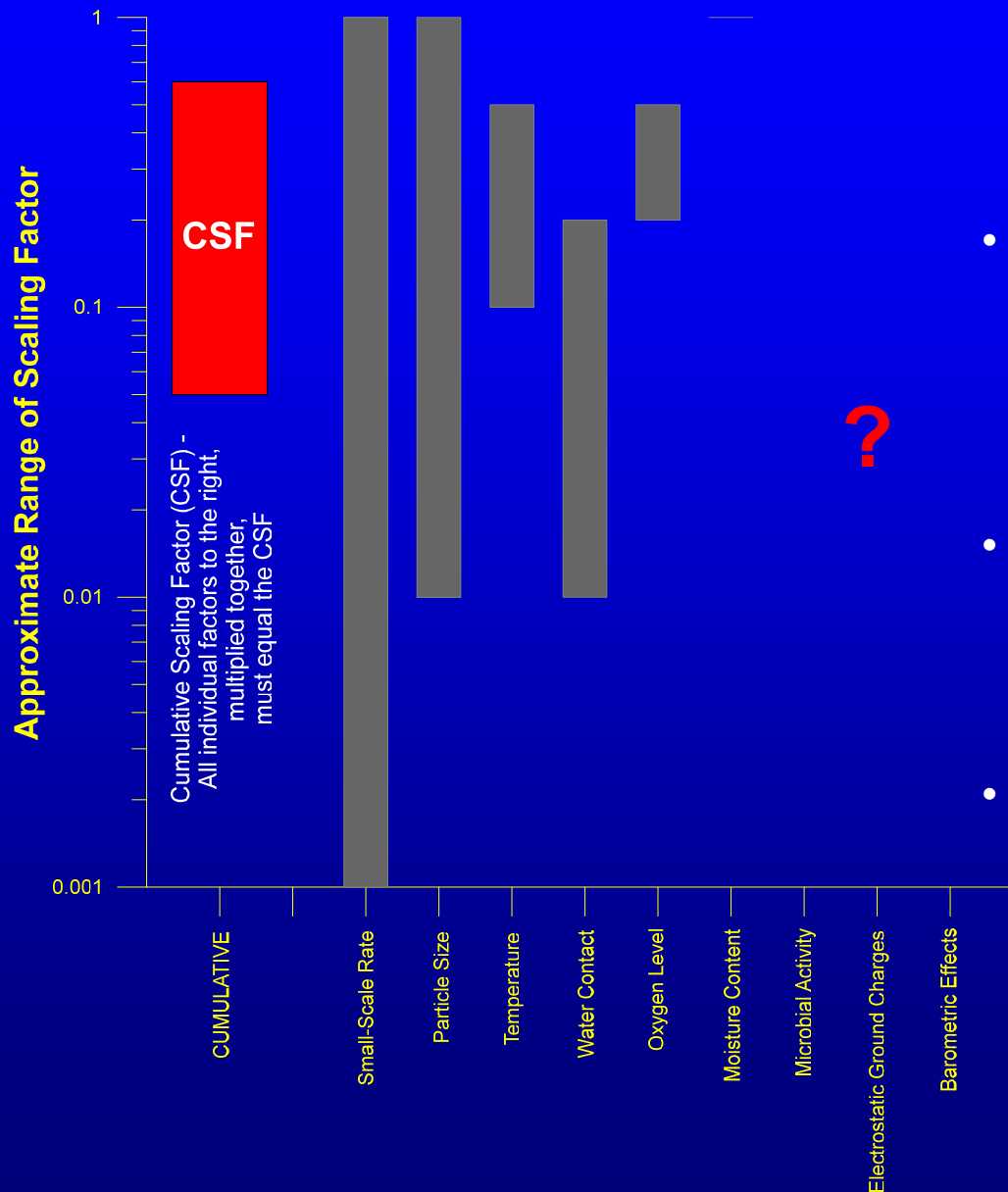
Another Factor: Temperature

- Another common scaling factor for minesite-drainage chemistry is temperature, using the “Arrhenius Equation” for sulphide oxidation. 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 and in environmental assessments is woefully misleading.
- There are many problems and misconceptions. A few are listed below.
 - The Arrhenius Equation, used to adjust sulphide-oxidation rate, is also often applied without adjustment to the leaching of every element. In any case, emergent full-scale chemistry is often independent of rate.
 - In Canada, recent environmental assessments that I have reviewed used average annual air temperature at the sites! 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.

Another Factor: Temperature

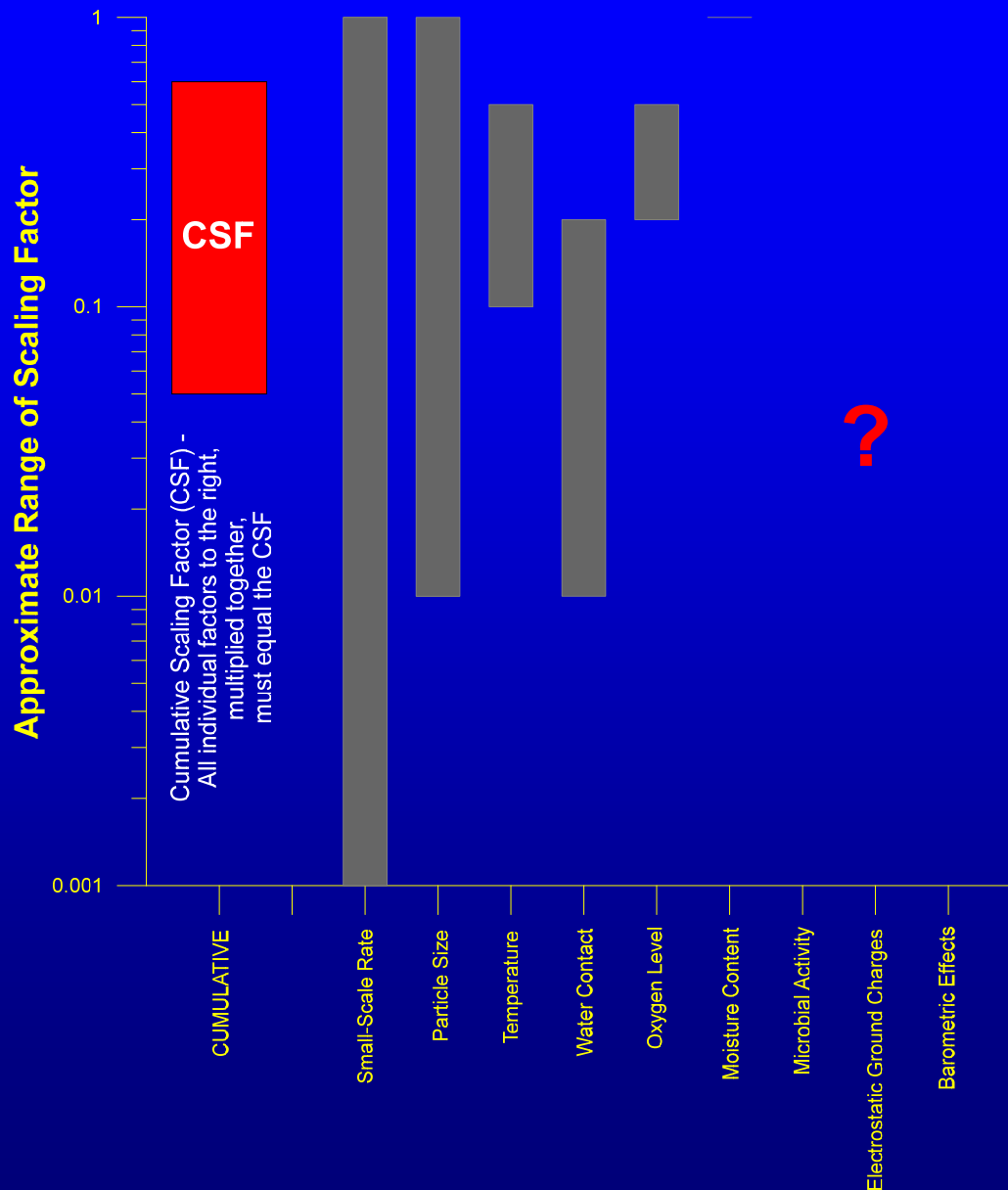
- Most people in Canada know that, under snow cover in winter, ground temperatures are often warmer than winter air temperatures. So why would winter air temperatures be included in an average annual temperature for ground conditions?
- Where sulphide oxidation occurs, the usage of any air or background ground temperatures ignores the well documented, abundant heat produced by that exothermic reaction. Furthermore, micro-scale temperatures around mineral grains does not necessarily match macro-scale atmospheric temperature.
- Thus, Canadian ML-ARD experts often underestimate the severity of full-scale drainage chemistry by using the Arrhenius Equation with these and other incorrect values and assumptions.
- In any case, for temperature differences of 10-20°C, the resulting scaling factors of 0.17-0.50 encompass the measured Cumulative Scaling Factors. Therefore, no additional scaling factors should be used if temperature correction is used.

Cumulative vs. Individual Scaling Factors



- Based on a literature reviews and studies, the general ranges of individual factors tend to overlap.
- Several factors have lowest values below measured CSF values, suggesting these lowest values should not be used.
- More importantly, the general range for each individual factor overlaps the measured CSF range.
- This means that using more than one individual factor to scale up a kinetic rate will typically underestimate the full-scale chemistry. The underprediction becomes worse as more factors are included.

Cumulative vs. Individual Scaling Factors



- Furthermore, what about all the other unexplored or undocumented factors that apply in reality under full scale?
- All these documented and undocumented factors multiplied together equal the CSF (the red bar to left). Some must be greater than 1.0.

Conclusion – Page 1 of 3

- Predictions of full-scale minesite-drainage chemistry continue to underestimate actual concentrations. This happens more than 50% of the time and thus this error is not random.
- Some younger people have told me that predictions are becoming more accurate (their optimism is refreshing!). However, I have been studying full-scale minesite-drainage chemistry for 36 years now, and sadly I find they are wrong based on the many errors still occurring. That is fact, not opinion. These errors are almost invariably underestimations, not overestimations, of full-scale concentrations, and thus the errors are not random.

Conclusion – Page 2 of 3

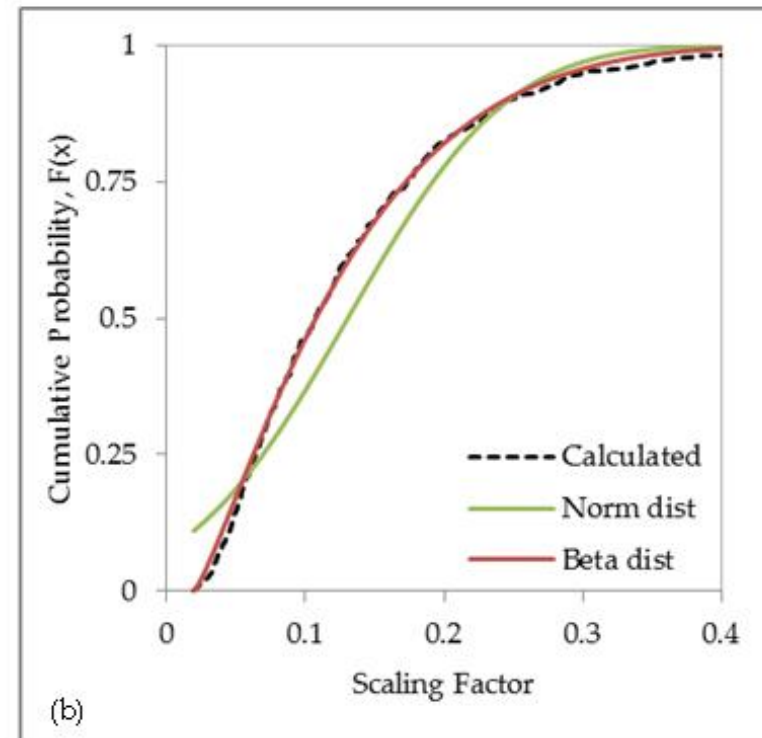
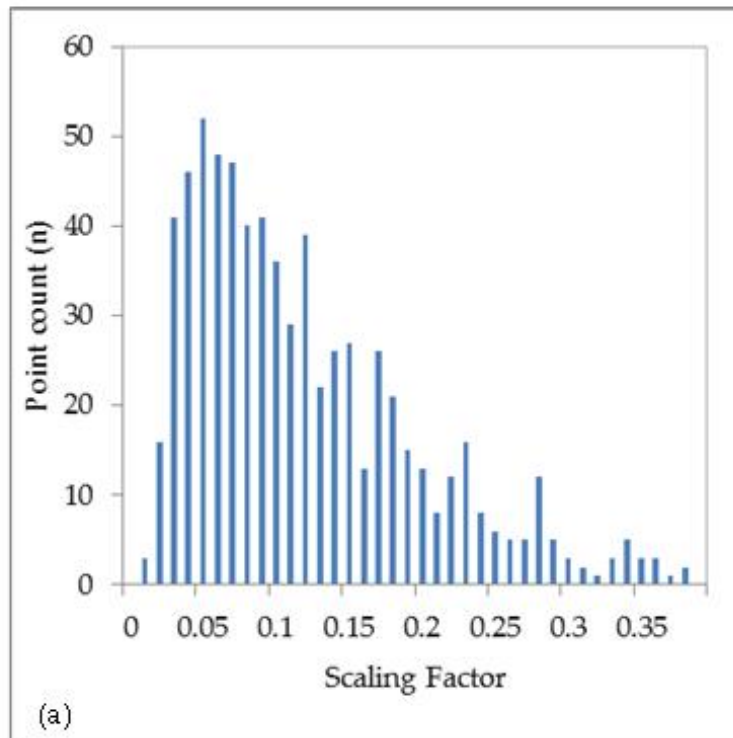
- Why is drainage chemistry typically underpredicted?
- In my opinion, one reason is that scaling/ correction/ translation/ adjustment factors are applied to small-scale kinetic tests to predict full-scale chemistry. Remember the two Important Points earlier? Above the scale transition, full-scale chemistry is instead often controlled by emergent equilibrium processes not encountered in, and independent of, most kinetic tests. Thus, small-scale kinetic rates often cannot lead to reasonable predictions of full-scale chemistry.
 - “... emergence of new structures at a high level of scale [is] difficult if not impossible to predict from constituent parts”.
- However, because it has become standard procedure, let us assume small-scale kinetic scaling factors can be used to predict drainage chemistry at any scale including emergent-controlled full-scale equilibrium chemistry.

Conclusion – Page 3 of 3

- Only a few examples of measured Cumulative Scaling Factors (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.
- Typical values of common individual scaling factors (those often considered while others remain ignored or unknown) are typically within this CSF range. As a result, a single commonly-considered scaling factor alone may reasonably represent the entire CSF used for upscaling.
- Therefore, the inclusion of additional individual factors can lead to the commonly observed underprediction of drainage chemistry.
- Additionally, some individual factors have their lowest values below the measured CSF range. These lowest values should not be used for prediction.

Conclusion Addendum: Something New and Interesting about CSF

- A new example of a measured CSF for aqueous sulphate is presented by Lapakko and Olson (submitted). In this case, the CSF is not a single value, but a statistical distribution based on 714 values. Note: this CSF is normalized to %S and weeks of testing, and thus include other scaling factors not discussed here.
 - *(Many thanks to Kim Lapakko and Michael Olson for letting me show this in advance!)*



THE END

