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KMP SO₂ EEM Program – Technical Memo W05

Power Analyses Technical Appendix

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1 Methods

1.1 Overview

We used empirically based simulation modeling to quantify the power to detect changes in lake Gran ANC, SO_4^{-2} and pH (a true positive) as well as the probability of falsely detecting changes in lake chemistry when they had not occurred (a false positive). Our overall approach (Figure 1) was to first simulate a time series of lake chemistry variables under alternative Kitimat Modernization Project (KMP) "effects" (the *signal*, reflecting a range of possible lake chemistry changes associated with a change in pH) while also incorporating the *noise* generated by natural within-year variability, between-year variability and measurement error. We then "sampled" the simulated time series to generate a data set of pre- and post-KMP lake chemistry observations. Lastly, we fit alternative models to the observed lake chemistry variables in the data set to statistically test for evidence of a KMP effect and compared the estimated KMP effect with the "*true*" KMP effect built into the model to ultimately quantifying statistical power, false negative and false positive rates. This approach was repeated across 8 different scenarios consisting of alternative combinations of KMP "effects", magnitudes of variability in lake chemistry, statistical tests to detect effects, within year sampling frequency and the inclusion of control lakes (Figure 2).



Figure 1: Conceptual diagram of the steps involved in the simulations. Boxes with dice indicate steps that included stochastic elements.



Figure 2: The eight separate scenarios considered in the power analyses. Each scenario (denoted by a number in the top left corner of the boxes) was run with and without a KMP "effect" to quantify power and false positive rates with 1 to 20 years of post-KMP observations.

1.2 Lake chemistry submodel

We simulated time series of lake chemistry variables across alternative KMP "effects" (Table 1). These "effects" describe how lake chemistry is predicted to vary in the absence of KMP influence as well as under two alternative ways in which the KMP may influence lake chemistry as:

$$\begin{aligned} X_{i,j,t,z} &= X_{i,2012-2014,j,z} + \omega_{i,t,z} + \phi_{t,z} + v_{i,t,z} + \varepsilon_{i,j,t,z}, \\ \phi_z &= N(0, \sigma_{\phi,t,z}^2), \\ v_{i,z} &= N(0, \sigma_{v,i,t,z}^2), \\ \varepsilon_{i,l,z} &= N(0, \sigma_{e,i,t,z}^2). \end{aligned}$$
(1)

where X is the true state of lake chemistry variable z (ANC, SO_4^{-2} , and pH) in lake *i*, on sampling event *j*, in year *t* and the influence of the KMP on lake *i* in year *t* is ω . We assumed variability in lake chemistry variable *z* was comprised of three independent components: among year variation common to all lakes (ϕ ; a common "year effect" due to, for example, shared regional climatic conditions), among year variation unique to each lake (υ), and within year variation unique to each lake (ε). These sources of variability were each assumed to be additive and identically and independently normally distributed with a mean of zero and variance-covariance as estimated under two alternative scenarios (Table 1 and next section). The first three observations of each simulated time series were fixed as the empirical measurements from each lake from 2012-2014. We then simulated lake chemistry variable states over the subsequent 20 years as random deviations from baseline conditions (i.e., the average of those observed in 2012-2014) due to among and within year variability plus the predicted KMP effect.

Table 1: Summary of the key components of the simulations explored in combination with one
another. Note not all possible combinations were explored see Figure 2 and Section 7 for further
details.

Component	Description
Post-KMP period	Number of years of post-KMP monitoring (1-20 years)
KMP effect	A Δ pH of 0 or -0.3 pH units and corresponding predicted change in
	ANC and SO_4^{-21} occurring either (1) abruptly one year after the KMP
	or (2) gradually (i.e., linearly) over 10 years ² .
Variability	The magnitude of inter- and intra-annual variability in the EEM lakes either (1) based on empirical estimates (as described in Section 3) or (2) with inter- and intra-annual variability reduced by an amount equal to the ratio of average Environmental Canada to EEM lake chemistry variability.
Analytic test	Either a statistical test of (1) a difference in mean lake chemistry between pre- and post-KMP periods or (2) a difference in the rate of change in lake chemistry between EEM and control lakes.
Frequency of within year sampling	Number of observations of lake chemistry during fall monitoring period (1, 3, 5 or continuous samples; only applicable to LAK006, LAK012 and LAK023).
Control lakes	The inclusion of three sensitive lakes from the North Coast that were outside the predicted KMP deposition area.
Alternative detection thresholds	Lake specific detection thresholds (0, -0.1, -0.2 or -0.3 pH unit changes and corresponding changes in Gran ANC and SO_4^{-2}) used to statistically test for a -0.3 pH unit KMP "effect".

1.3 Variance estimates

We used two datasets (Figure 3) to generate empirical estimates of inter- and intra-annual variability that were subsequently used in our simulations. The first dataset consisted of estimates of ANC, SO_4^{-2} , and pH from samples taken once each year in seven EEM lakes in 2012 (summer), 2013 (fall), and 2014 (fall) (Technical memo W01 in ESSA Technologies Ltd. 2015) as well as a single sample taken in 2013 (fall) from three sensitive lakes outside the predicted KMP deposition area which we treated as control lakes. In addition to the annual samples, three of the seven EEM lakes also had five within-season samples taken during the fall in 2014 and continuous (every half hour) monitoring of lake pH from late August to late November (Technical memo WO2 in ESSA Technologies Ltd. 2015; Perrin and Bennett 2015).

¹ The calculation of changes in ANC and SO_4^{2-} corresponding to a pH change of 0.3 pH units is explained in Appendix 2.

² Note: For the scenarios in which it is applied, the gradual KMP effect means that by 5 years post-KMP the underlying pH change is 0.15 pH units, and that by 20 years post-KMP the underlying change is 0.6 pH units. This is important to keep in mind when interpreting the results for such scenarios because it means that compared to the abrupt KMP effect, power should be much lower in earlier years (detecting a smaller effect) and much higher in later years (detecting a larger effect) – over time both the amount of data and magnitude of the effect are increasing.



Figure 3: Lake chemistry variables though time in the Environment Canada (EC) and EEM lakes.

The second data set consisted of lake chemistry data (total alkalinity, SO_4^{-2} , and pH) from 10 lakes monitored by Environment Canada and sampled between 2005 and 2014 in southwestern British Columbia (Pat Shaw, personal communication). We converted total alkalinity from the Environment Canada dataset into Gran ANC according to the relationship between the two metrics as described in ESSA et al. (2014a) (Gran ANC = [total alkalinity -11.589]/1.0124; R²=0.9987).

Shared inter-annual variation

To generate an estimate of the proportion of inter-annual variability that we should simulate as being comprised of a shared "year effect" for each lake chemistry variable we fit generalized linear mixed effects models (Pinheiro and Bates 2000) to the lake chemistry data from the Environment Canada lakes. There were not a sufficient number of years of data from the EEM lakes to fit equation 2. The model took the form:

$$Y_{i,j,t,z} = b_z + \theta_{lake,z} + \theta_{year,lake,z} + \varepsilon_{i,z},$$

$$\theta_{lake,z} = N(0, \sigma_{lake,z}^2),$$

$$\theta_{year,z} = N(0, \sigma_{year,z}^2),$$

$$\theta_{year,lake,z} = N(0, \sigma_{year,lake,z}^2),$$

$$\varepsilon_{i,z} = N(0, \sigma^2).$$

(2)

where Y is the observed value of lake chemistry variable z taken from lake i in year t, b is the average of lake chemistry variable z across years and lakes, and the remaining terms capture four independent components of observed variation: (1) variation due to persistent differences among lakes ($\theta_{lake,z}$), (2) variation due to synchronous or coherent yearly variation among lakes (i.e., common year effects; $\theta_{year,z}$), (3) unique or non-synchronized inter-annual variation among lakes ($\theta_{year,lake,z}$), and (4) residual variation ($\varepsilon_{i,z}$) due to, for example, measurement error or intra-annual variation. Based on the Environment Canada lakes, the estimated proportion of inter-annual variability that would be expected to be due to shared year effects ($p_{shared,z}$) was then estimated as $\theta_{year,z}/(\theta_{year,z} + \theta_{lake;year,z})$ and corresponded to 0.28, 0.09, and 0.11 for ANC and SO₄⁻², and pH, respectively.

To generate a common year effect in our simulated time series a single draw from a multivariate normal distribution with variance and co-variance equal to the average scaled (i.e., standard deviation units) variance-covariance matrix for the EEM lakes was taken and multiplied by $p_{shared,z}$. The resulting scaled year effect for each lake chemistry variable was then applied to each lake by multiplying the scaled year effect by the lake chemistry variable standard deviation for each individual lake to generate a raw estimate of the shared deviation in a given year (i.e., ϕ in equation 1). For the control lakes, which did not have empirical variance-covariance estimates because there was only one year of observations, we used the average variance covariance matrix from the Environment Canada lakes.

Unique inter-annual variation

To generate unique, lake specific random deviations (i.e., $v_{i,z}$ in equation 1), in each year of the simulated time series we drew a random deviation for each lake chemistry variable from a multivariate normal distribution with variance and co-variance as estimated for each EEM lake. As described above, control lake deviations were drawn from a variance-covariance matrix that was the average of the Environment Canada lakes. The lake specific deviations were then multiplied by $1 - p_{shared,z}$ to account for the fact that they only make up a portion of total inter-annual variation in a given year.

Intra-annual variation

For the three EEM lakes with estimates of intra-annual variation (LAK006 (End Lake), LAK012 (Little End Lake) and LAK023 (West Lake)), intra-annual variation was simulated as draws from a multivariate normal distribution with variance and co-variance as estimated for each lake. The four EEM and three control lakes without empirical estimates of intra-annual variability were assigned the average variance-covariance from LAK006 and LAK023 based on their similar water residence times, which is assumed to be an important determinant of variation in lake chemistry. LAK012 (Little End Lake) was not used to inform the simulation of intra-annual variation in the lakes without empirical estimates because the available evidence suggests that its intra-annual dynamics are fundamentally different than the other lakes and therefore not representative of the EEM lakes in general. The estimated intra-annual variability for LAK012 was considerably larger than LAK006 and LAK023 and its water residence time is substantially different from both the two other lakes with intra-annual sampling and all of the other lakes.

Alternative variation scenario

It is possible that the short time series used to estimate within and among year variation in the EEM lakes resulted in over-estimates of "true" natural variation in lake chemistry. We therefore also considered an alternative variation scenario where shared and unique inter-annual variation as well as intra-annual variation were reduced by an amount equal to the ratio of Environmental Canada to

EEM lake chemistry variability. This correction corresponded to a ratio of 0.003, 0.001 and 0.44 for Gran ANC, SO_4^{-2} , and pH respectively.

1.4 Observation submodel

We simulated lake chemistry observations from each lake as:

$$Y_{i,j,t,z} = X_{i,t,z} + \delta_{z,s},$$

$$\delta_{z,s} = N(0, \sigma_{\delta_{j,j,z,s}}^2).$$
(3)

where *Y* is the observed value of lake chemistry variable *z* taken in sampling event *j* from lake *i* in year *t* and δ is measurement error associated with methodology *s* to quantify lake chemistry variable *z*. We assumed that Gran ANC and SO_4^{-2} both had measurement error equal to a 10% coefficient of variation (CV) (Perrin and Bennett 2015) while pH had a measurement error equal approximately a 3% CV (+/- 0.2 pH units; Perrin and Bennett 2015).

1.5 Analysis submodel

We used two alternative statistical models to test for KMP effects in the simulated lake chemistry time series. The first model tested whether there was a difference in mean lake chemistry between pre- and post-KMP observations (i.e., 2012-2014 vs. 2015 onward). Specifically, we fit a general linear model to the data generated from the observation submodel:

$$Y_{i,j,t,z} = \beta_{0,z} + \beta_{1,z} X_{postKMP} + \gamma_{i,j,t,z},$$

$$\gamma_{i,j,t,z} = N(0, \sigma^2).$$
(4)

where $\beta_{0,z}$ is the average of lake chemistry variable z prior to the KMP, $\beta_{l,z}$ is the difference between the average lake chemistry variable z pre- and post-KMP and $X_{postKMP}$ is a dummy variable to identify post-KMP observations.

The second statistical model we used tested whether there was a difference in the rate of change in lake chemistry over time between control and EEM lakes. Specifically we fit a general linear mixed effects model to the data generated from the observation submodel:

$$Y_{i,j,t,z} = \beta_{0,l,z} + \theta_{year,z} + \theta_{lake,z} + \beta_{1,l,z} X_{KMP,t} + \gamma_{i,j,t,z},$$

$$\theta_{lake,z} = N(0, \sigma_{lake,z}^2),$$

$$\theta_{year,z} = N(0, \sigma_{year,z}^2),$$

$$\gamma_{i,l,t,z} = N(0, \sigma^2).$$
(5)

where $\beta_{0,l,z}$ is the average of lake chemistry variable z in lake group l (control or EEM) in 2014 prior to the KMP (the intercept), $\beta_{1,l,z}$ is the per year rate of change in lake chemistry variable z in lake group l (the slope), and γ is residual error. The terms $\theta_{lake,z}$ and $\theta_{year,z}$ were included to capture variation among lakes due to intrinsic differences in baseline lake chemistry and random variation in lake chemistry common to all lakes among years both of which were assumed to normally distributed with a mean of zero and variance that was estimated.

1.6 Multiple lake chemistry observations per year

For simulations where we explored the influence of multiple within-year sampling events on statistical power, false positives and false negatives, equations 3 and 4 were modified to include a within-year random effect, and fit as a general linear mixed model to account for the non-independence of observations within years. These simulations were performed for lakes LAK006, LAK012 and LAK023, all of which can be sampled multiple times per year, for either 3 or 5 sampling events each fall.

We also quantified power, false positives and false negatives for the same lakes assuming continuous monitoring of pH during the fall period using Manta pH meters³. Empirical observations of lake pH were collected every half hour continuously from late August to late November in 2014 (Perrin and Bennett 2014). The Manta meter has three probes that each detect lake pH. We averaged the pH estimates across the probes for each half hour interval for the 2014 observations and then took a subset of the continuous data to provide an observation every 6 hours. We then simulated the same number of observations post-KMP to quantify power and false positives rates based on continuous monitoring. As with the simulations above for 3 or 5 samples per fall, we fit a general linear mixed model to account for the non-independence of observations within years. We did not simulate temporal autocorrelation in the post KMP "observations" and so did not include an autocorrelated error structure in the model we fit to the simulated time series. However, we note that there was clear evidence of temporal autocorrelation in the 2014 continuous pH measurements.

1.7 Alternative thresholds for detecting KMP effect

To explore how increasing the threshold for detecting a KMP effect affected power while reducing false positives we also ran simulations under alternative lake chemistry thresholds for classifying lakes as having been affected by the KMP. Specifically, we considered changes of -0.1, -0.2 and -0.3 pH units and corresponding change in ANC and for SO_4^{-2} , as alternative thresholds (Figure 4). These thresholds were added to post-KMP observations so as to test whether the observed change was of a larger magnitude than the threshold change. For example, if the estimate for $\beta_{1,l,z}$ in equation 5 was significantly greater than 0 for SO_4^{-2} (at $\alpha = 0.1$ because it is a one-tailed hypothesis test), after the threshold value had been applied to the post-KMP observation, then the estimated change in SO_4^{-2} could be said to be significantly greater than the threshold value.

1.8 Quantifying error rates

We quantified power, the rates of false positives and the rates of false negatives across a range of observation windows (i.e., number of years of observations) across the eight scenarios covering alternative combinations of KMP effect, variance and statistical models to test for KMP effects (Figure 2). For all scenarios we ran 1000 Monte Carlo trials and scored the outcome of each trial as one of 4 possible classifications (Figure 4):

³ Perrin and Bennett (2014) compared the different methods of measuring pH to determine whether there were significant differences among methods. For the methods relevant to the current work (i.e., Manta continuous meters and lab-based measurements for the annual and within-season samples), they concluded that there is no instrument effect – the differences were less than the reported measurement error of the instruments and not statistically significant.

<u>**True positive**</u>: the analysis submodel correctly detected a KMP induced change in lake chemistry as large or larger than the detection threshold.

<u>**True negative**</u>: the analysis submodel correctly did not detect a KMP induced change in lake chemistry as large or larger than the detection threshold.

<u>False positive</u>: the analysis submodel incorrectly detected a KMP induced change in lake chemistry as large or larger than the detection threshold.

<u>False negative</u>: the analysis submodel failed to detect a KMP induced change in lake chemistry, as large or larger than the detection threshold, that had actually occurred.

To quantify power for scenarios that involved simulating KMP effects on lake chemistry we calculated the proportion of Monte Carlo trials that were true positives. To quantify false positive rates for scenarios that involved no simulated KMP effect on lake chemistry we calculated the proportion of Monte Carlo trials that were false positives.



Figure 4: The four possible classifications for each Monte Carlo trial based on a simulated -0.3 pH unit KMP effect. The terms α , β , and $1 - \beta$ are equivalent to type I error, type II error, and power in traditional hypotheses testing.

2 Results

This section includes descriptions and graphical illustrations of the results of the analyses. Appendix 1 includes tables of all of the results for all of the lakes for each scenario, at 3, 5 and 10 years post-KMP. The results for 3 years post-KMP most closely align with the end of the final year of monitoring in the present phase of the EEM (i.e., 2018). Although KMP was initiated in 2015, it is likely that the timing and phased nature of the implementation of KMP will mean that 2015 annual emissions are not meaningfully different than 2014. It is therefore expected that 2016 will be the first truly "post-KMP" year of monitoring.

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2.1 Lake chemistry variability



In general, for those EEM lakes with empirical observations, lake chemistry was more variable among year than within years, particularly for Gran ANC and SO_4^{-2} (

Figure 5). Both within and among year variability tended to be largest for SO_4^{-2} followed by Gran ANC and then pH. There was considerable variability among lakes within each lake chemistry variable (Figure 5). In contrast, lake chemistry variability in the Environment Canada lakes was much lower than the EEM lakes, particularly for Gran ANC and SO_4^{-2} (Figure 5 and Figure 6).



Figure 5: Inter- and intra-annual coefficients of variation for each lake chemistry variable from EEM lakes for which there were empirical observations.



Figure 6: Inter-annual coefficients of variation for each for each lake chemistry variable from EEM and Environment Canada (EC) lakes as well as the average for each group of lakes.

2.2 Detecting abrupt change in lake chemistry under alternative variance

assumptions

Changes in Gran ANC and SO_4^{-2} were easier to detect than changes in pH. For most EEM lakes, within about 5 years of post-KMP monitoring, there was high power (i.e., > 0.8) to detect changes in Gran ANC and SO_4^{-2} that corresponded to an abrupt -0.3 pH unit change (Figure 7A and Appendix 1). However, those lakes with the greatest among and/or within year variability in Gran ANC and SO_4^{-2} , and/or relatively modest changes in Gran ANC and SO_4^{-2} that corresponded to a - 0.3 pH unit change (see Table 2), had low (i.e., < 0.2) or moderate (< 0.8) power regardless of the number of years of post-KMP observations. In contrast, all lakes had low to moderate power to detect an abrupt -0.3 unit change in pH (Figure 7A and Appendix 1).

Table 2. Baseline measures of pH, ANC and SO₄⁻² and changes associated with a -0.3 pH unit change (ΔpH), and per year change assuming a -0.3 pH unit change after 10 years (ΔpH yr⁻¹), for each of the 7 acid-sensitive lakes in the EEM program.

Lake	Baseline ¹ pH	∆рН	∆pH yr ⁻¹	Baseline Gran ANC	∆Gran ANC ²	∆Gran ANC yr ⁻¹	$\begin{array}{c} \textbf{Baseline} \\ \text{SO}_4^{-2} \end{array}$	$\Delta \mathrm{SO}_4^{-2}$	ΔSO_4^{-2} yr ⁻¹
LAK006	6.1	-0.3	-0.03	30.49	-16.3	-1.63	12.99	20.67	2.07
LAK012	6.1	-0.3	-0.03	66.97	-33.91	-3.39	8.61	54.25	5.43
LAK022	6.1	-0.3	-0.03	37.02	-19.37	-1.94	39.33	29.48	2.95
LAK023	5.9	-0.3	-0.03	26.36	-14.41	-1.44	20.54	18.81	1.88
LAK028	5.2	-0.3	-0.03	7.82	-7.29	-0.73	94.34	18.95	1.90
LAK042	5.1	-0.3	-0.03	4.35	-6.77	-0.68	6.2	7.8	0.78
LAK044	5.6	-0.3	-0.03	5.24	-6.85	-0.69	6.37	7.14	0.71

¹ baseline values are the average of samples taken in 2012-2014

² change in lake chemistry value corresponding to a -0.3 pH unit change



Figure 7: Power to detect a -0.3 unit change in pH, and corresponding changes in Gran ANC and SO₄⁻², both individually and in combination, under alternative variance scenarios (A: inter-annual EEM lake variability; B: inter-annual EC lake variability). Power is defined here as the proportion of 1000 Monte Carlo trials where a statistical model that tested for a pre- vs. post-KMP difference in mean lake chemistry correctly estimated a significant change (Scenarios 1 and 2 in Figure 2). False positive rates for the same scenarios but for simulations without a KMP effect are presented in panel C (assuming EEM lake variability) and D (assuming EC lake variability), respectively.

False positive rates for all three lake chemistry variables were very low (i.e., < 0.02) with the exception of SO₄⁻² which had false positive rates as high as 0.3 after 1 year of post-KMP observations before dropping rapidly to less than 0.1 within 5 years (Figure 7C and Appendix 1).

Considering all three lake chemistry variables simultaneously (i.e., only saying a change in lake chemistry had truly occurred if it had been detected in all three lake chemistry variables) led to lower or equal power relative to any single lake chemistry variable, but also eliminated the chance of a false positive occurring (Figure 7C and Appendix 1).

Changes in lake chemistry are easier to detect when there is less natural variation. For simulations that assumed that magnitude of natural variability in lake chemistry is best approximated by that observed in the EC lakes, as opposed to the EEM lakes, power was higher for any given lake after a given number of years of observations (Figure 7B and Appendix 1). However, these improvements in power were not as large as might be expected based on the magnitude of the reduction in assumed among year variation from the EEM to EC lakes (i.e., 99%, 99%, and 56% for Gran ANC, SO_4^{-2} and pH, respectively), because within year variation remained the same in both scenarios. False positive rates did not differ appreciably under the two alternative variance scenarios (Figure 7C and Appendix 1).

2.3 Detecting gradual changes in lake chemistry with and without control lakes

Gradual changes in lake chemistry were harder to detect than abrupt ones. When lake chemistry was simulated to change gradually over time, i.e., by -0.3 pH units every ten years as opposed to abruptly one year after the KMP, power to detect true changes in lake chemistry was lower (Figure 8A), and false positives were higher (Figure 8C and Appendix 1), for any given number of post-KMP observations (compare to panels A and C in Figure 7). For example, after 10 years, power to detect a linear increase in pH of -0.3 units was only ~ 20% for any given lake compared to ~40% for most lakes when pH changed abruptly one year after the KMP. These reductions in power occurred because it is harder to detect a gradual change in lake chemistry as opposed to an abrupt one. False positive rates were higher when lake chemistry changed gradually because natural variation, particularly for SO_4^{-2} , led to a higher probability of chance variation leading to the appearance of gradual change, when none had actually occurred.

Control lakes helped detect changes in lake chemistry, but not a lot. The inclusion of control lakes, which help to isolate shared regional variation in lake chemistry due to natural processes from changes due to the KMP, resulted in increased power to detect a KMP effect, relative to simulations without control lakes. However, increases in power were minor and most pronounced during the first couple of years of post-KMP observations (Figure 8A vs. B). The relatively modest benefit of including control lakes in the analysis was due to the fact that the simulated degree of regional coherence in lake chemistry variability (i.e., shared year "effects"), as estimated from the EC lakes where there was sufficient data to try and quantify it, was small (28%, 9%, and 11% for ANC and SO_4^{-2} , and pH, respectively). As a result the benefit of accounting for regional variation was also small. However, the risk of incorrectly detecting a KMP induced change in lake chemistry, particularly for SO_4^{-2} , was higher than when control lakes were considered. This arose because, with small shared year effects, natural variation in the chemistry of control lakes increased the probability of the appearance of a gradual change in lake chemistry in the EEM lakes when none had actually occurred.



Figure 8: Power to detect a linear rate of change in lake chemistry corresponding to a -0.3 unit change in pH every 10 years, both for individual lake chemistry variables and for all three in combination without (A) and with (B) the inclusion of control lakes. Power is defined here as the proportion of 1000 Monte Carlo trials where a statistical model that tested for positive (SO₄²⁻) or negative (Gran ANC and pH) rates of change in lake chemistry estimated a significant change (Scenarios 3 and 5 in Figure 2). False positive rates for the same scenarios but for simulations without a KMP effect are presented in panel C (without control lakes) and D (with control lakes). Note that the gradual linear change continues throughout the entire period (i.e., by 20 years, the underlying change has doubled from 10 years) and therefore the power increases substantially in later years for all the metrics because there is a much larger underlying effect to detect.

2.4 Applying the "wrong" statistical model to detect changes in lake

chemistry

Applying the wrong statistical test to detect KMP induced changes in lake chemistry resulted in reduced power. Specifically, testing for a difference in mean lake chemistry from before to after



2.5 Multiple within-year samples

Increasing the number of samples collected during the fall increased power to detect change in lake chemistry (Figure 10 and Appendix 1). The benefits of increased sampling were most pronounced for pH where increasing the numbers of samples from 1 to 5 doubled the power to detect a KMP induced change in pH. The benefit of increased sampling during fall was most pronounced when only a few years of post-KMP monitoring had occurred. However, these increases in power came at the cost of increased false positive rates when there were less than 5 years of post-KMP observations. This occurred because additional samples resulted in increased variability within years which, when there were only a few years of post-KMP observations, resulted in the appearance of a change in lake chemistry when in fact there was none.

Continuous monitoring of lake pH led to increase in power to detect true changes in pH for the three lakes for which continuous monitoring is currently possible (Table 7a). However, these increases in power were less pronounced than the benefits of increasing sampling from 1 to 3 samples per fall and they came at the cost of increased false positives rates relative to only a few fall samples of lake chemistry (Table 7b).

For the three lakes with multiple samples and continuous monitoring, increasing sampling from 1 to 3 samples per fall increased power by 1.5-2.6 times. Although the benefit of increasing from 5 samples to continuous monitoring is least for LAK012 (1.1x, compared to 1.3-1.4x), it shows by far the greatest benefit of increasing sampling from 1 to 3 samples per fall (power increases by 2.6x). However, even though the increase in power is less than for the other two lakes, the increase in power due to continuous monitoring is important for LAK012 because even with the multiple/continuous sampling, its power for detecting changes in pH is still much lower than most of the other lakes.

2.6 Alternative detection thresholds

Increasing the threshold for detecting a KMP induced change in lake chemistry, from -0.1 to -0.3 pH units, reduced false positive rates but at the cost of reduced power (Figure 11A and Appendix 1). For example, in LAK022, which had the highest false positives rates of any of the lakes, increasing the detection threshold to 0 to -0.1 pH units (and corresponding changes in Gran ANC and SO_4^{2-}) reduced false positive rates to near zero within the first few years of post-KMP observations (Figure 11B and Appendix 1) but also reduced power substantially. However, the

3 Discussion Points

This section includes discussion points regarding the results of the power analyses. Most of these points are addressed in the discussion section of the summary report; however, the text below includes further details on some of these points as well as some more detailed observations.

- Power to detect KMP induced changes in lake chemistry increased with the numbers of years of post-KMP observations and was highest for Gran ANC followed closely by SO₄²⁻ and then pH, which had the lowest power of the other lake chemistry variables considered. False positives were low for all lake chemistry variables except when there was only a few post-KMP observation of SO₄²⁻.
- Variability in power and false positives among lake chemistry variables, and among lakes, was due to differences in inter- and intra-annual variation in lake chemistry and the magnitude of the change in lake chemistry that corresponded to a -0.3 unit pH change (e.g., for a -0.3 pH unit change some lakes like LAK012 had a much larger magnitude change in Gran ANC than others like LAK042).
- Not surprisingly, it was easier to detect a rapid change in lake chemistry than a gradual change of the same magnitude but over ten years.

- Considering all three lake chemistry variables simultaneously when testing for a KMP effect, led to lower or equal power relative to any single lake chemistry variable, but also lower false positives. Because false positives were already very low in most cases there does not appear to be much benefit to considering all three lake chemistry variables together.
- The inclusion of control lakes increased power to detect changes in lake chemistry for the first few years of post-KMP observations but thereafter had little benefit relative to analyses without controls. The modest benefit of control lakes occurred because the degree of regional coherence in lake chemistry variability (i.e., shared year "effects"), as estimated from the EC lakes where there was sufficient data to try and quantify shared regional variation in lake chemistry, was relatively small. If the true degree of shared regional variation in lake chemistry is higher than that assumed in our analysis the benefit of controls would be expected to be more pronounced.
- An additional benefit of the control lakes is that they allow for ongoing monitoring of the magnitude of natural inter-annual variability in lake chemistry that would be predicted to occur in the region. Because the estimates of lake chemistry variability used in the power analyses were based on the EEM lakes, which could be confounded by the effects of the pre-KMP emissions, these estimates of natural variation from the control lakes should help to inform future power analyses and interpretations of monitoring data.
- False positive rates were low for Gran ANC and pH but higher for SO₄²⁻ when only a few years of post-KMP observations were analyzed. False positive rates were highest when lake chemistry was simulated to change gradually, especially when the "test" for a KMP effect was incorrectly based on testing for a difference of means.
- Applying the wrong statistical test to lake chemistry data (i.e., testing for a difference in means when the true change is gradual over time) led to reduced power. This highlights that the statistical test that is used to test for KMP effects on lake chemistry should be based on the observed changes in emission from the smelter such that if there is abrupt change in emission a before-after type statistical comparison should be made. However, if changes in emissions are observed to be more gradual then testing for significant rates of change in lake chemistry over time would be more appropriate.
- Increasing sampling frequency increased power but also came at the cost of high false positives for the first few years of post-KMP monitoring. The benefit of increased sampling was greatest for pH and most pronounced for the first few years of post-KMP observations.
- Most scenarios had low or very low false positives rates. The exception was detecting gradual changes over time when control lakes were also considered. Increasing the detection threshold used in the statistical tests reduced false positives but also came at the cost of reduced power. However, the reductions in power were most pronounced after numerous years of post-KMP observations while the reduction in false positives were most pronounced with only a few post-KMP observations.
- Monitoring and analysis recommendations that emerge from the analyses include:
 - Use Gran ANC as the primary indicator of KMP induced change in lake chemistry because it had a higher power to detect true changes than pH but lower false positive rate than SO₄²⁻ (i.e., it is the "Goldilocks" lake chemistry variable).
 - For some lakes we are going to have to accept that we are not likely to ever have high power to detect KMP induced changes:
 - LAK028 low power for ANC and SO_4^{2-}
 - LAK042 low power for ANC and pH (and 2nd/3rd lowest for SO_4^{2-} , though at moderate level)

- LAK012 low power for pH (but already a continuous monitoring site, which is helping)
- LAK044 typically next lowest for ANC (2nd/3rd) for ANC and SO_4^{2-} (2nd) but at moderate power (for abrupt change), though power is low for gradual KMP; similar to others re: pH.
- Continue taking continuous and multiple samples from those lakes where it is logistically feasible.
- Generally speaking, there is not a clear need to use detection thresholds greater than 0 because false positives were so low without having to increase the detection threshold and doing so led to fairly pronounced losses in power.
- Continue with control lakes, primarily to characterize natural variability in the system.
- There was clear evidence of autocorrelation in the 2014 continuous pH monitoring data (i.e., the pH observation were dominated by low-frequency variability). We did not simulate autocorrelation in the post KMP pH observation in our analyses but we recommend the incorporation of autocorrelation into both simulated data and the error structure of the statistical model fit to the data to test for a KMP effect be considered in subsequent power analyses and actual analyses of empirical data. The presence of autocorrelation violates the assumption of serial independence required for most classical statistical tests (Hurlbert 1984). A consequence of this is that the correlation between two variables has fewer degrees of freedom (or a larger variance) than that assumed under the classical significance test. Consequently, autocorrelation can lead to an increased Type I error rate or increased chance of concluding that a correlation is statistically significant when in fact no correlation is present).

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5 Appendix 1: Summary of Results

The following tables summarize the results of the power analyses for each of the scenarios. Each table has two sub-tables for power and false positive rates. For each lake and metric, results are shown for 3, 5 and 10 years of post-KMP observations. Note that "0.00" indicates a non-zero value that rounds to 0.00 (i.e., <0.005), whereas "-" indicates a true zero value (i.e., 0.000).

Table 2: Power (A) and false positives (B) for individual lake chemistry variables, and in combination for each EEM lake at 3, 5 and 10 years of post KMP monitoring under the conditions assumed in Scenario 1.

(A) Power	
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Laka	ANC			SO4				рН		combined			
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	
LAK006	0.95	0.99	1.00	0.99	1.00	1.00	0.22	0.29	0.31	0.20	0.29	0.31	
LAK012	0.75	0.87	0.98	1.00	1.00	1.00	0.10	0.09	0.13	0.10	0.09	0.13	
LAK022	0.77	0.94	1.00	0.95	0.99	1.00	0.34	0.37	0.47	0.28	0.35	0.47	
LAK023	0.60	0.82	0.98	0.91	0.97	1.00	0.33	0.37	0.44	0.23	0.34	0.44	
LAK028	0.03	0.06	0.07	0.04	0.05	0.05	0.31	0.37	0.43	-	-	-	
LAK042	0.01	0.01	0.01	0.51	0.51	0.54	0.09	0.11	0.14	0.00	0.01	0.01	
LAK044	0.50	0.65	0.83	0.46	0.43	0.46	0.33	0.36	0.42	0.10	0.11	0.17	

(B) False positives

Lako	ANC			SO4			рН			combined		
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
LAK006	0.00	0.00	0.00	0.05	0.03	0.00	0.02	0.01	-	-	-	-
LAK012	0.02	0.01	0.00	0.07	0.02	0.00	0.01	0.01	0.00	0.00	0.00	-
LAK022	0.00	0.00	-	0.02	0.01	0.00	0.02	0.01	0.00	-	-	-
LAK023	0.00	0.00	-	0.04	0.01	0.00	0.02	0.01	-	-	-	-
LAK028	-	0.00	0.00	0.00	0.01	0.00	0.03	0.01	0.00	-	-	-
LAK042	0.00	0.00	0.00	0.07	0.02	0.00	0.00	0.01	0.00	-	-	-
LAK044	0.01	0.01	-	0.08	0.04	-	0.03	0.01	0.00	-	-	-

Table 3: Power (A) and false positives (B) for individual lake chemistry variables, and in combination for each EEM lake at 3, 5 and 10 years of post KMP monitoring under the conditions assumed in Scenario 2.

(A) Power												
Laka	ANC			SO4				рН		combined		
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
LAK006	1.00	1.00	1.00	0.98	1.00	1.00	0.29	0.44	0.63	0.29	0.44	0.63
LAK012	1.00	1.00	1.00	1.00	1.00	1.00	0.07	0.19	0.36	0.07	0.19	0.36
LAK022	1.00	1.00	1.00	1.00	1.00	1.00	0.40	0.57	0.73	0.39	0.57	0.73
LAK023	0.98	1.00	1.00	0.97	1.00	1.00	0.41	0.54	0.73	0.38	0.54	0.73
LAK028	-	0.00	0.39	-	-	0.37	0.42	0.54	0.73	-	-	0.11
LAK042	-	-	-	0.48	0.54	0.59	0.05	0.15	0.34	-	-	-
LAK044	0.72	0.94	1.00	0.48	0.45	0.49	0.42	0.55	0.72	0.15	0.24	0.36

(B) False positives

Lako	ANC			SO4			рН			combined		
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
LAK006	-	-	-	0.06	0.02	0.00	0.01	0.00	-	-	-	-
LAK012	-	-	-	0.03	0.02	0.01	0.00	0.00	-	-	-	-
LAK022	-	-	-	0.00	0.00	0.00	0.01	0.01	0.00	-	-	-
LAK023	-	-	-	0.03	0.02	0.01	0.01	0.01	-	-	-	-
LAK028	-	-	-	-	-	-	0.01	0.01	0.00	-	-	-
LAK042	-	-	-	0.08	0.03	0.00	-	0.00	-	-	-	-
LAK044	0.00	-	0.00	0.07	0.03	0.00	0.02	0.01	0.00	-	-	-

Table 4: Power (A) and false positives (B) for individual lake chemistry variables, and in combination for each EEM lake at 3, 5 and 10 years of post KMP monitoring under the conditions assumed in Scenario 3.

Power

Lako	ANC			SO4				рН		combined		
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
LAK006	0.09	0.21	0.95	0.33	0.58	0.99	0.01	0.03	0.16	-	0.02	0.16
LAK012	0.10	0.16	0.70	0.46	0.81	1.00	0.01	0.02	0.08	0.01	0.01	0.08
LAK022	0.02	0.06	0.75	0.22	0.58	0.99	0.05	0.06	0.28	-	0.01	0.24
LAK023	0.04	0.06	0.55	0.21	0.42	0.94	0.04	0.06	0.26	-	0.01	0.19
LAK028	0.01	0.01	0.02	0.07	0.15	0.35	0.04	0.07	0.25	-	-	0.01
LAK042	-	0.00	0.01	0.16	0.19	0.48	0.01	0.02	0.12	-	-	0.00
LAK044	0.03	0.07	0.47	0.16	0.19	0.44	0.05	0.05	0.26	-	0.00	0.08

False positives

Lake		ANC		SO4			pH			combined			
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	
LAK006	0.02	0.01	0.00	0.12	0.08	0.07	0.01	0.01	0.01	-	-	-	
LAK012	0.03	0.01	0.01	0.10	0.07	0.07	0.00	0.01	0.01	-	-	0.00	
LAK022	0.01	0.00	0.00	0.06	0.08	0.11	0.02	0.01	0.02	-	-	-	
LAK023	0.01	0.01	0.00	0.08	0.05	0.04	0.02	0.01	0.01	-	-	-	
LAK028	0.01	0.00	-	0.04	0.07	0.12	0.03	0.01	0.02	-	-	-	
LAK042	-	-	0.00	0.11	0.07	0.05	0.00	0.00	0.01	-	-	-	
LAK044	0.01	0.01	0.02	0.12	0.06	0.05	0.03	0.02	0.01	-	-	-	

Table 5: Power (A) and false positives (B) for individual lake chemistry variables, and in combination for each EEM lake at 3, 5 and 10 years of post KMP monitoring under the conditions assumed in Scenario 4.

(A) Power												
Laka		ANC			SO4			рН			combined	
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
LAK006	0.03	0.13	0.53	0.20	0.23	0.58	0.04	0.04	0.04	0.00	0.00	0.01
LAK012	0.08	0.11	0.24	0.30	0.39	0.80	0.03	0.03	0.02	0.01	0.02	0.02
LAK022	0.01	0.05	0.31	0.07	0.14	0.50	0.05	0.05	0.06	-	0.00	0.01
LAK023	0.02	0.03	0.20	0.12	0.14	0.39	0.05	0.04	0.07	0.00	-	0.01
LAK028	0.00	0.01	0.01	0.01	0.01	0.01	0.04	0.05	0.04	-	-	-
LAK042	0.00	0.00	0.00	0.13	0.09	0.10	0.01	0.01	0.01	-	-	-
LAK044	0.02	0.06	0.13	0.13	0.08	0.07	0.05	0.07	0.06	-	-	-

(B) False positives

Lake		ANC			SO4			pH			combined			
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years		
LAK006	0.01	0.01	0.00	0.07	0.03	0.01	0.02	0.01	0.00	-	-	-		
LAK012	0.02	0.01	0.00	0.06	0.02	0.00	0.01	0.01	-	0.00	0.00	-		
LAK022	0.00	-	-	0.02	0.01	0.00	0.03	0.01	0.00	-	-	-		
LAK023	0.00	0.00	-	0.04	0.02	-	0.02	0.01	0.00	-	-	-		
LAK028	-	0.00	-	0.00	0.00	0.00	0.03	0.01	0.00	-	-	-		
LAK042	-	0.00	-	0.08	0.04	0.00	0.01	0.00	-	-	-	-		
LAK044	0.01	0.01	0.00	0.08	0.03	0.00	0.03	0.01	0.00	-	-	-		

Table 6: Power (A) and false positives (B) for individual lake chemistry variables, and in combination for each EEM lake at 3, 5 and 10 years of post KMP monitoring under the conditions assumed in Scenario 5.

Power

Lako		ANC		\$04				рН		combined			
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	
LAK006	0.09	0.35	0.91	0.27	0.46	0.92	0.03	0.07	0.22	0.00	0.02	0.20	
LAK012	0.20	0.35	0.80	0.58	0.81	1.00	0.04	0.05	0.16	0.03	0.04	0.16	
LAK022	0.06	0.19	0.80	0.57	0.70	0.98	0.04	0.06	0.22	0.00	0.02	0.20	
LAK023	0.07	0.20	0.71	0.27	0.44	0.83	0.04	0.08	0.23	0.00	0.02	0.18	
LAK028	0.02	0.06	0.23	0.59	0.57	0.64	0.03	0.07	0.21	0.00	0.00	0.03	
LAK042	0.01	0.02	0.10	0.10	0.16	0.37	0.02	0.06	0.18	0.00	0.00	0.03	
LAK044	0.04	0.10	0.44	0.11	0.15	0.34	0.04	0.06	0.26	-	0.00	0.06	

False positives

Lake		ANC		SO4			pH			combined			
Lake	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	
LAK006	0.03	0.03	0.05	0.11	0.11	0.10	0.02	0.03	0.03	-	-	0.00	
LAK012	0.08	0.10	0.13	0.18	0.18	0.18	0.01	0.03	0.05	0.00	0.02	0.01	
LAK022	0.01	0.02	0.05	0.33	0.30	0.24	0.03	0.04	0.06	-	-	0.00	
LAK023	0.02	0.04	0.09	0.10	0.12	0.12	0.02	0.04	0.05	0.00	0.00	0.00	
LAK028	0.01	0.03	0.08	0.56	0.51	0.41	0.01	0.03	0.04	-	0.00	0.00	
LAK042	0.00	0.01	0.05	0.06	0.07	0.08	0.02	0.03	0.06	-	-	0.00	
LAK044	0.02	0.02	0.06	0.08	0.09	0.09	0.02	0.03	0.04	-	-	-	

Table 7: Power (A) and false positives (B) for individual lake chemistry variables, and incombination for each EEM lake with multiple or continuous fall samples at 3, 5 and 10 years of postKMP monitoring under the conditions assumed in Scenarios 6 and 7.

(A) Power													
Lako	Samples		ANC			SO4			рН			combined	
Lake	Samples	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
	1	0.95	0.99	1.00	0.99	1.00	1.00	0.22	0.29	0.31	0.20	0.29	0.31
1 4 K 006	3	0.99	1.00	1.00	1.00	1.00	1.00	0.46	0.43	0.53	0.45	0.43	0.53
LANOUU	5	0.99	1.00	1.00	1.00	1.00	1.00	0.50	0.46	0.55	0.49	0.46	0.55
	cont.							0.52	0.63	0.80			
	1	0.75	0.87	0.98	1.00	1.00	1.00	0.10	0.09	0.13	0.10	0.09	0.13
1 4 6012	3	0.96	0.99	1.00	1.00	1.00	1.00	0.25	0.25	0.18	0.25	0.25	0.18
LANUIZ	5	0.98	1.00	1.00	1.00	1.00	1.00	0.27	0.22	0.17	0.27	0.22	0.17
	cont.							0.32	0.25	0.23			
	1	0.60	0.82	0.98	0.91	0.97	1.00	0.33	0.37	0.44	0.23	0.34	0.44
LAK023	3	0.85	0.94	1.00	1.00	1.00	1.00	0.56	0.62	0.73	0.51	0.61	0.73
	5	0.85	0.94	0.99	1.00	1.00	1.00	0.59	0.65	0.78	0.55	0.64	0.78
	cont.							0.64	0.85	0.98			

(B) False positives

Lako	Samples		ANC			SO4			рН		combined		
Lake S LAK006 - LAK012 - LAK023 -	Samples	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
	1	0.00	0.00	0.00	0.05	0.03	0.00	0.02	0.01	-	-	-	-
1 4 K 006	3	0.00	0.01	-	0.02	0.01	-	0.03	0.02	0.00	-	-	-
LANOUU	5	0.00	0.01	0.00	0.01	0.00	-	0.03	0.02	0.00	-	-	-
	cont.							0.10	0.06	0.02			
	1	0.02	0.01	0.00	0.07	0.02	0.00	0.01	0.01	0.00	0.00	0.00	-
1 4 6012	3	0.03	0.02	0.01	0.02	0.00	0.00	0.02	0.01	0.00	-	-	-
LANUIZ	5	0.04	0.02	0.00	0.00	-	-	0.03	0.02	-	-	-	-
	cont.							0.06	0.01	0.00			
	1	0.00	0.00	-	0.04	0.01	0.00	0.02	0.01	-	-	-	-
LAK023 -	3	0.02	0.01	0.00	0.03	0.01	0.00	0.04	0.01	0.00	-	-	-
	5	0.02	0.01	0.00	0.03	0.01	0.00	0.05	0.01	-	-	-	-
	cont.							0.12	0.13	0.12			

Table 8: Power (A) and false positives (B) for individual lake chemistry variables, and in combination for each EEM lake with multiple fall samples at 3, 5 and 10 years of post KMP monitoring under the conditions assumed in **Scenario 8**.

(A) Power													
Laka	Detection		ANC			SO4			рН			combined	
Lake	threshold	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
	0.0	0.95	0.99	1.00	0.99	1.00	1.00	0.22	0.29	0.31	0.20	0.29	0.31
1 4 6 006	-0.1	0.53	0.73	0.93	0.76	0.83	0.93	0.13	0.14	0.11	0.06	0.10	0.10
LANOUU	-0.2	0.09	0.14	0.14	0.31	0.29	0.25	0.04	0.05	0.02	0.00	0.01	0.00
	-0.3	-	-	-	-	-	-	0.00	-	-	-	-	-
	0.0	0.75	0.87	0.98	1.00	1.00	1.00	0.10	0.09	0.13	0.10	0.09	0.13
1 4 16 0 1 2	-0.1	0.36	0.41	0.53	0.91	0.97	1.00	0.05	0.05	0.04	0.04	0.04	0.04
LARUIZ	-0.2	0.11	0.09	0.05	0.48	0.46	0.43	0.02	0.02	0.01	0.01	0.01	0.00
	-0.3	-	-	-	-	-	-	0.00	0.00	-	-	-	-
	0.0	0.77	0.94	1.00	0.95	0.99	1.00	0.34	0.37	0.47	0.28	0.35	0.47
1 4 16 0 2 2	-0.1	0.25	0.42	0.69	0.59	0.74	0.90	0.18	0.16	0.16	0.03	0.06	0.12
LANUZZ	-0.2	0.03	0.05	0.05	0.12	0.15	0.14	0.09	0.08	0.03	0.00	0.00	-
	-0.3	-	-	-	-	-	-	0.00	-	-	-	-	-
	0.0	0.60	0.82	0.98	0.91	0.97	1.00	0.33	0.37	0.44	0.23	0.34	0.44
1 4 16 0 2 2	-0.1	0.16	0.28	0.49	0.57	0.66	0.76	0.17	0.17	0.13	0.04	0.05	0.08
LARUZJ	-0.2	0.03	0.04	0.04	0.19	0.17	0.14	0.07	0.05	0.03	0.00	0.00	0.00
	-0.3	-	-	-	-	-	-	-	-	-	-	-	-
	0.0	0.03	0.06	0.07	0.04	0.05	0.05	0.31	0.37	0.43	-	-	-
1 4 14 0 2 9	-0.1	0.01	0.02	0.02	0.01	0.02	0.01	0.20	0.16	0.15	-	-	-
LANUZU	-0.2	0.01	0.01	0.00	0.01	0.00	0.00	0.08	0.06	0.04	-	-	-
	-0.3	0.00	-	-	-	-	-	-	-	-	-	-	-
	0.0	0.01	0.01	0.01	0.51	0.51	0.54	0.09	0.11	0.14	0.00	0.01	0.01
1 4 1 0 1 2	-0.1	0.00	0.01	0.01	0.33	0.27	0.21	0.04	0.05	0.04	-	-	0.00
LANU42	-0.2	0.00	0.01	-	0.17	0.11	0.03	0.02	0.02	0.01	-	-	-
	-0.3	-	-	-	0.01	-	-	-	-	-	-	-	-
	0.0	0.50	0.65	0.83	0.46	0.43	0.46	0.33	0.36	0.42	0.10	0.11	0.17
	-0.1	0.21	0.31	0.34	0.30	0.25	0.14	0.20	0.19	0.13	0.02	0.02	0.01
LAN044	-0.2	0.07	0.05	0.05	0.15	0.09	0.03	0.07	0.05	0.02	0.00	-	-
	-0.3	-	-	-	0.00	-	-	0.00	-	-	-	-	-

Laba	Detection		ANC			SO4			рН			combined	
Lake	threshold	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years	3 years	5 years	10 years
	0.0	0.00	0.00	0.00	0.05	0.03	0.00	0.02	0.01	-	-	-	-
1 4 1 006	-0.1	-	-	-	-	-	-	0.00	0.00	0.00	-	-	-
LANUUU	-0.2	-	-	-	-	-	-	-	-	-	-	-	-
	-0.3	0.01	0.00	0.00	0.06	0.03	0.00	0.01	0.01	-	-	-	-
	0.0	0.02	0.01	0.00	0.07	0.02	0.00	0.01	0.01	0.00	0.00	0.00	-
I AK012	-0.1	0.00	-	-	-	-	-	0.01	0.00	0.00	-	-	-
LANVIZ	-0.2	-	-	-	-	-	-	0.00	-	-	-	-	-
	-0.3	0.02	0.01	0.00	0.06	0.02	0.00	0.02	0.00	0.00	0.00	0.00	-
	0.0	0.00	0.00	-	0.02	0.01	0.00	0.02	0.01	0.00	-	-	-
I AK022	-0.1	-	-	-	-	-	-	0.01	0.00	-	-	-	-
LANULL	-0.2	-	-	-	-	-	-	-	-	-	-	-	-
	-0.3	-	0.00	-	0.01	0.01	0.00	0.04	0.02	0.00	-	-	-
	0.0	0.00	0.00	-	0.04	0.01	0.00	0.02	0.01	-	-	-	-
I AK023	-0.1	-	-	-	-	-	-	0.01	0.00	-	-	-	-
LANGEO	-0.2	-	-	-	-	-	-	0.00	-	-	-	-	-
	-0.3	0.00	0.00	0.00	0.05	0.03	0.00	0.02	0.02	0.00	-	-	-
	0.0	-	0.00	0.00	0.00	0.01	0.00	0.03	0.01	0.00	-	-	-
I AK028	-0.1	-	0.00	-	-	-	-	0.01	-	-	-	-	-
2,0020	-0.2	-	-	-	-	0.00	-	0.00	-	-	-	-	-
	-0.3	-	0.00	0.00	0.00	0.00	-	0.02	0.02	0.00	-	-	-
	0.0	0.00	0.00	0.00	0.07	0.02	0.00	0.00	0.01	0.00	-	-	-
LAK042	-0.1	0.00	0.00	-	0.03	0.00	-	0.00	0.00	-	0.00	-	-
	-0.2	-	-	-	0.00	0.00	-	-	0.00	-	-	-	-
	-0.3	0.00	0.00	-	0.08	0.03	0.01	0.01	0.00	0.00	0.00	-	-
	0.0	0.01	0.01	-	0.08	0.04	-	0.03	0.01	0.00	-	-	-
LAK044	-0.1	0.00	-	-	0.03	0.00	0.00	0.01	0.00	-	-	-	-
	-0.2	-	-	-	0.00	-	-	0.00	-	-	-	-	-
	-0.3	0.01	0.01	0.0	0.08	0.03	0.00	0.02	0.01	0.00	-	-	-

6 Appendix 2: Determination of ANC and SO₄²⁻ Thresholds

The EEM thresholds for ANC and SO₄²⁻ corresponding to a 0.3 unit change in pH were calculated independently for each lake. Due to the non-linear relationship between pH and ANC, the change in ANC corresponding to a decrease of 0.3 pH units is dependent on the shape of the relationship and the initial ANC value. In the present case, the same pH-ANC relationship was used for all of the lakes (i.e., the Small and Sutton (1986) pH-alkalinity curve fit to the STAR lakes, as applied by ESSA et al. (2013)). However, it is still necessary to make lake-specific calculations because the initial ANC values vary widely by lake. Given that the baseline values for pH and ANC for these lakes do not fall directly on the curve (due to natural variability and the use a single pH-alkalinity curve), it is necessary to account for the deviation from the curve in the calculation of the Δ ANC that corresponds to Δ pH of 0.3 units. The approach we have applied assumes that the deviation from the curve is primarily due to variability in pH and apply an adjustment to the calculation of Δ ANC based on how far the baseline values are above or below the curve (i.e., adjusting for "errors in Ys"). An alternative approach is to assume that the deviation from the curve is primarily due to variability in ANC and apply an adjustment based on "errors in Xs". In either case, once Δ ANC is calculated, Δ SO₄²⁻ can be calculated as Δ SO₄²⁻⁼ Δ ANC / (1 – F-factor). See ESSA et al. (2013) for additional discussion of F-factor.

Table 9 shows the thresholds used in the present analyses. Table 10 shows the thresholds based on the alternative approach for determining Δ ANC based on Δ pH and the pH-alkalinity curve. For some of the lakes, the alternative approach results in more conservative thresholds (i.e., a smaller change would be required to reach the threshold), but for others the alternative results would be slightly less conservative thresholds. For most the lakes, the difference between the two approaches is not large. The only exception is LAK012, for which the change required to reach its ANC and SO₄²⁻ thresholds would be roughly half as much under the alternative thresholds.

As more data is collected, it will eventually be possible to derive lake-specific pH-ANC curves, which will improve our ability to estimate the change in ANC associated with specific changes in pH. The baseline values for LAK012 have by far the most deviation from the common pH-alkalinity curve and therefore the development of lake-specific pH-alkalinity curves would be particularly beneficial to improving the estimation of its thresholds.

		pН			Gran A	NC	SO4 ²⁻		
	Baseline	Three	shold	Baseline	Three	shold	Baseline	Three	shold
Lake	value	Value	Δ	value	Value	Δ	value	Value	Δ
LAK006	6.06	5.76	-0.3	30.5	14.2	-16.3	13.0	33.7	20.7
LAK012	6.07	5.77	-0.3	67.0	33.1	-33.9	8.6	62.9	54.3
LAK022	6.11	5.81	-0.3	37.0	17.6	-19.4	39.3	68.8	29.5
LAK023	5.90	5.60	-0.3	26.4	12.0	-14.4	20.5	39.3	18.8
LAK028	5.17	4.87	-0.3	7.8	0.5	-7.3	94.3	113.3	18.9
LAK042	5.08	4.78	-0.3	4.4	-2.4	-6.8	6.2	14.0	7.8
LAK044	5.61	5.31	-0.3	5.2	-1.6	-6.8	6.4	13.5	7.1

Table 9. Thresholds for pH, ANC and SO_4^{2-} as applied in the analyses presented in this report.

Table 10.Thresholds for pH, ANC and SO_4^{2-} based on the alternative approach for
calculating changes in ANC from a given change in pH based on the pH-alkalinity curve. The

		pН			Gran ANC			SO4 ²⁻	
	Baseline	Three	shold	Baseline	Thre	shold	Baseline	Thre	shold
Lake	value	Value	Δ	value	Value	Δ	value	Value	Δ
LAK006	6.06	5.76	-0.3	30.5	14.2	-16.3	13.0	33.7	20.7
LAK012	6.07	5.77	-0.3	67.0	50.6	-16.4	8.6	34.9	26.3
LAK022	6.11	5.81	-0.3	37.0	19.1	-18.0	39.3	66.7	27.3
LAK023	5.90	5.60	-0.3	26.4	14.6	-11.8	20.5	36.0	15.4
LAK028	5.17	4.87	-0.3	7.8	0.1	-7.7	94.3	114.3	20.0
LAK042	5.08	4.78	-0.3	4.4	-4.3	-8.6	6.2	16.1	9.9
LAK044	5.61	5.31	-0.3	5.2	-2.3	-7.5	6.4	14.2	7.8

thresholds (value and Δ) for ANC and SO₄²⁻ differ from the values in Table 9 but other values are identical.