REPORT

MAGIC library for Swedish lakes: evaluation of multiple calibrations

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Project title

Känslighetsanalys med MAGIC på 146 sjöar

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Title and subtitle of the report

MAGIC library for Swedish lakes: evaluation of multiple calibrations

Summary

Sweden has an official procedure for determining whether or not a water body is acidified, and thereby qualified for remedial measures such as liming. The criterion of anthropogenic acidification is that the decrease in lake pH relative to pre-industrial status be more than 0.4 pH units (ΔpH). The pre-industrial pH is estimated by means of the dynamic biogeochemical model MAGIC. In cases for which data are insufficient to calibrate MAGIC, an estimation of pre-industrial pH can be obtained by use of the MAGIC library (www.ivl.se/magicbibliotek). The MAGIC library consists of calibrations for hundreds of lakes and streams in Sweden. The library has a matching procedure to select the lake in the library that most closely resembles the lake to be evaluated. The ΔpH of the evaluation lake is then assumed to be that of the library lake.

The MAGIC library has been updated in 2012 with MAGIC calibrations for 2903 lakes covering the whole country. Water chemistry data for these comes from three separate datasets: 163 "trend" lakes (TRN), sampled four-times annually since the mid-1980s; 1373 "synoptic" lakes (SNP), sampled in nationwide surveys conducted in 1995, 2000, and 2005; and 1367 "liming reference" lakes (MAL), sampled in 2007 - 2008. The MAGIC calibrations put into the library consist of the most recent lake chemistry data from the period 2005-2010 for each lake.

In all 307 of the lakes were included in more than one of these three datasets. These were thus calibrated two or three times using different water chemistry inputs. For the purpose of the MAGIC library, only one calibration was used, preferring TRN above both SNP and MAL lakes due to most extensive sampling and most robust data generated by the TRN sampling scheme. SNP lakes were sampled at multiple years and SNP model calibrations were preferred over MAL lakes sampled once in 2007 and once in 2008. Here we use these multiple calibrations to quantify the differences in MAGIC historical reconstructions of water chemistry due solely to variations in modern lake water chemistry.

In general there was very good correlation between the ΔpH obtained from the calibration used in the library with the ΔpH obtained from the duplicate calibration not used in the library. Of the 307 lakes with multiple calibrations, fully 85% were classified the same by both the calibration in the library and the calibration not used in the library.

Keyword

Acidification, lakes, MAGIC model, MAGIC bibliotek

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Sammanfattning

Den svenska definitionen på antropogen försurning är att pH har sjunkit med 0.4 pH-enheter från förindustriell tid. pH från mitten av 1800-talet uppskattas med hjälp av den dynamiska biogeokemiska modellen MAGIC. Om det inte finns tillräckligt med bakgrundsdata för att modellera kan verktyget MAGIC-biblioteket användas (www.ivl.se/magicbibliotek). Sjödelen av MAGIC-biblioteket består av knappt 3000 sjöar i Sverige som har modellerats med MAGIC. Biblioteket har en matchningsrutin som letar fram den sjö i biblioteket som mest liknar den sjö man vill försurningsbedöma. Den pH-förändring som har modellerats fram för sjön i biblioteket antas då även beskriva pH-förändringen i bedömningssjön.

Under 2012 har MAGIC-biblioteket byggts ut och kalibreringar för 2903 unika sjöar från hela landet har tagits fram. Den vattenkemidata som har använts vid kalibreringarna kommer från tre olika dataset: 163 trendsjöar (TRN), som har provtagits fyra gånger årligen sedan i mitten av 1980-talet, 1373 synoptiska sjöar (SNP), som provtagits i nationell övervakning 1995, 2000 och 2005, och 1367 kalkreferenssjöar (MAL), som provtogs 2007-2008. De MAGIC-kalibreringar som lagts in i MAGIC-biblioteket är baserade på den senaste sjökemidatan från perioden 2005-2010, för respektive sjö.

En del sjöar har funnits med och provtagits i mer än en av de tre undersökningarna (TRN, SNP och MAL) och har därför modellerats med MAGIC vid mer än ett tillfälle. 307 sjöar finns med i minst två av dataseten och 29 sjöar finns med i alla tre. Detta innebär att sjöarna har kalibrerats två eller tre gånger med olika nutida vattenkemidata. I MAGIC-biblioteket används endast en av dessa kalibreringar. I första hand används en sjö som har kalibrerats i TRN-undersökningen, eftersom de sjöarna har provtagits flest gånger och har mest robusta data. I andra hand används en sjö från SNP-undersökningen, eftersom de har provtagits flera år medan sjöarna i MAL-undersökningen endast provtagits en gång 2007 och en gång 2008. I den här rapporten använder vi dessa multipla kalibreringar för att kvantifiera skillnader i den historiska rekonstruktionen av MAGIC, med hjälp av enbart variationer i dagens sjövattenkemi.

Generellt sett var det god överensstämmelse mellan den pH-förändring som erhålls i biblioteket och den pH-förändring som duplikaten eller triplikaten visar. Av de totalt 336 alternativa kalibreringarna klassades 85 % på samma sätt som den kalibrering som används i MAGIC-biblioteket. 12 % gav bedömningen försurad istället för den nu opåverkade bedömningen och drygt 2 % gav bedömningen opåverkad istället för den nu försurade bedömningen.

Summary

Sweden has an official procedure for determining whether or not a water body is acidified, and thereby qualified for remedial measures such as liming. The criterion of anthropogenic acidification is that the decrease in lake pH relative to pre-industrial status be more than 0.4 pH units (ΔpH). The pre-industrial pH is estimated by means of the dynamic biogeochemical model MAGIC. In cases for which data are insufficient to calibrate MAGIC, an estimation of pre-industrial pH can be obtained by use of the MAGIC library (www.ivl.se/magicbibliotek). The MAGIC library consists of calibrations for hundreds of lakes and streams in Sweden. The library has a matching procedure to select the lake in the library that most closely resembles the lake to be evaluated. The ΔpH of the evaluation lake is then assumed to be that of the library lake.

The MAGIC library has been updated in 2012 with MAGIC calibrations for 2903 lakes covering the whole country. Water chemistry data for these comes from three separate datasets: 163 "trend" lakes (TRN), sampled four-times annually since the mid-1980s; 1373 "synoptic" lakes (SNP), sampled in nationwide surveys conducted in 1995, 2000, and 2005; and 1367 "liming reference" lakes (MAL), sampled in 2007 - 2008. The MAGIC calibrations put into the library consist of the most recent lake chemistry data from the period 2005-2010 for each lake.

In all 307 of the lakes were included in more than one of these three datasets. These were thus calibrated two or three times using different water chemistry inputs. For the purpose of the MAGIC library, only one calibration was used, preferring TRN above both SNP and MAL lakes due to most extensive sampling and most robust data generated by the TRN sampling scheme. SNP lakes were sampled at multiple years and SNP model calibrations were preferred over MAL lakes sampled once in 2007 and once in 2008. Here we use these multiple calibrations to quantify the differences in MAGIC historical reconstructions of water chemistry due solely to variations in modern lake water chemistry.

In general there was very good correlation between the ΔpH obtained from the calibration used in the library with the ΔpH obtained from the duplicate calibration not used in the library. Of the 307 lakes with multiple calibrations, fully 85% were classified the same by both the calibration in the library and the calibration not used in the library.

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1 Introduction

Decades of acid deposition have caused acidification of lakes and streams in large areas of Sweden (Almer et al. 1974). Ecological effects include impairment and loss of thousands of fish populations (Tammi et al. 2003). Since the mid-1980s international agreements conducted as part of the United Nations Economic Commission for Europe (UN-ECE) Convention on Long-Range Transboundary Air Pollution (CLRTAP) have achieved several major international agreements leading to substantial reductions in the emissions of sulphur and nitrogen compounds to the atmosphere (UNECE 2012). In response, lakes in Sweden (Wilander and Fölster 2007) and elsewhere in Fennoscandia have begun to recover from acidification (Skjelkvåle et al. 2001).

In 1999, Sweden adopted 15 Environmental Objectives as part of an environmental policy for a sustainable Sweden (http://www.sweden.gov.se/sb/d/5775). These are to be achieved by the year 2020. One of these is "Natural Acidification Only". Determination of natural acidification of lakes necessitates assessment of the chemical status in pre-industrial times. The official Swedish criterion of anthropogenic acidification is that the decrease in lake (stream, river) pH relative to pre-industrial status be less than 0.4 pH units (ΔpH) (Fölster et al. 2007). This criterion is based primarily on analyses of lakewater chemistry and biological status of two organism groups, fish and littoral invertebrate fauna (Fölster et al. 2007).

Sweden has an official procedure for determining whether or not a water body is acidified, and thereby qualified for remedial measures such as liming. This procedure entails estimation of the pre-industrial pH by means of the dynamic biogeochemical model MAGIC (Cosby et al. 1985a, 1985b, Cosby et al. 2001). In cases for which data are insufficient to calibrate MAGIC, an estimation of pre-industrial pH can be obtained by use of the MAGIC library (in Swedish "MAGIC biblioteket", www.ivl.se/magicbibliotek). The MAGIC library consists of calibrations for almost 3000 lakes and streams in Sweden. The library has a matching procedure to select the lake in the library that most closely resembles the lake to be evaluated. The ΔpH of the evaluation lake is then assumed to be that of the library lake. The matching is with respect to present-day chemistry and geographic location. The MAGIC library is maintained and operated by IVL Swedish Environmental Research Institute.

The MAGIC library has been updated in 2012 with MAGIC calibrations for 2903 lakes covering the whole country (Moldan et al. 2009, Moldan et al. in press). Water chemistry data for these comes from three separate datasets: 163 "trend" lakes (TRN), sampled four-times annually since the mid-1980s; 1373 "synoptic" lakes (SNP), sampled in nationwide surveys conducted in 1995, 2000, and 2005; and 1367 "liming reference" lakes (MAL), sampled in 2007 - 2008. Since 2005 one-fifth of the synoptic lakes have been sampled each year. The MAGIC calibrations put into the library consist of the most recent lake chemistry data from the period 2005-2010 for each lake. Water chemistry data are held at the Swedish University of Agricultural Sciences, Department of Aquatic Sciences and Assessment (http://info1.ma.slu.se). Since the purpose of the MAGIC library is to make lake-acidification assessments the current version of the MAGIC library contains 2631 lakes. Lakes with a pH above 7.3 and/or lakes with a Ca-concentration above 400 $\mu eq\ l^{-1}$ were not included in the final version of the library, and lakes with these characteristics are always evaluated as non-acidified.

In all 307 of the lakes were included in more than one of these three datasets (Figure 1). These were thus calibrated two or three times using different water chemistry inputs. For the purpose of the MAGIC library, only one calibration was used, preferring TRN above both SNP and MAL lakes due to most extensive sampling and most robust data generated by the TRN sampling scheme. SNP lakes were sampled at multiple years and SNP model calibrations were preferred over MAL lakes sampled once in 2007 and once in 2008. Here we use these multiple calibrations to quantify the uncertainty in MAGIC historical reconstructions of water chemistry due solely to variations in modern lake water chemistry.

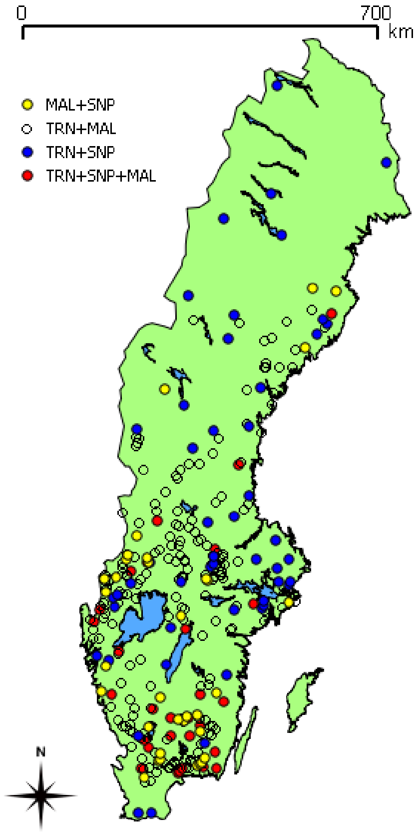


Figure 1. Lakes with multiple calibrations included in the analyses. Liming reference lakes (MAL (kalkreferenser inom målsjöprovtagningen, in total 258), trend lakes (TRN, trendsjöar, in total 112), synoptic lakes (SNP, synoptiska sjöar, in total 273).

2 Data sources, materials and methods

2.1 The MAGIC Model

MAGIC is a lumped-parameter model of intermediate complexity, developed to predict the long-term effects of acidic deposition on soils and surface water chemistry (Cosby et al. 1985a, 1985b, 2001). The model simulates soil solution chemistry and surface water chemistry to predict the annual average concentrations of the major ions in lakes and streams. MAGIC represents the catchment with aggregated, uniform soil compartments (one or two) and a surface water compartment that can be either a lake or a stream. MAGIC consists of (1) a section in which the concentrations of major ions are assumed to be governed by simultaneous reactions involving sulphate adsorption, cation exchange, dissolution-precipitation-speciation of aluminium and dissolution-speciation of inorganic and organic carbon, and (2) a mass balance section in which the flux of major ions to and from the soil is assumed to be controlled by atmospheric inputs, chemical weathering inputs, net uptake in biomass and losses to runoff. At the heart of MAGIC is the size of the pool of exchangeable base cations in the soil. As the fluxes to and from this pool change over time owing to changes in atmospheric deposition, the chemical equilibria between soil and soil solution shift to give changes in surface water chemistry. The degree and rate of change in surface water acidity thus depend both of flux factors and the inherent characteristics of the affected soils. Additional details and information on calibration procedures and data sources are given by Moldan et al. (2009) and (Moldan et al. in press).

2.2 Calibration and calculation of pH

In each case MAGIC was calibrated to the observed water chemistry data for the year of the sample such that the simulated matched the observed major ion chemistry for the ions contributing to the acid neutralising capacity (ANC). ANC is defined as the equivalent difference between the sum of base cations (Ca, Mg, Na, K) and sum of strong acid anions (SO_4, Cl, NO_3). The calibration was then run forward in time to the year 2010. For the calibration an automated optimization procedure was used.

Pre-industrial pH is then calculated from ANC using the official Swedish procedure given by (Fölster 2006):

$$ANC = ([CO_3^{2-}] + [HCO_3^-] + [org^-]) – ([H^+] + [Al^{n+}]),$$

where org^- is the sum of organic anions, Al^{n+} is the sum of cationic aluminium species, and units are $\mu eq\ L^{-1}$. Org^- is calculated from present-day DOC concentration and the tri-protic model of Hruška et al. (2003) assuming no change over time. Concentrations of bicarbonate and carbonate are calculated assuming CO_2 content is 4 times atmospheric (0.156% by volume). Concentrations of cationic Al are assumed negligible (Fölster 2006). For the comparisons here, delta pH is given as pH for the year 1860 minus pH for the year 2010, both calculated from ANC using the above procedure.

2.3 Calibrated lake datasets

MAGIC was calibrated to 2903 unique lakes. Due to overlaps of the three datasets, the number of model calibrations was 3239. Of the 3239 calibrations, 336 were a duplicate or a triplicate calibration of a lake in another dataset. 278 lakes were calibrated twice and 29 lakes three times (Figure 2).

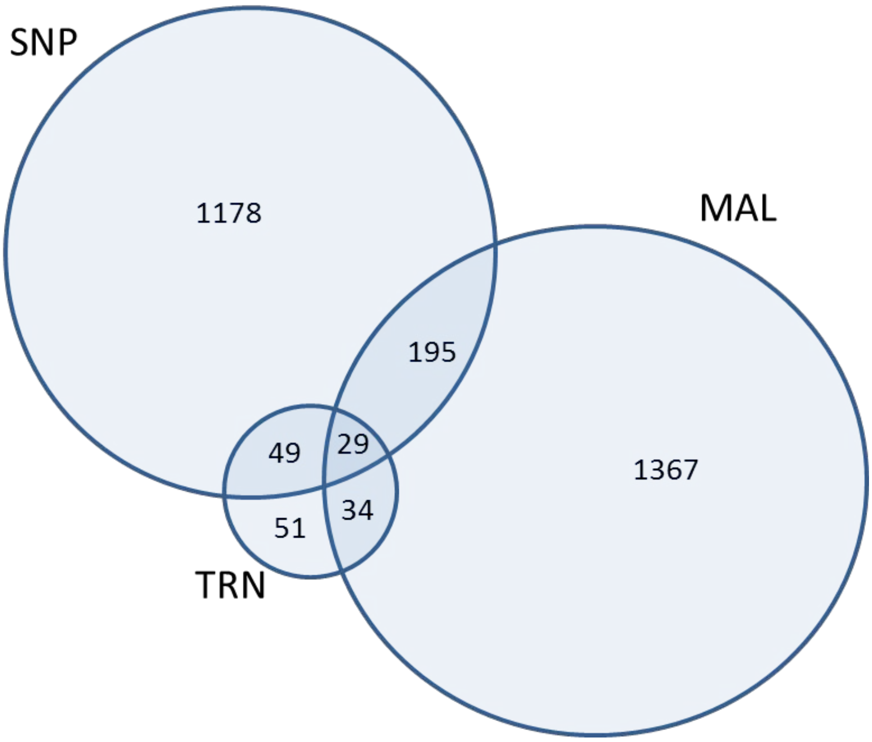


Figure 2. Venn diagram showing the numbers of calibrated lakes in the three datasets and duplicates and triplicates. SNP = synoptic lakes; TRN = trend lakes; MAL = liming reference lakes.

The following calibrations were entered into the MAGIC library: the TRN calibrations for all the TRN lakes (51+49+34+29), the calibrations for the remaining unique SNP lakes (1178), the calibrations for the remaining unique MAL lakes (1367), and the SNP calibrations of the duplicated SNP and MAL lakes (195). The remaining calibrations of SNP and MAL lakes were not entered into the library but used here for testing. These are the MAL calibrations for those duplicated only with SNP (195), the MAL calibrations for those duplicated only with TRN (34), the SNP calibrations for those duplicated only with TRN (49), and the MAL and SNP calibrations for the lakes with triplicates (29). These are termed here as “not used in library”.

3 Results and discussion

In general there was very good correlation between the ΔpH obtained from the calibration used in the library with the ΔpH obtained from the duplicate calibration not used in the library (Figure 3). The linear regression falls very close to the 1:1 line with correlation coefficient R^2 of 0.65. Most of the 336 lake pair calibrations (and indeed most of the 2631 lakes entered into the library) are classified as “not acidified”, as they have ΔpH < 0.4 (Moldan et al. 2013).

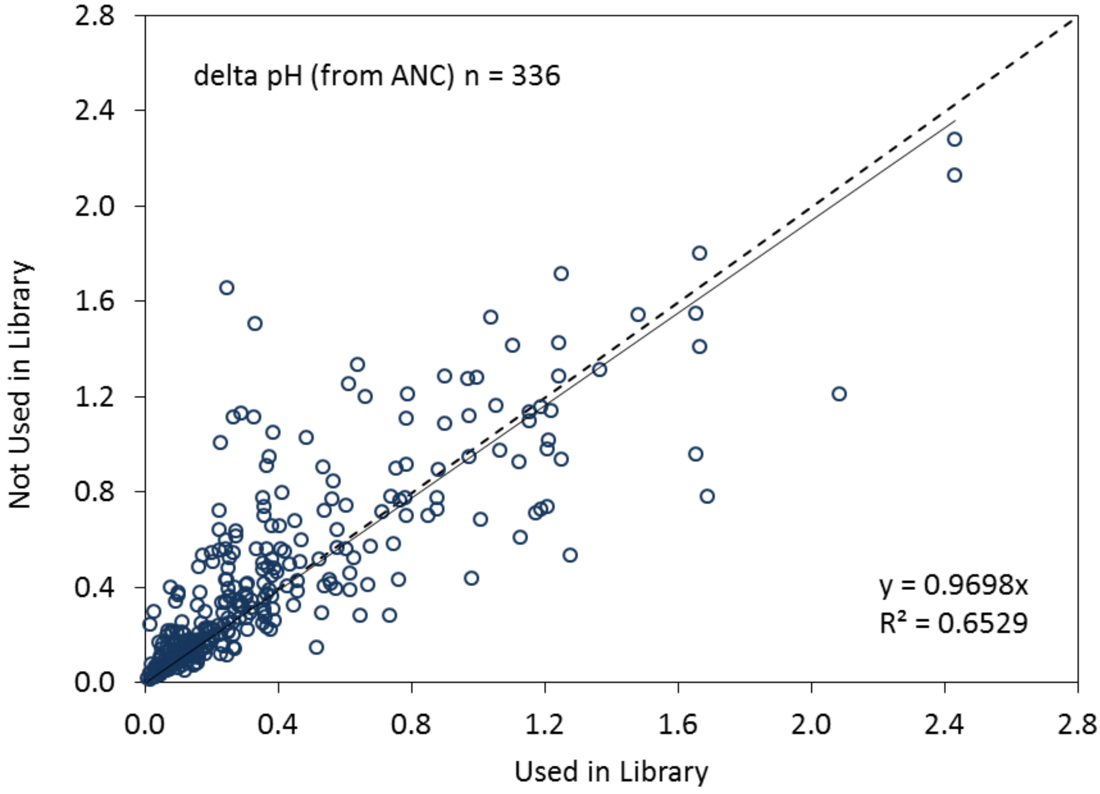


Figure 3. ΔpH (pH year 1860 minus pH year 2010) simulated by MAGIC for 307 Swedish lakes included in more than one of the three datasets. On the x-axis is the ΔpH for the calibration that is included in the MAGIC library and on the y-axis is the ΔpH for the calibration not included in the library.

Of more interest perhaps is whether lakes would be classified differently by each of the two calibrations. Of the 307 lakes with multiple calibrations, fully 85% were classified the same by both calibrations (Figures 4 and 5). And many of the 49 lake calibration pairs that were classified differently between the two calibrations were very close one or the other of the 0.4 ΔpH lines.

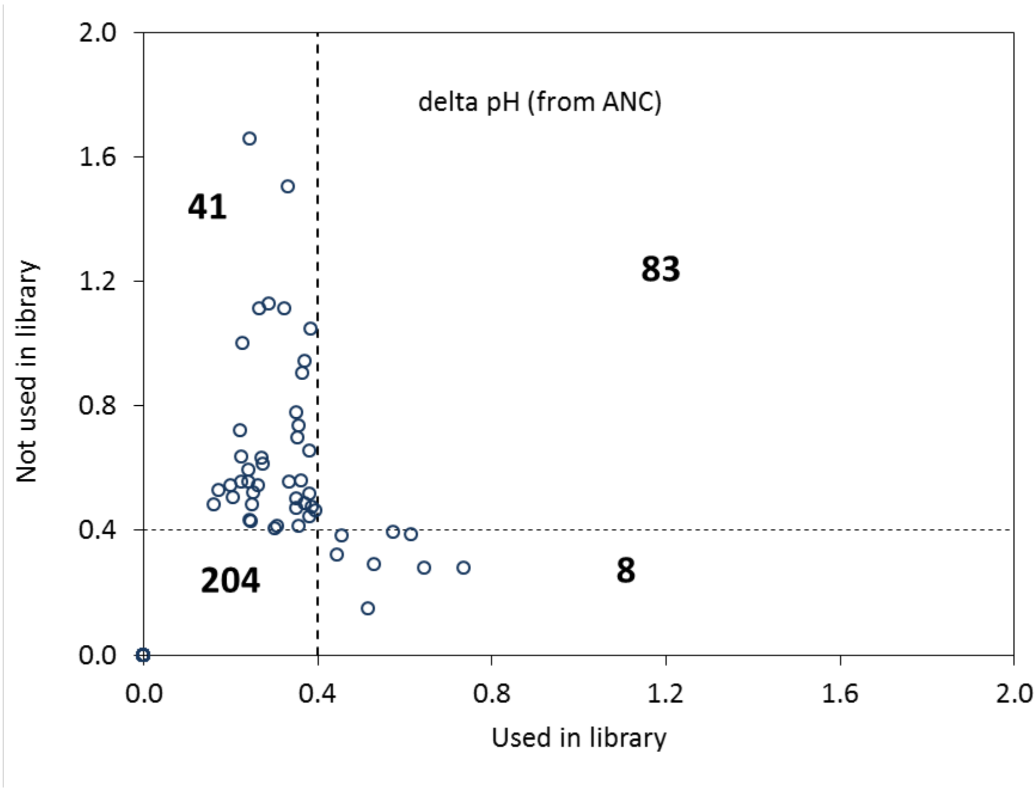


Figure 4. ΔpH (pH year 2010 minus pH year 1860) simulated by MAGIC for 307 Swedish lakes included in more than one of the three datasets. The large numbers indicate the number of lakes in each of the four quadrants. Data points for only the 49 duplicates with disagreement in classification are shown.

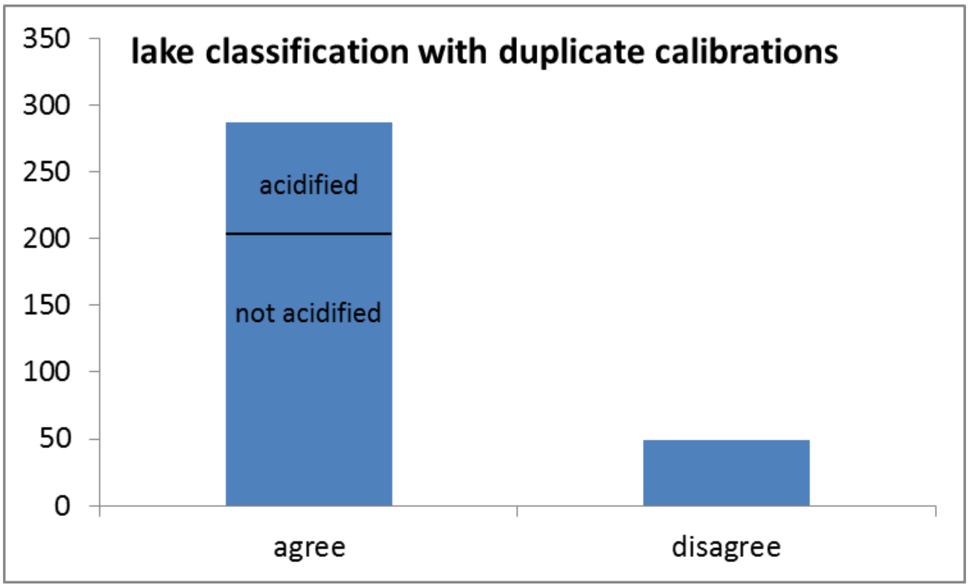
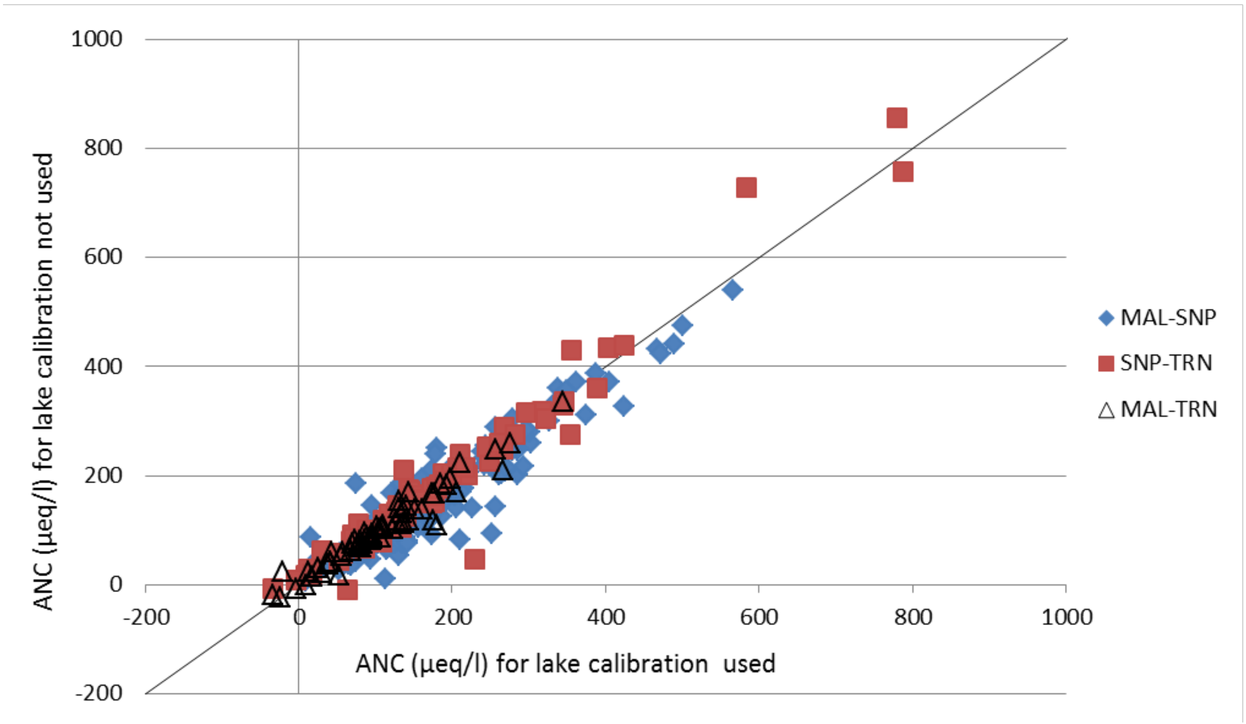


Figure 5. Classification of lake acidification under the criterion of ΔpH (pH year 1860 minus pH year 2010) greater than 0.4 units for the 307 Swedish lakes with duplicate or triplicate MAGIC calibrations. The 49 lake calibration pairs in the "disagree" category are plotted in Figure 4.



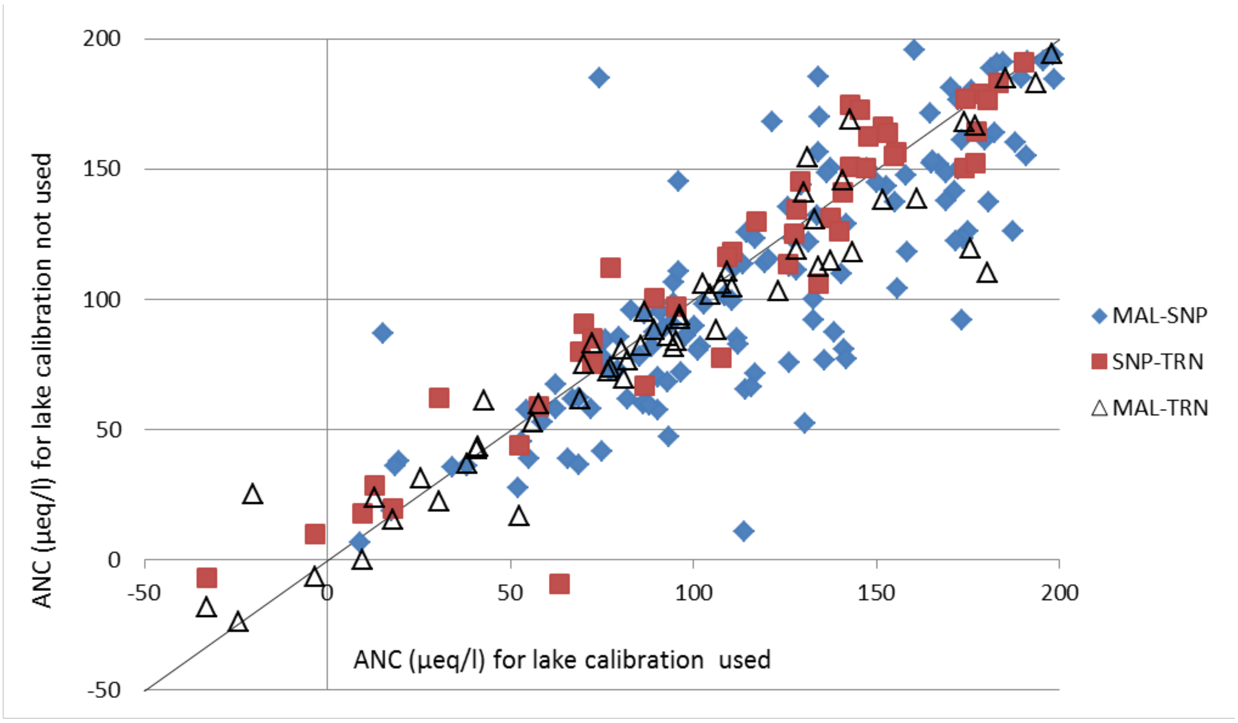
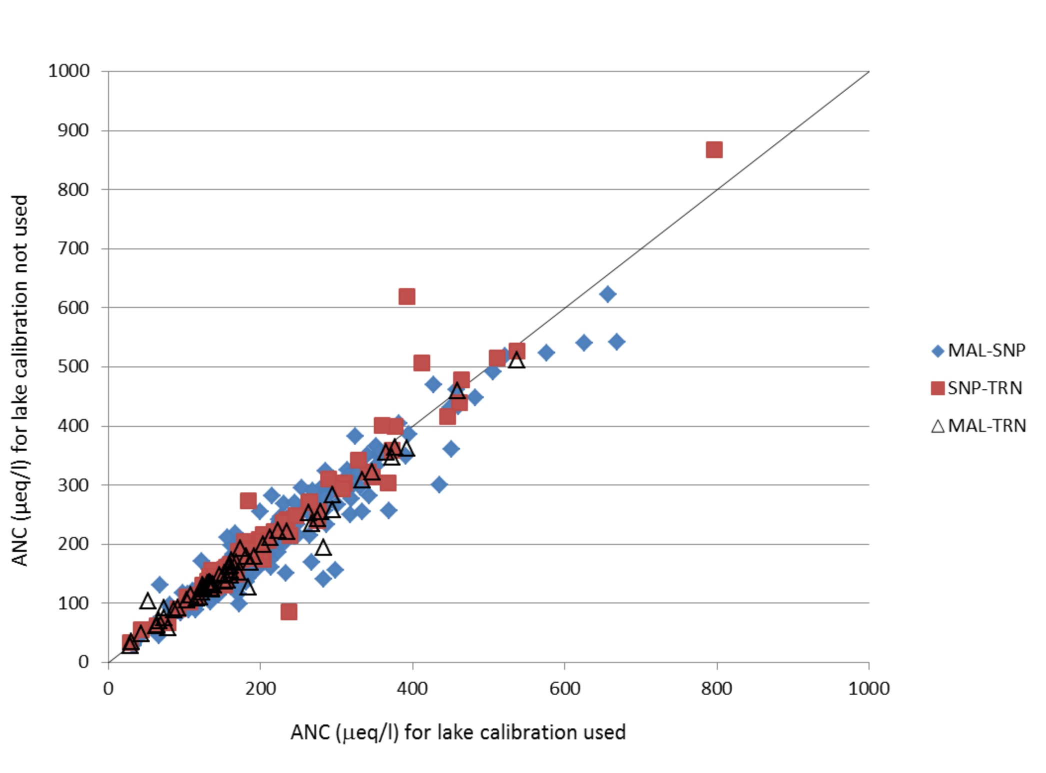


Figure 6. ANC 2007 for the duplicate and triplicate lake calibrations covering wide ANC range (upper panel) and lower ANC range only (lower panel). ANC was in average lower for MAL than for SNP in the MAL-calibration year 2007. Nine lakes had extremely high ANC (>1 000 µeq/l) and were not included in the graph.



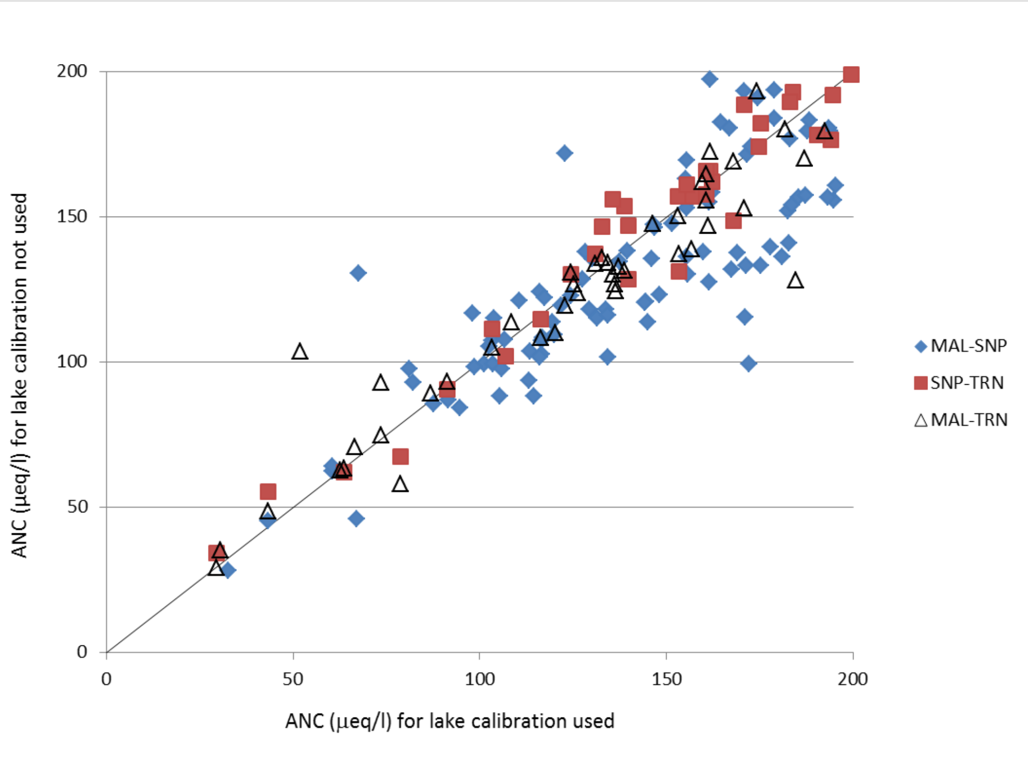


Figure 7. ANC 1860 for the duplicate and triplicate lake calibrations covering wide ANC range (upper panel) and lower ANC range only (lower panel). ANC was often lower for MAL than for SNP in the MAL-calibration year 2007. Nine lakes had extremely high ANC (>1 000 µeq/l) and were not included in the graph.

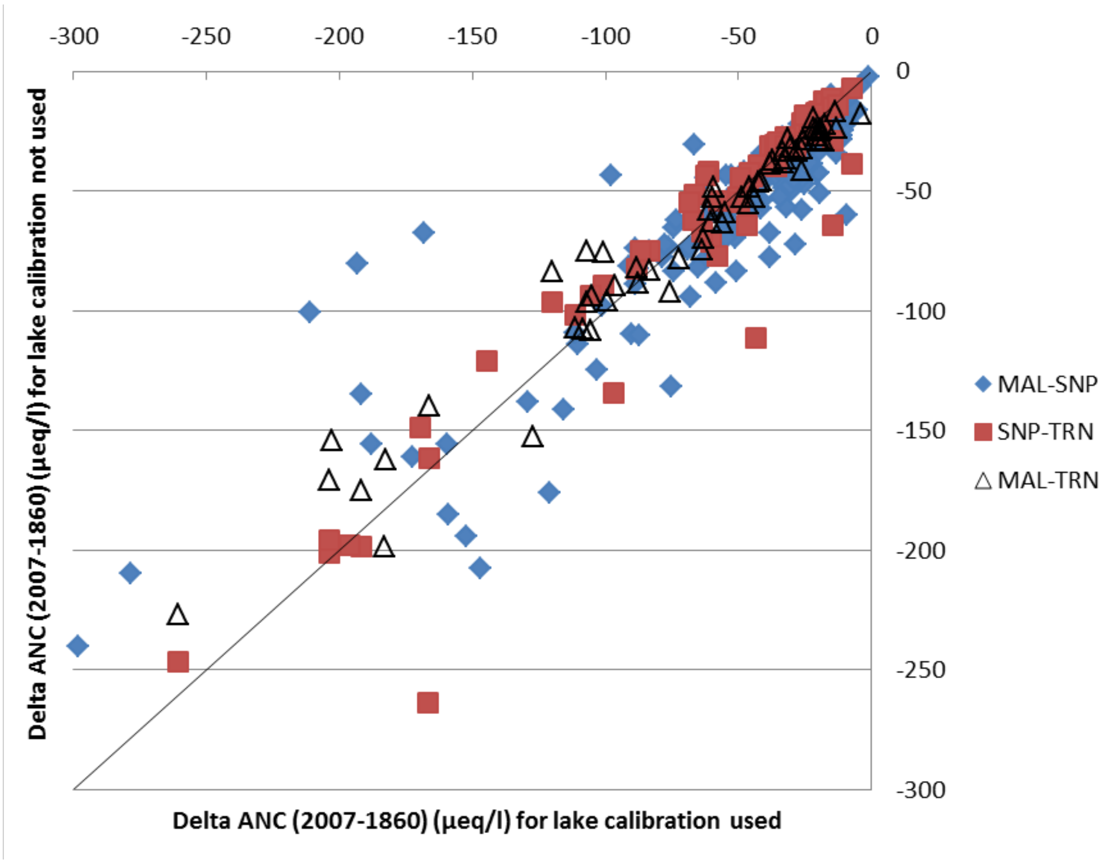


Figure 8. ANC changes (2007-1860) in the used and not used lake calibrations. ANC in general decreased more in the MAL lakes not used in the MAGIC library than in the SNP lakes used in the MAGIC library.

There are many possible reasons why the two calibrations do not give the same ΔpH values. Foremost is the different water chemistry to which the calibration is made. Lake water chemistry can vary from day-to-day, month-to-month and year-to-year. All the lake samples used here in the calibrations were collected in the autumn, so seasonal variations are probably minimised. Year-to-year variations can be caused by such factors as storms with large inputs of seasalts or heavy rains with dilution of high pH baseflow water. The long-term trends in rising DOC concentrations in many lakes may also affect the calibrations. Two calibrations made on the same lake with water samples separated in time by many years and with different DOC concentrations will give different ΔpH, as in all these calibrations the observed DOC value from the sample year is assumed constant over the entire 150 year simulation period.

All three data sets have, for a specific lake, been calibrated with the same soil data, hydrology, land use and deposition data over time. It is therefore unlikely that the MAGIC calibration procedure itself generates significant uncertainty. However, ANC in year 2007 (calibration year/close to the calibration year) and 1860 was lower in the MAL lake calibrations compared to the SNP lake calibrations for the same lake (Figure 6 and Figure 7). *This is due to lower ANC in the samples collected in the MAL study in 2007/2008*. Moreover, the change in ANC from 1860 to 2007 was larger for MAL lakes than SNP lakes (Figure 8). For the lakes with duplicate calibrations MAL and SNP, the SNP lake calibration is included in the MAGIC library. There are, however, other MAL lakes in the library, sampled and calibrated to the same year, and if they have the same characteristics the library might have a tendency of giving a larger ΔpH than if a SNP lake is chosen from the library. Previous studies with MAGIC using the automatic optimizer procedure for calibration showed that given the same inputs, the optimizer generates nearly identical past and future values of ANC.

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