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Modelling Long-Term Acidification: A Comparison with Diatom Reconstructions and the Implications for Reversibility [and Discussion]

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Modelling long-term acidification: a comparison with diatom reconstructions and the implications for reversibility

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A model of long term acidification (MAGIC) is applied to a range of catchments in Scotland that are subject to different pollution inputs and land uses. The simulated historical trends in pH are compared with data from palaeolimnological reconstructions undertaken at the same sites. Both techniques produce similar historical acidification trends and, with some exceptions, closely match observed present day pH. The MAGIC model results indicate that pollution inputs and land-use, particularly afforestation, have significant effects on surface water acidification. Moreover, the model indicates that reversibility may be occurring at several sites. Reversibility of acidification is further explored by using the model in predictive mode under several scenarios for reduction deposition.

INTRODUCTION

In recent years many lakes and streams in upland Scotland have demonstrated increased surface water acidity (Harriman & Morrison 1981). This has been attributed to the effect of increased anthropogenic sulphur deposition since pre-industrial times in both moorland catchments and afforested systems (Flower *et al.* 1987). The timing of response of the surface water to increased input of anthropogenic sulphate is thought to be controlled by the physiochemical characteristics of the catchment, namely, bedrock, soils and vegetation. Evidence for the processes and mechanisms involved in the titration of acidity from catchment inputs to outputs is still being gathered, but a quantification of the change in water acidity and the timing of changes in acid status has been derived from two approaches: long-term hydrochemical simulation models and palaeolimnological reconstructions. The two approaches differ in that the palaeolimnological reconstruction may be viewed as a direct measure of a surrogate acidity indicator whereas the models, although having their roots in hydrochemical laws, draw largely on a conceptualized representation of the major processes thought to be operating, and so at best can only be regarded as a simplification of the catchment system. Given this situation, model hindcast simulations require validation against long-term water-quality data sets. Clearly, few data sets of sufficient time period exist with which to test and validate either approach but increased confidence in both techniques would be gained if the reconstructions from the two are found to be consistent. Furthermore, the international concern over the problem of surface water acidification and its ecological effects and a stated policy of promoting amelioration strategies (Mason & Seip 1985) demands that predictions of surface water quality are made to assess the ability of systems to reverse acidification under different emissions and land-use strategies.

We use the model of acidification of groundwater in catchments (MAGIC) to simulate historical water quality and to compare the pH reconstruction to those determined by diatom analysis of sediment cores from the same lake sites. Six sites are chosen to cover a range of deposition loadings, land-use and bedrock geology in Scotland (Battarbee & Renberg, this symposium). The results from the calibrated models are compared both historically and to present-day water chemistry; the models are run forward to assess reversibility under a range of scenarios for deposition reduction.

The study sites and data sources

The sites selected are Round Loch of Glenhead, Lochan Uaine, Loch Tinker, Loch Chon, Loch Doilet and Lochan Dubh (Battarbee & Renberg, this symposium). Rainfall amount and chemistry are taken, wherever possible, from nearby collectors operated by the Warren Springs Laboratory under the Department of the Environment monitoring network (Warren Spring Laboratory 1987). At L. Tinker and L. Uaine, because of the lack of a nearby D.O.E. collector, mean bulk precipitation data for 1987 for the L. Chon (Jenkins *et al.* 1989*a*) and Allt a Mharcaidh (Jenkins *et al.* 1988) catchments were used, respectively. Sea-salts dominate rainfall at the sites in the west and although sulphate concentrations are at a consistent level at all of the sites, rainfall quantity is substantially greater on the west coast thereby increasing the total loading. Mean present day observed water chemistry is taken from the SWAP Palaeolimnology Programme data-base (Munro *et al.*, this symposium).

To achieve a charge balance to both input and output it was necessary in some cases to add or subtract cations or anions. Where this was necessary concentrations of chloride or sodium, or both, were adjusted and the result of the changes generally improved the sea-salt ratio. In all cases, the changes implemented were within the annual variation in chemistry at each site.

Reconstruction techniques

Details of diatom analysis (Jones *et al.* and Kreiser *et al.*, this symposium), dating procedures (Appleby *et al.*, this symposium) and techniques for reconstructing historical pH (Birks *et al.*, this symposium) are fully documented in this volume. A full description of the MAGIC model is given by Cosby *et al.* (1985*a*, *b*, 1986) and details of the optimization and calibration procedure used for these applications are identical to those given in Jenkins and Cosby (1989). Partial pressure of CO_2 in soil and lake water was identical for all applications. Organic matter concentration in soil water was 100 mmol m^{-3} at all sites and proportional to measured total organic carbon (TOC) in the surface water.

Comparison of reconstruction techniques

The historical pH reconstructions at each site are given in figure 1. The MAGIC pH reconstruction is shown as an envelope curve, the width of which represents uncertainty in the model output; the 'true' pH value may lie anywhere within the envelope. These uncertainty bands encompass the range of variable values that were simulated given the specified uncertainty in the fixed parameter values and measured target values used in the optimization procedure (Jenkins & Cosby 1989). Values for pH inferred from the diatoms are represented

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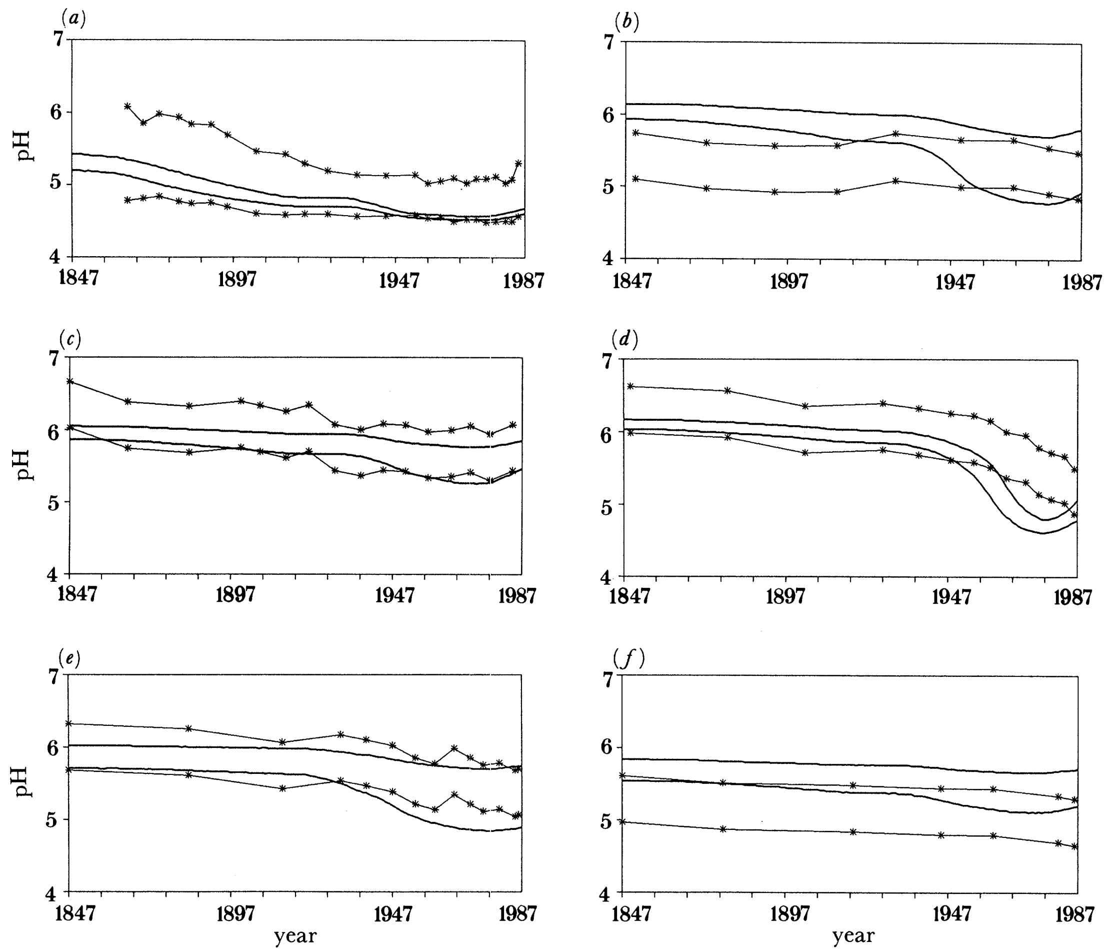

FIGURE 1. Historical pH trends reconstructed by MAGIC (thick lines) and diatoms (thin lines with asterisks) at (*a*) Round Loch of Glenhead, (*b*) Lochan Uaine, (*c*) Loch Tinker, (*d*) Loch Chon, (*e*) Loch Doilet and (*f*) Lochan Dubh.

as a series of points (asterisks), connected by thin lines. These represent the upper and lower standard errors of prediction for the weighted average pH reconstructions, estimated by bootstrapping (Birks *et al.*, this symposium). The overlap between the two reconstructions demonstrates a close agreement between the techniques in terms of the general pattern of historical acidification and timing of change. At L. Dubh and L. Uaine, however, the uncertainty bands from the two methods demonstrate the poorest agreement. These are high altitude sites where little pH change is predicted from a slightly acidic (pH 5.5–6.0) background (1847) level. At L. Uaine, MAGIC predicts a higher background pH although the uncertainty bands converge from 1940 onwards. At L. Dubh the diatom reconstructed pH is consistently lower than the MAGIC reconstruction. The predicted magnitude of pH change through the reconstruction period is consistent, however, being only *ca* 0.3 pH units for both methods. The background pH derived from both techniques for all lakes are in close agreement (figure 2*a*) and neither method shows a systematic bias. Comparison of observed and simulated present day pH (figure 2*b*), however, shows that both the MAGIC reconstructions, and to a lesser extent the diatom reconstructions, tend to underestimate observed mean pH. This problem

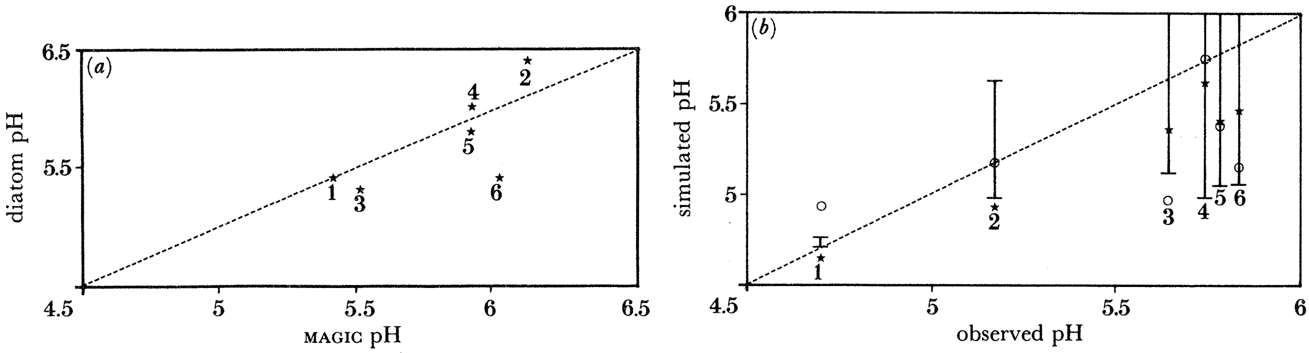

FIGURE 2. A comparison of (*a*) MAGIC and diatom reconstructed background (*ca.* 1850) pH and (*b*) present-day observed mean pH and that predicted from MAGIC (★) and diatom (○) reconstructions at Round Loch of Glenhead (1), L. Chon (2), L. Dubh (3), L. Tinker (4), L. Doilet (5) and L. Uaine (6). Solid bars represent the range of present-day measured pH values at each site.

tends to be exacerbated at pH greater than 5.5 although the simulated pH is almost always within the range of measured pH values at any site (figure 2*b*).

5. Reversibility of acidification

All of the MAGIC reconstructions demonstrate some degree of reversibility since the late 1970s (figure 1) as a direct consequence of the reduction in sulphate deposition since 1970. The deposition trajectory used in the model is based on data from the Warren Spring Laboratory (1987), which reports an almost linear decrease to approximately 50% of the 1970 level. This simulated recovery in pH is not always consistent with the diatom reconstructions although at Round Loch of Glenhead there is an agreement between the two techniques. A possible recovery is also indicated in the diatom reconstruction at L. Tinker. Battarbee *et al.* (1988) note a trend towards improved pH conditions at several other moorland sites in Scotland. The implication at the other four sites included in this analysis, however, is that the deposition trajectory is not applicable at all of the sites or that the pH change is as yet too small to be identified by diatom analysis.

It is predicted by MAGIC that under a range of deposition reduction scenarios reversibility of surface water acidification will continue and that greater deposition reductions will lead to increased surface water recovery (table 1). The simulations are run forward for 50 years to

TABLE 1. SIMULATIONS FROM MAGIC OF MEAN pH BY YEAR 2037 UNDER THREE FUTURE DEPOSITION REDUCTION SCENARIOS

(See text for details.)

	deposition reduction		
site	no reduction	30% reduction	70% reduction
Loch Doilet	5.0	5.2	5.4
Loch Chon	5.0	5.4	5.7
Lochan Dubh	5.2	5.3	5.4
Round Loch of Glenhead	4.7	4.8	5.0
Lochan Uaine	5.6	5.7	5.9
Loch Tinker	5.6	5.7	5.8

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2037 on the basis of three different scenarios: no deposition reduction from the present day; a 30 % linear reduction to the year 2000, then held constant at that level until 2037; a 70 % reduction to the year 2000, then held constant until 2037. At Round Loch of Glenhead, L. Chon and L. Doilet, a decrease of 70 % does not return the surface water to its background pH level and indeed, the predicted pH may still be too low for a self-sustaining fish population to be maintained (i.e. mean pH < 5.5) although this will depend on other chemical and biological factors. It is clear that at these sites further recovery of the surface water pH will only occur following more rapid recovery of the soil-base exchange capacity. A modelling analysis of the L. Chon system by Jenkins *et al.* (1989*b*) demonstrates that soil recovery occurs more slowly than surface water, even with relatively large reductions in sulphate input. At L. Chon and L. Doilet, however, the simulated pH reported in table 1 depends not only upon sulphate deposition levels but also on land management. The reported pH assumes that the forest, planted in the 1920s and 1950s at L. Doilet and L. Chon, respectively, remains in place for a further 50 years. This is unlikely in a commercial forest where trees are normally harvested after about 60 years. The surface water pH will then depend upon whether the forest is replanted or not and such considerations are detailed by Jenkins *et al.* (1989*b*). Furthermore, at L. Chon the high degree of recovery, simulated by MAGIC, in recent years (figure 1) and the level of future recovery (table 1) is greatly influenced by the very high calcium weathering rates, associated with a doleritic dyke, within the catchment. From this point of view L. Chon is not necessarily typical of forested catchments on bedrock with very low acid neutralizing capacity, which will recover only slowly (cf. L. Doilet).

Soil physical and chemical data were provided by Bob Ferrier, Bruce Walker, Basil Smith and Cyril Bown of the Macaulay Land Use Research Institute.

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Discussion

D. F. Charles (*Indiana University, Indiana, U.S.A.*). A concern has been raised at this meeting and elsewhere that computer models such as MAGIC do not account well for organic acids, especially for any change in output of organic acids from watersheds that may occur in response to increased acidic deposition.

A. Jenkins. The MAGIC model incorporates only a simple representation of the effects of organics on water chemistry. Organic matter concentrations for the soil water and stream water are specified, usually in proportion to TOC, together with dissociation constants derived from empirical relations. Organic concentrations are held constant at the specified level throughout the model simulation. In this form, the model has been applied to a Finnish lake (Liuhapuro) with high DOC (17.2 mg l^{-1}) and succesfully reproduces the pH decline indicated by palaeolimnological reconstruction. At present, the effect of increased acid deposition on the output of organic acid is not well documented and so cannot be represented in the model.

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