Chapter (non-refereed)

Jenkins, A.; Shaw, C.. 1993 Comparison of empirical and dynamic model approaches for surface waters. In: Hornung, M.; Skeffington, R. A., (eds.) *Critical loads: concept and applications.* London, HMSO, 109-114. (ITE Symposium, 28).

Comparison of empirical and dynamic model approaches for surface waters

A Jenkins & C Shaw

Institute of Hydrology, Wallingford, Oxfordshire OX10 8BB

INTRODUCTION

The purpose of determining critical loads is to set goals for a future deposition rate of acidifying compounds such that the environment is protected. The definition of the critical load for freshwater is: 'the highest load that will not lead in the long term (within 50 years) to harmful effects on biological systems' (Nilsson & Grennfelt 1988). Critical loads for water are defined, therefore, with the purpose of protecting a chosen sensitive receptor; for example, water acidification can lead to the decline or disappearance of natural fish populations. Commonly used criteria to protect aquatic organisms are that the runoff water should have positive alkalinity and a concentration of labile inorganic aluminium less than 50 $\mu g \, l^{-1}$ (Nilsson & Grennfelt 1988; Henriksen & Brakke 1988).

Once the protective criteria have been set and the timescale for these criteria to be met has been decided, the concept of the critical load for a catchment can then be regarded as a fixed value, altering only with major changes in chemical processes occurring within a catchment, eg brought on by afforestation. It represents a threshold specific to that catchment, below which no harmful effects should occur. Critical loads will differ for a given area as well as from site to site, depending upon the inherent sensitivity of the natural environment. Two methods have been advanced for calculating critical loads for freshwaters: steady-state water chemistry and dynamic modelling (Sverdrup, De Vries & Henriksen 1990). Dynamic models ('level 2' approach to critical load determination), however, are difficult to parameterise and calibrate for a site, requiring substantial data input, but perform an essential role within the critical loads exercise. The empirical ('level 1') approach assumes a steady state with respect to inputs to a catchment from the atmosphere, and take no account of timelags in response or of changes in land use; it therefore does not describe the time dependence of critical loads or assess the influence of land use. Only dynamic modelling can account for changes over time, such as the depletion of element pools in soils (Henriksen, Lien & Traaen 1990). This paper compares the two approaches, explores the impact of afforestation on critical load calculation, and assesses the inter-

relationships between sulphur and nitrogen deposition in estimating critical loads.

THE HENRIKSEN EMPIRICAL MODEL

This static model for surface waters is based upon the empirical link between present-day water and precipitation chemistry identified by Henriksen (1980), based on a regional study of lakes in Norway. The model is static in that it specifies the water chemistry resulting from a given change in deposition without specifying the time at which this new water chemistry will exist. Information as to the length of time required to achieve steady state following a change in acid deposition can be gained, but only through further experimentation. Conversely, the model cannot calculate a required deposition loading to achieve a specified water chemistry if a time limit is set. The empirical model takes no account of any future changes in land use and assumes that soils will de-acidify at the same rate at which they acidified. This soil buffering ability is represented in the model by an empirical factor relating the ratio of Ca and Mg to SO_4^{2-} ions in solution.

THE DYNAMIC MAGIC MODEL

MAGIC (Model for Acidification of Groundwater In Catchments) is an intermediate-complexity process-oriented model for constructing acidification history and predicting future acidification over time periods of decades to centuries (Cosby *et al.* 1985a, b). MAGIC makes use of lumped parameters on a catchment scale and focuses on chemical changes in the soil caused by atmospheric deposition, vegetation, and leaching to runoff. The processes in MAGIC include atmospheric deposition, sulphate adsorption, cation exchange, CO_2 dissolution, precipitation and dissolution of aluminum, chemical weathering, uptake and release of cations by vegetation, and export in runoff.

MAGIC has been used extensively in a variety of applications at sites in both North America and Europe. Application of MAGIC to the whole-catchment experimental manipulations of the RAIN project shows that this intermediate-complexity lumped model predicts the response of water and
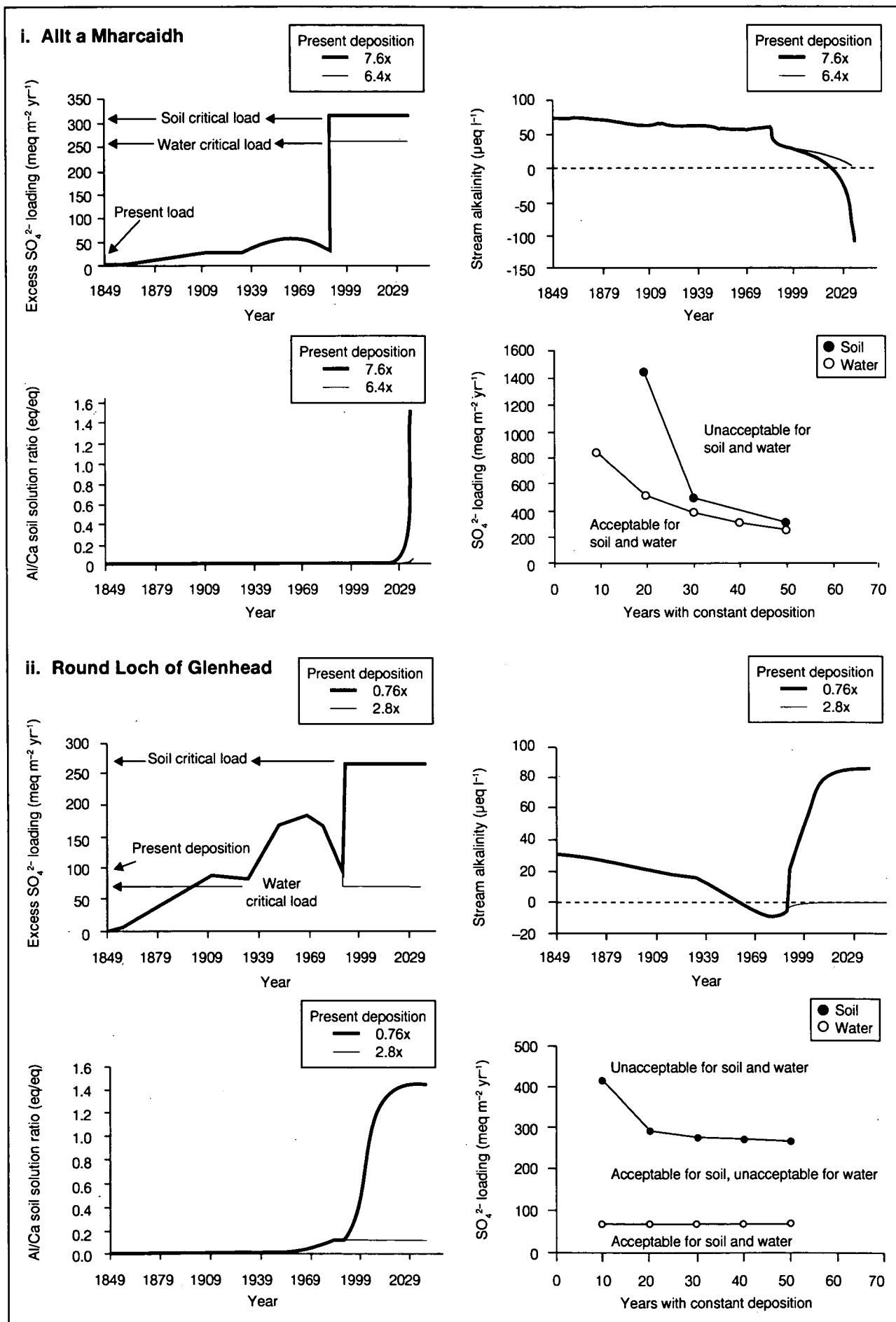
Figure 1. The historical sulphate deposition, stream alkalinity and soil water Al/Ca response at (i) Allt a Mharcaidh and (ii) Round Loch of Glenhead. Predictions of future response assume deposition held constant at the relevant sulphur loading into the future. A lower sulphur load is necessary if the critical chemistry is to be achieved over a shorter timescale

soil acidification to large and rapid changes in acid deposition (Wright et al. 1990). These results reinforce other evaluations of MAGIC, such as comparison with palaeolimnological reconstructions of lake acidification (Jenkins et al. 1990). The major processes by which forests influence surface water and soil acidification are also represented in MAGIC (Jenkins et al. 1990). In addition, several of the assumptions in MAGIC have been tested experimentally (Grieve 1989). Together, these applications indicate that MAGIC provides a robust tool for predicting future soil and water acidification following changes in acid deposition. It is one of several dynamic models included in the handbook on mapping critical loads, produced by the United Nations Economic Commission for Europe (Henriksen et al. 1989).

To calculate critical loads, the model is calibrated to a catchment using available soil and water chemistry and land use data. The model is then used in predictive mode to determine the sulphur deposition required to achieve some predefined critical chemistry in soil or surface water at some predefined time in the future. This critical chemistry is conventionally taken as a surface water alkalinity of zero (to protect brown trout (Salmo trutta)) and soil solution Al/Ca ratio (eq/eq) of 1.5 to protect forests, although, in practice, a critical load can be determined on any chemical parameter in the soil/water system. The timescale is taken as 50 years as this is the most appropriate timescale over which deposition reductions and critical chemistry should be achievable. The level of deposition required is assumed to be reached immediately and held constant at that level for 50 years. MAGIC is then run repeatedly with different levels of deposition until the critical chemistry is achieved. This deposition is assumed to be the critical load for sulphur, assuming that the loading and retention of nitrogen compounds are not changed from present-day conditions.

These concepts are illustrated in Figure 1. In Figure 1(i) (Allt a Mharcaidh), current and past sulphur deposition is not sufficient to depress stream alkalinity below zero or the Al/Ca ratio above 1.5, because the critical load is not currently exceeded at this site, and so the sulphur deposition is increased in the model to achieve alkalinity zero and thereby quantify the critical load. Figure 1(ii) (Round Loch of Glenhead) shows a site where present deposition exceeds the critical load for water and so must be reduced to achieve zero alkalinity, although the soil is not as sensitive.

COMPARISON OF TECHNIQUES

The empirical and MAGIC techniques for calculating critical loads generally compare favourably (Figure 2), and in most cases produce the same critical load category. There are, however, differences between the two methods caused by differences in the dynamic and equilibrium assumptions utilised (Figure 2). Across a wide range of critical loads, from
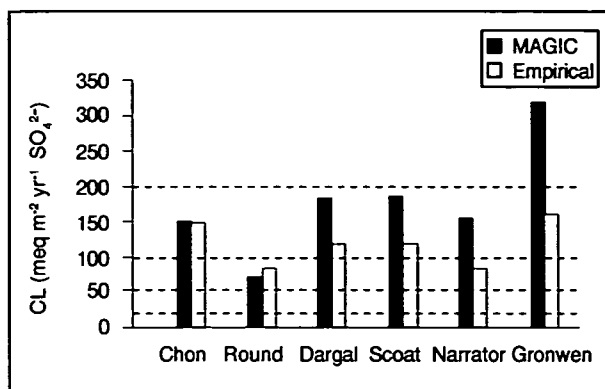

Figure 2. MAGIC and empirically calculated critical loads are in general agreement as regards critical load class

sensitive to insensitive, differences mainly occur at the least sensitive sites (ie high critical loads), where the MAGIC critical load is generally higher than the Henriksen empirical critical load, whilst at the most sensitive end of the range (ie low critical loads) the opposite is true. The less sensitive sites are characterised by well-buffered chemistry with high pH and alkalinity, influenced by soils which have retained a high acid buffering capacity. To deplete this soil store of base cations will either take many years of acid deposition at a relatively low sulphur loading, ie as described by the equilibrium concept assumed in the empirical critical load, or 50 years of a higher sulphur loading, as described by the dynamic MAGIC model. Sensitive sites are characterised by low pH and low, or in many cases negative, alkalinity and have soils with low base saturation and a large adsorbed sulphate pool. At these sites, the MAGIC critical load is lower than the empirical critical load, because the empirical approach assumes equilibrium conditions over an indefinite timescale whereas the dynamic modelling approach assumes a finite timescale. The MAGIC critical load is lower because these systems require longer than 50 years to recover, and the base cation store in the catchment soils which have been depleted by many years of acidic deposition and forest growth must be replenished by weathering inputs before recovery can occur.

The question of uncertainty in critical load calculation is difficult to address as much of the variance in surface waters will be due to the changing flow regime, and in particular the chemical changes associated with high flows. It must be remembered that the MAGIC model simulates only mean annual chemistry and takes no account of these flow/chemistry relationships. Uncertainty can be introduced into the model simulations, however, by incorporating known measurement errors and spatial variability in the parameters within the catchment at the calibration stage (Jenkins & Cosby 1989). In this way, uncertainty bands for the model simulations can be presented as maximum and minimum values for output variables, including target loads (Figure 3). A range of critical loads can also be calculated
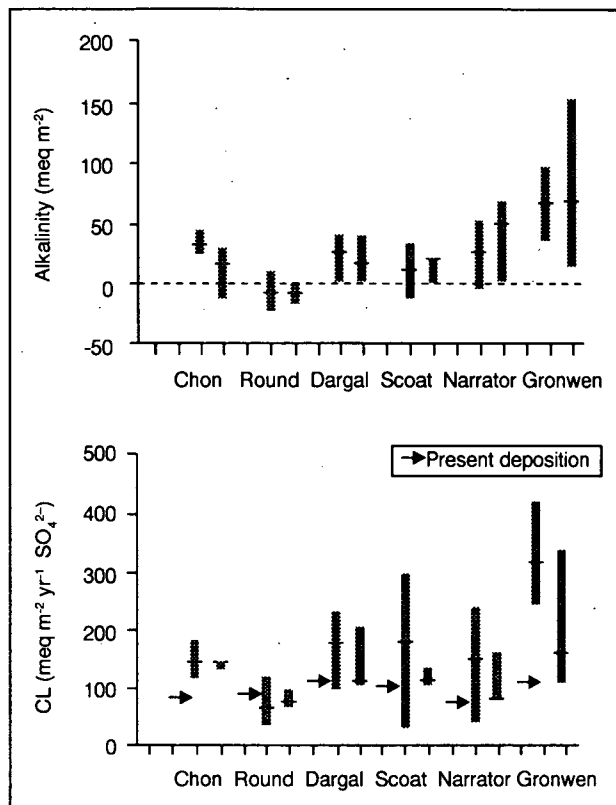
Figure 4. The time dependency of the critical load calculation using MAGIC. The longer the timescale over which the critical chemistry is to be achieved, the lower the critical load required to protect sites currently in exceedance, such as Round Loch. Where a site has to acidify in order to reach the critical load, as at Narrator, the opposite is true

Figure 3. Comparison of the uncertainty in model simulations of stream or lake alkalinity (top) or critical loads (bottom). In each case, the vertical bars represent the range of observations, or of model simulations derived by varying the input parameters across a likely range of error, and the horizontal bar is the mean. For each site, two values are shown: MAGIC simulations on the left in each case; observed (top) or empirical model simulations (bottom)

sulphate). This time-dependent effect can be identified using MAGIC, and Figure 4 (also illustrated in Figure 1) indicates that the target year by which the critical chemistry is to be reached produces variation in the calculated critical load.

THE INFLUENCE OF AFFORESTATION

The role of trees in the critical loads concept requires careful consideration. As well as being sensitive receptors for which critical loads need to be determined, trees play a crucial role in the soil and water acidification process by the uptake of base cations for growth, changing hydrological behaviour, and by scavenging pollutants from the atmosphere thereby increasing the deposition. Figure 5 shows critical loads calculated for the forested Loch Chon catchment in central Scotland using the MAGIC model (see Jenkins *et al.* 1990 for details). Three future afforestation scenarios are utilised in the critical load calculations:

empirically for samples collected across a wide range of flows. The ranges calculated from the two techniques demonstrate a good match (Figure 3), although the representations of uncertainty have little statistical significance, and further work is necessary, in particular to assess the importance of episodes to biological response and to relate the mean chemistry to extreme events.

The empirical approach to critical load calculation, based on the long-term weathering rate at a site, is time-independent, ie steady-state conditions are assumed, so that the timescale over which the new equilibrium at the critical chemistry will be achieved is irrelevant in the calculation. It is also assumed, perhaps more crucially, that the site is capable of recovering to the target chemistry level and that, prior to the onset of acidification, the water chemistry was equivalent to, or less acidic than, the target chemistry. Furthermore, the influence of the catchment soils, in particular their ability to adsorb and desorb ions through time, is only implicitly included in the empirical model, which assumes that the soil acidification process is completely reversible in the very long, or equilibrium, timescale. Soil chemical processes may mitigate or delay acidification through sulphate adsorption and base cation exchange, or extend the acidification effect after acidic deposition is reduced through soil recovery (adsorbing base cations and desorbing
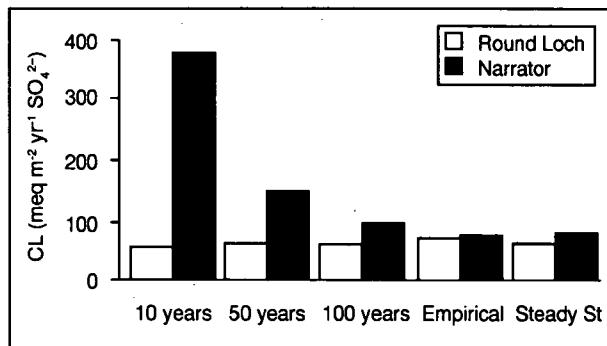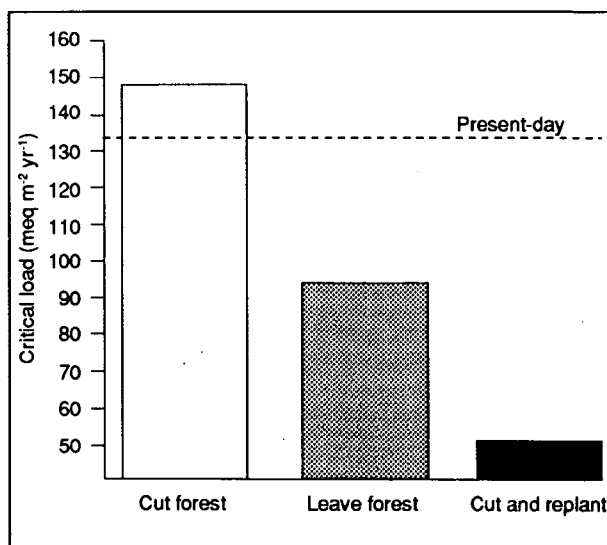

Figure 5. Critical loads calculated using MAGIC under three future afforestation scenarios

- leave the forest in place for a further 50 years;
- cut the forest immediately and leave as a moorland site for 50 years;
- cut the forest immediately and replant the entire area.

The results (Figure 5) show that the acidification stress occurring within the catchment, due to the second-rotation forest, is clearly reflected in the calculation of a low critical load, whilst the relative recovery following deforestation with no subsequent replanting changes the catchment processes to afford a slightly higher critical load than for the 'constant' forest scenario. Clearly, the calculation of critical loads for soil and freshwaters in areas where plantation forestry is a major land use requires that these impacts be considered.

THE INFLUENCE OF NITROGEN DYNAMICS

Although nitrogen is dealt with in an extremely simplified manner in MAGIC, uptake being modelled as a first-order function, the model can be used to illustrate the influence of nitrogen dynamics in calculating critical loads for sulphur. An increase in nitrate leaching from a catchment in surface waters may occur as a result of increased nitrate deposition, decreased plant uptake of nitrate (perhaps due to sulphur-induced stress on the organisms), or through a change in climatic conditions leading to increased mineralisation of nitrogen in the soil. Describing this increased nitrate leakage simply as a decrease in catchment uptake, we can evaluate the relative effect on sulphur target load. If nitrate increases in surface water, the target load of sulphur decreases (Figure 6).

CONCLUSIONS

In addition to the factors considered here, long-term climate change will potentially have an important effect on calculated critical loads for soils and water. This effect can o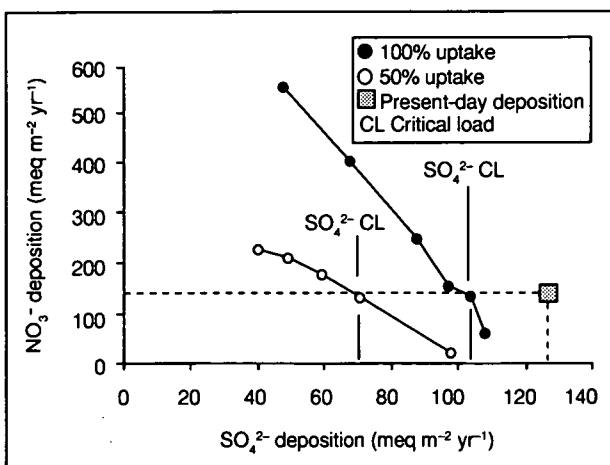nly be realistically quantified through the application of dynamic models. Such models will, however, need to incorporate explicitly the processes and driving variables leading to increased nitrate leaching from catchment soils. The role of land use and climate change and the interaction between sulphur and nitrogen dynamics make the use of dynamic models mandatory within the critical loads framework. It is also clear that the models represent a powerful tool in the determination of target load strategies and for assessing the consequences of not achieving critical loads.

Critical loads estimated using MAGIC represent the change in deposition flux which must be made immediately to achieve zero alkalinity, and so must be regarded as a 'best case', as sulphur deposition is more likely to be reduced gradually over a long time period. On the other hand, if an equilibrium timescale is considered such that the recovery time of the system is of no great importance, then the empirical calculations are adequate. Under the empirical critical load deposition scenario, however, it is possible that a number of surface waters in the UK will not be restored to positive alkalinity within the lifespan of the existing population.

Figure 6. The interaction between sulphur and nitrogen critical loads. The graph shows MAGIC calculations of critical loads for sulphate at a given N deposition, assuming 100% or only 50% N uptake. Sulphate critical loadings for these two assumptions at the present rate of N deposition are shown on the graph

REFERENCES

Cosby, B.J., Hornberger, G.M., Galloway, J.N. & Wright, R.F. 1985a. Modelling the effects of acid deposition: assessment of a lumped-parameter model of soil water and streamwater chemistry. *Water Resources Research*, **21**, 51-63.

Cosby, B.J., Wright, R.F., Hornberger, G.M. & Galloway, J.N. 1985b. Modelling the effects of acid deposition: estimation of long-term water quality responses in a small forested catchment. *Water Resources Research*, **21**, 1591-1601.

Grieve, I.C. 1989. A laboratory test of the soil chemical submodels of two models of catchment acidification. *Hydrological Processes*, **3**, 339-346.

Henriksen, A. 1980. Acidification of freshwaters - a large-scale titration. In: *Ecological impact of acid precipitation*, edited by D. Drablos & A.Tollan, 68-74. Oslo: SNSF.

Henriksen, A. & Brakke, D.F. 1988. Increasing contributions of nitrogen to the acidity of surface waters in Norway. *Water, Air and Soil Pollution*, **42**, 183-201.

Henriksen, A., Lien, L., Rosseland, B.J., Traaen, T.S. & Sevaldrud, I.S. 1989. Lake acidification in Norway - present and predicted fish status. *Ambio*, **18**, 314-321.

Henriksen, A., Lien, L. & Traaen, T.S. 1990. *Critical loads for surface waters: chemical criteria for inputs of strong acids.* (Report 0-89210.) Oslo: Norwegian Institute for Water Research.

Jenkins, A., Whitehead, P.G., Cosby, B.J. & Birks, H.J.B. 1990. Modelling long-term acidification: a comparison with diatom reconstructions and the implications for reversibility. *Philosophical Transactions of the Royal Society of London B*, **327**, 435-440.

Jenkins, A. & Cosby, B.J. 1989. Modelling surface water acidification using one and two soil layers and simple flow routing. In: *Regional acidification models*, edited by J. Kamari, D. Brakke, A. Jenkins, S. Norton & R. Wright, 253-267. Heidelberg: Springer-Verlag.

Nilsson, J. & Grennfelt, P., eds. 1988. *Critical loads for sulphur and nitrogen.* (Report 1988: 15.) Copenhagen: Nordic Council of Ministers.

Sverdrup, H., De Vries, W. & Henriksen, A. 1990. *Mapping critical loads. Guidance to criteria, methods and examples for mapping critical loads and areas where they have been exceeded.* Annex to the UN-ECE Task Force on mapping manual on methodologies and criteria for mapping critical levels/loads and geographical areas where they are exceeded. (Report 1990: 14, Nord 1990: 98.) Copenhagen: Nordic Council of Ministers.

Wright, R.F., Cosby, B.J., Flaten, M.B. & Reuss, J.O. 1990. Evaluation of an acidification model with data from manipulated catchments in Norway. *Nature, London,* **343,** 53-55.