Integrated Assessment of Acid Deposition Impacts Using Reduced-Form Modelling

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ABSTRACT

Emissions of sulphates and other acidic pollutants from anthropogenic sources result in the deposition of these acidic pollutants on the earth's surface, downwind of the source. These pollutants reach surface waters, including streams and lakes, and acidify them, resulting in a change in the chemical composition of the surface water. Sometimes the water chemistry is sufficiently altered so that the lake can no longer support aquatic life. This document traces the efforts by many researchers to understand and quantify the effect of acid deposition on the water chemistry of populations of lakes, in particular the improvements to the MAGIC (Model of Acidification of Groundwater in Catchments) modelling effort, and describes its reduced-form representation in a decision and uncertainty analysis tool. Previous reduced-form approximations to the MAGIC model are discussed in detail, and their drawbacks are highlighted. An improved reduced-form model for acid neutralising capacity is presented, which incorporates long-term depletion of the watershed acid neutralisation fraction. In addition, improved fish biota models are incorporated in the integrated assessment model, which includes reduced-form models for other physical and chemical processes of acid deposition, as well as the resulting socio-economic and health related effects. The new reduced-form lake chemistry and fish biota models are applied to the Adirondacks region of New York.

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NOTATION

a, b, c, d	Parameters for the pH-ANC relationship
b'	Intercept factor for the Equilibrium lake calcium relationship
Al	Lake Aluminium (in $\mu\text{eq/L}$ unless stated otherwise)
ANC_t	Lake Acid Neutralising Capacity at t (in $\mu\text{eq/L}$ unless stated otherwise)
$\text{ANC}_{s,t}$	Soil Water ANC (in $\mu\text{eq/L}$ unless stated otherwise)
ANC_{se}	Equilibrium Soil Water ANC (in $\mu\text{eq/L}$ unless stated otherwise)
ASI	Acid Stress Index
CA	Total Acid Anion Concentration
Ca_t	Lake Calcium at time t (in $\mu\text{eq/L}$ unless stated otherwise)
Ca_e	Equilibrium value of Lake Calcium (in $\mu\text{eq/L}$ unless stated otherwise)
CB	Total Base Cation Concentration
CMR	Conditional Mortality Rate
CPUE	Catch Per Unit Effort
d_f	Fraction of direct runoff without neutralisation of acid
D_0	Acid deposition in the base year (1985), in $\mu\text{eq/L}$
D_t	Acid deposition at time t, in $\mu\text{eq/L}$
Dep_t	Average acid deposition over a time period, in $\mu\text{eq/L}$
DNF	Nominal Deposition for no change in N_F , in $\mu\text{eq/L}$
δt	Time period between successive data points, in years

IA	Integrated Assessment
m	Slope factor in the Neutralisation Fraction, Ca_t and Ca_e relationships
μ	Mean
v	Coefficient of variation
N	Total number of fish species present in a lake
$N(0,1)$	Unit normal distribution
$N_{F,0}$	Initial watershed Neutralisation Fraction in the base year (1985)
$N_{F,t}$	Watershed Neutralisation Fraction at time t
pH	Lake pH
$P(\bullet)$	Probability of ...
RFM	Reduced Form Model
σ	Standard deviation
t	Time in years
τ	Lag factor for the Soil Water ANC and Calcium relationships
θ, ξ, ϕ	Parameters for the 3-parameter lognormal regional ANC distribution
tp	Time periods elapsed till time t ($=t/\delta t$)
WTP	Willingness-to-Pay, a measure of how much money for increased travel costs an angler is willing to pay to go to a fishing site.

SYMBOLS

g	Gram (= 1000 mg)
ha	Hectare (= 10000 m ²)
kg	Kilogram, S.I. Unit of Mass (= 1000 g)
L	Litre (= 1000 cm ³)
m	Metre, S.I. Unit of Length (= 100 cm)
mg	Milligram (= 1000 µg)
meq/L	Milli-equivalents per litre (= 1000 µeq/L)
µeq/L	Micro-equivalents per litre
µg	Microgram
s	Second, S.I. Unit of Time
yr	Year ($\approx 3.154 \times 10^7$ s)

1. INTRODUCTION

1.1. EXECUTIVE SUMMARY

The National Acid Precipitation Assessment Program was mandated by the Congress to track compliance with Title IV of The Clean Air Act Amendment of 1990. In order to link science to policy, it was proposed to create the Tracking and Analysis Framework which is a modular, integrated modelling and decision analysis tool incorporating the relevant science and policy issues.

The Tracking and Analysis Framework (TAF) project provides an integrated assessment framework for the National Acid Precipitation Assessment Program (NAPAP) with which to evaluate the environmental and economic impacts of acidic deposition. The TAF prototype includes a series of linked reduced-form models incorporating uncertainty and intended to provide the foundation for informed decision-making regarding emissions controls and regulations for nitrogen and sulphur. Each of the reduced-form models in TAF is based on a state-of-the-art full-form model, and provides input and output specifications for one or more components of the acidic deposition effects problem (e.g. deposition, aquatic effects, valuation, etc.). The aquatic chemistry module is constructed as a reduced-form representation of the Model of Acidification of Groundwater in Catchments (MAGIC). The soil solution chemistry module is also a reduced-form approximation to MAGIC, and is closely related to the aquatics module. The Aquatics module and the Soils module share information regarding watershed characteristics in the Adirondacks. So closely related are they that in TAF they have been combined into a single Soils-Aquatics Module. This document describes the Aquatics portion, and references to the Soils portion

are made wherever relevant. The Soils-Aquatics Module is demonstrated and applied using a representative set of lakes for the Adirondacks region of New York.

Since TAF is an integrated assessment effort, each module provides an output to another "downstream" module for further effects or economic analysis. The Aquatics module relates wet and dry deposition of sulphate, nitrate and other ions to changes in lake chemical properties such as acid neutralising capacity (ANC), lake calcium, lake pH, lake aluminium and measures of the ability of a lake to support each of three fish species. TAF is implemented in Analytica™, which is a decision modelling and analysis software. Analytica propagates uncertainty through all the sub-modules of TAF by Monte Carlo simulation. Therefore, the effect of proposed emission reductions from power utilities on the benefits accrued from recreational fishing in lakes can be studied and evaluated in an efficient manner. Sensitivity analysis of the input parameters can be performed to determine the most important parameters in the model. Analytica uses a modular, layered design that allows for rapid prototyping of models, and provides a ready-made framework to compare alternative models.

The aquatic chemistry module generates uncertain time series outputs for lake chemistry variables such as Acid Neutralising Capacity (ANC), pH, calcium and aluminium. Changes in lake chemistry are used to estimate the ability of the lake to support fish life. This information is used by the TAF economic benefits module.

1.2. ORGANISATION

This document is divided into sections, each of which deals with a different aspect of this research effort. Section 1 describes the overall *raison d'être* for this work and the

structure and organisation of the document. Section 2 is a description of the reduced-form modelling methodology and its application to integrated modelling in general and to TAF in particular. Section 3 deals with the efforts to study and model surface water systems affected by acid deposition. The MAGIC model is described, along with the improvements implemented for the TAF project. Significant conclusions from the NAPAP Integrated Assessment in 1990 are presented. Section 4 starts with a brief description of earlier reduced-form models for aquatic chemistry. A detailed description of the aquatics reduced-form models for TAF follows. The mathematical formulation, calibration to MAGIC and a description of how MAGIC and reduced-form model uncertainty are incorporated into TAF are documented in this section. Section 5 is a discussion of how changes in lake chemistry influence the ability to support fish. Three different measures of the ability of a lake to support fish are presented. The TAF aquatics module contains all three measures, one of which is used by the TAF economic benefits module to assign a dollar value to lakes which are not acidified and can therefore support recreational fishing. Section 6 is a short conclusion and discussion of possible future work. This document concludes with a bibliography and Appendices containing excerpts from the SASTM program code used to generate and test the reduced-form models and evaluate uncertainty over the parent MAGIC model and the Analytica implementation of the reduced-form models. All physical and chemical quantities are in S.I. units.

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2. REDUCED-FORM AND INTEGRATED MODELLING

2.1. HOW REDUCED FORM MODELLING WORKS

Traditional modelling is domain specific and involves deriving a mathematical formulation based on empirical data and the underlying physical or chemical processes for the domain. The model is then checked against other data sets. However, the modeller receives his or her input data from experimentalists or other models and produces output from the model in a proprietary format. Output data from an atmospheric transport and deposition model may be of use to a surface water chemistry modeller. However, this data exchange is fraught with problems of incompatibility of format, type, numerical precision or range. Each modeller is aware only of his or her particular domain, and not of the "big picture". Another problem arises when a model is changed - all downstream models have to be rerun with the new outputs from the altered model. Even more complicated is the issue of characterising uncertainty. It is very difficult to decide which parameters in a model influence a certain output in another model to the greatest extent. It is in such situations that Integrated Modelling is appropriate.

An integrated modelling tool provides an environment where all modellers can construct their models in a common, standardised setting. Data structures can be global, which would allow them to be visible to other models. This allows seamless exchange of data between models. Data structures can also be local, meaning that they are visible only to the model in which they are defined. A change in one model will automatically be propagated to all other dependent models. If the tool supports uncertainty, Monte Carlo sampling will allow uncertainty to be propagated from one model to another. However,

combining several models into a single structure can be a daunting task, and is often limited by problems of computer storage.

This is why a “reduced-form” model is created from a larger model. A reduced-form model mimics to a large extent the behaviour of the more complicated parent model, but at a very significant savings in terms of storage, computation time and complexity. The simplest type of reduced-form model is a look-up table, which contains all the possible inputs and outputs (or a sufficiently dense grid so that interpolation is possible without much error) in a multidimensional table. If the model has n inputs and m outputs, the look-up table has dimensions of $n+m$. For a large number of inputs and outputs, however, this is not practical. A slightly more complicated reduced-form model is a curve-fit to the inputs and outputs using linear or non-linear regression techniques. Such a curve fit is also called a response surface when its dimensionality is more than 2. This method is more storage efficient than the look-up table method, but fails to capture any of the domain-specific processes in the mathematical formulation. It is a purely mathematical construct used to match the input data to the outputs. The “third generation” of reduced-form models are those which incorporate some domain knowledge in the form of equations and variables that represent the physical or chemical quantities in the processes being modelled. The reduced-form models presented here all fall into this category.

The Tracking and Analysis Framework (abbreviated as TAF for the remainder of this document) is a combination of several first, second and third generation reduced-form models (called “modules”), each of which represents a particular domain related to acid deposition. Most of these modules incorporate uncertainty. The TAF Soils-Aquatics Module incorporates the uncertainty in MAGIC as well as the error in the reduced-form model fit to MAGIC. Such a framework is called an Integrated Model.

Similarly, integrated modelling has been successfully applied to multidisciplinary problems in the behaviour of non-crystalline solids (Kamihori et al., 1994), in control systems (Blankenship et al., 1995) and in hardware and software systems (Stoy and Peng, 1994). This methodology allows for easy linkage of several models from diverse domains in such a way as to allow for propagation of uncertainty throughout the system. Rapid prototyping is also possible, since a working prototype can be assembled in a fraction of the time it takes to run each individual module separately and pass the output to all dependent modules. If the tool used offers an intuitive interface, then communicating the suite of models to other researchers is also possible.

2.2. PREVIOUS ATTEMPTS AT INTEGRATED ASSESSMENT

The tool used in TAF is Analytica™ (earlier versions of which were called Demos™), which provides an easy-to-use graphical user interface for model creation and uncertainty propagation. Figure 1 shows the top-level TAF influence diagram.

Figure 1. TAF Top-Level Influence Diagram

Several integrated assessment models have been constructed using this tool. One such work-in-progress is the Integrated Environmental Control Model (IECM), which quantifies the performance and cost of power plant designs incorporating user-specified combinations of pre-combustion, combustion and post-combustion methods of environmental control (Small and Kalagnamam, 1994). It is possible to analyse advanced technologies at an early stage of development, and to compare them against conventional technologies where uncertainties are usually smaller. Each performance module is augmented with an economic model which estimates the capital cost, the annual operating cost and the total levelised cost of each technology. Input parameters can be specified, after which the model takes over and computes the desired outputs. Analytica propagates

uncertainty through the model, and outputs are typically viewed as cumulative probability distributions.

An earlier version of TAF, which incorporated an implementation of the Direct Distribution Model (Small and Sutton, 1986b) was also implemented in Demos. Some climate models are modelled in Analytica, including ICAM (Integrated Climate Assessment Model), developed by Dowlatabadi and co-workers (Dowlatabadi and Morgan, 1993).

2.3. ABOUT TAF

As part of the Clean Air Act Amendments (CAAA) of 1990, the National Acid Precipitation Assessment Program (NAPAP) was asked to evaluate the status of implementation, the effectiveness and the costs and benefits of the acid-deposition control program created by Title IV of this Act, and to determine whether additional reductions in deposition are necessary to prevent adverse ecological effects. To be able to perform such an evaluation, the Tracking Analysis Framework (TAF), an integrated assessment model was developed. This is one of the first tools of its kind to explicitly link science and policy in a single framework. TAF links the important components of acid deposition together, namely emissions, permit trading and control costs, atmospheric transport and deposition, and environmental effects on lakes, soils, visibility and crops.

The goal of TAF is to integrate credible models of the science and technology into an assessment framework that can directly address key policy issues, and in doing so act as a bridge between science and policy (Henrion et al., 1995). This framework helps to support co-ordination and communication among scientific researchers, to support

communication with policy makers, to provide rapid response for analysing newly emerging policy issues and to provide guidance for prioritising research programs.

Integrated assessment is a complex activity requiring the participation of several organisations with different interests. The TAF development group consists of a team of researchers from national laboratories, universities, private companies and non-profit research institutes who have developed the TAF software using the Analytica™ development environment. TAF provides comprehensive coverage of the costs, benefits and effectiveness of the CAAA Title IV. It incorporates technically credible models and up-to-date databases to track compliance with Title IV. It provides the ability to do cost-benefit analysis. Uncertainty is represented and propagated through all the models in TAF. It is possible to use TAF to identify sensitive indicators of atmospheric pollution and acid deposition. It is also possible through analysis of data from ongoing monitoring programs to detect trends in these indicators. Finally, TAF models are transparent and model documentation is incorporated within each model. This approach minimises the chances of inconsistency and incompleteness in the documentation.

3. DATA AND MODELS FOR SURFACE WATER SYSTEMS

3.1. HISTORICAL BACKGROUND

In the 1970s and early 80s, evidence from site-specific studies in the United States and Canada indicated that declines of pH and ANC in surface waters had occurred over time. These conditions had been caused by acidic deposition from anthropogenic sources releasing acidic pollutants into the atmosphere.

There was considerable uncertainty in extrapolating the site specific results to a regional or national scale because of (1) the degree to which individual study sites represent larger regional populations, (2) unknown bias in lake selection, (3) absence of measurements of chemical variables that are critical to assessing chemical or biological effects, (4) difficulty in comparing data collected by different and sometimes unknown methods and (5) inconsistent documentation of quality assurance protocols. The Eastern Lake Survey (ELS: Overton et al., 1986 and Kanciruk et al., 1986) was conducted to determine the chemical variables pH, ANC, major ions like Al^{3+} , Ca^{2+} and others for the lakes in the Eastern United States. The critical issue in the design of the survey was the chemical characterisation of regional lake populations. Chemical measurements for a lake, such as pH and ANC, are subject to spatial and temporal variability. It was recognised that it was not essential that the index sample be taken at a time of worst-case conditions. It was more important that the index sample be collected at a time when within lake spatial variability is small. Samples were collected in the fall when spatial variation within the lake is reduced as the lake undergoes a period of mixing that may last four to eight weeks. Samples were collected in the deepest part of the lake to represent the dominant water mass.

A stratified sampling method was used by which sample lakes were allocated equally among strata (Landers et al., 1988). There were three levels of stratification. The first was by region, and there were three regions, namely the North East, the Upper Midwest and the South East. Each region was divided into subregions, where each subregion in each region was relatively homogeneous with respect to water quality, physiography, vegetation, climate and soils. Based on this homogeneity, five subregions were identified in the Northeast, four in the Upper Midwest and two in the Southeast. Each subregion was divided into alkalinity map classes, based on the predominant range of surface water alkalinity values, namely $< 100 \mu\text{eq/L}$, $100\text{-}200 \mu\text{eq/L}$ and $> 200 \mu\text{eq/L}$. All three alkalinity map classes were found within each of the eleven subregions. Lakes were selected in such a way that each lake in a stratum had an equal probability of inclusion. Lakes with a surface area < 4 ha were an important resource that were not considered in this survey. Small lakes are often lower in pH and ANC than larger lakes in the same geographic area.

There is substantial evidence that surface water chemical characteristics during Spring may be less favourable for biota than during Fall (Landers et al., 1988), possibly due to snow melt and subsequent runoff into surface waters. Florida has been shown to have a high percentage of acidic lakes (22%) and this may be due to the warmer climate in the Florida region. But Florida is an area receiving only moderate loadings of sulphur. At the time when the results of the survey were made available, this anomaly could not be explained. But these new data made it possible to apply empirical models to evaluate lake acidification associated with loadings of sulphur deposition, explore the importance of organic acids and to test the hypothesis of regional scale lake acidification caused by neutral salts.

3.2. CURRENT UNDERSTANDING OF THE PROBLEM

3.2.1. Dynamic Models

Since the collection of the Eastern Lake Survey, the state-of-the-art has advanced a great deal. Dynamic, mechanistic models have been developed to simulate the acidification processes with a high degree of detail. These models are useful to study individual lake systems in detail and they provide a framework for advancing the state of knowledge of the fundamental mechanisms of acidification (Small and Sutton, 1986). For assessing the acidification in an entire region, predictions are required for many lakes and generating and evaluating a dynamic model for each lake and calibrating the model for each lake system is a very difficult task. Dynamic models have been developed by Chen et al., 1982, Christophersen and Wright et al., 1981, Galloway et al., 1983, Cosby et al., 1985a and 1985b and other workers. A summary of MAGIC, the mechanistic model used for TAF is presented here. For a more detailed discussion, see § 3.3.

3.2.1.1. *MAGIC: The Model of Acidification of Groundwater in Catchments*

Regional mechanistic models attempt to represent actual chemical reactions in the catchment under consideration using kinetic and equilibrium expressions for the underlying geochemical processes. In such models, for the sake of simplicity, spatial variations within the watershed are not considered. Regionalisation is achieved using Monte Carlo methods which produce a set of statistically representative lakes for the region. This set of lakes (the artificial or simulated data set) is identified by selecting parameter distributions from the

expected range of values for typical lakes in the region. These distributions are randomly sampled and the model is calibrated by accepting a set of parameter inputs which generates the current distribution of lake chemistry. Accepted parameter sets are stored and form the set of simulated lakes. This set is then used to simulate the response of the region to future changes in deposition.

There are two principal regional mechanistic models currently in use, namely the RAINS Lake Model and the MAGIC model. RAINS is the Regional Acidification Information and Simulation Model (Alcamo et al., 1987; Kämäri, 1990; Posch and Kämäri, 1990), developed by the International Institute for Applied Systems Analysis and was formulated to help decision makers evaluate policies for controlling the impact of acidic deposition in Europe. The model was designed to be a simple dynamic model with a regional scale focus rather than a watershed focus. The model contains modules for sulphur emissions, meteorological atmospheric transport and deposition, hydrology and soil chemistry. The model uses a Monte Carlo approach for simulating distributions of effects on a regional basis.

MAGIC is an intermediate complexity process oriented model of catchment soil and stream water chemistry (Cosby et al., 1985a). It incorporates a small number of processes which are assumed to be important in influencing the long-term response of surface waters to acidic deposition. These soil processes are: (1) base cation exchange in soils, (2) dissolution of aluminium hydroxide, (3) solution of carbon dioxide in soil solution and subsequent carbonic acid dissociation, (4) sulphate adsorption in soils and (5) mineral weathering.

Processes 1 through 3 are modelled based on the Reuss-Johnson soil chemistry model (Thornton et al., 1990). Sulphate is assumed to have an adsorbed phase and to

follow a Langmuir isotherm. The first four processes equilibrate rapidly and are assumed to occur instantaneously in soils. A simultaneous equilibrium is computed at each time step. Changes over time steps are calculated by computing a mass balance for the total amount of base cations and strong acid cations in the watershed. Inputs are by acidic deposition and net uptake and release in the watershed, primarily mineral weathering minus biological uptake.

MAGIC represents the watershed with two soil-layer compartments arranged vertically and assumed to be areally homogeneous. Typical temporal resolution is annual, but monthly output can also be obtained. Numerical integration techniques are used in which the two soil compartments and the lake compartment are treated as continually stirred tank reactors. The efflux of a given chemical component from a compartment is calculated as the difference between the influx product of the rates and durations of reactions occurring within the compartment at each time step. Watershed flow data are averaged to obtain monthly or yearly values before being used in MAGIC.

MAGIC was specifically formulated for the purpose of conducting long-term simulations. It does not simulate short term episodic events. MAGIC has been modified to include organic acids, based on the work of Driscoll et al. (1994). Labieniec et al. (1989) showed that the Direct Distribution Model (DDM) of Small and Sutton (1986b) could approximately mimic the predictions of MAGIC for a set of lakes in southernmost Norway. More recently, Small et al. (1995) have shown that the Direct Distribution model can be used as a simplified approximation to MAGIC for the Adirondack subregion, albeit with two shortcomings :

1. The DDM fails to capture the slow, long-term acidification predicted by MAGIC.
2. The rate and magnitude of the regional recovery is overestimated by the DDM.

This systematic difference between the models is due to the ongoing loss of base saturation in soils simulated by MAGIC as acid loads ensue and persist (Small et al, 1995).

Simplified nitrogen cycling has recently been incorporated in MAGIC (Sullivan and Cosby, 1995a), based on the following processes. The two major pathways of nitrogen input to terrestrial ecosystems are atmospheric deposition and biological fixation. Deposited nitrogen can remain on plant surfaces for some time, only to be moved again by wind or dissolved by rain so that it can enter the soil or run off into surface waters. When atmospheric nitrogen is deposited on land, various processes determine its fate. Because many of these processes are mediated by biological agents, they are seasonal and highly dynamic.

Some specialised organisms convert atmospheric N to NH_3 , thereby making it biologically active. Nitrogen mineralisation is the conversion of organic nitrogen to inorganic forms, primarily NH_4^+ and NO_3^- . There are two processes involved in this conversion. The first is ammonification, by which organic nitrogen is converted to NH_3 which in turn is converted to NH_4^+ in the soil. The second is nitrification, which involves the bacterial conversion of NH_4^+ to NO_3^- . Ammonification is carried out by micro-organisms that are favoured by warm temperatures, high organic content and high soil moisture. As a result of the diversity of the micro-organisms involved, the process takes place over a wide range of environmental conditions. Nitrifying bacteria are very sensitive to soil moisture content. Nitrification is more rapid in well-aerated and drained soils. Total nitrogen in the soil declines sharply with depth, while the proportion of fixed NH_4^+ increases with depth. A simplified representation of nitrogen cycling has been incorporated in MAGIC.

3.2.2. Empirical Equilibrium/Steady State Models

Steady state models have no time component. Most steady-state models use information describing the current state of the water chemistry in the lake to predict: (1) the original water chemistry before any acid deposition and (2) the eventual future condition assuming a constant deposition rate. The major advantage over dynamic models is that they require less data and can be applied where insufficient data exist to apply dynamic models.

Most steady state models explicitly consider only some of the components of lake ANC, namely bicarbonate (HCO_3^-), carbonate (CO_3^{2-}) and hydroxide (OH^-), and not organic anions or Al (Wright and Henriksen, 1983). Therefore these models predict the effect of acid deposition on alkalinity and not on ANC. In estimating pH from alkalinity, most of these models use time-independent empirical relationships derived from lake surveys which implicitly account for the effect of other constituents on pH such as organic anions and Al (Schnoor et al., 1984 and 1986). None of these models consider the possibility of a change in organic acid concentrations as a result of acidification. However, recent studies suggest that this oversight is likely to cause only slight overestimates of acidification. Some steady-state models such as the Henriksen model (Wright and Henriksen, 1983) cannot be applied to systems with significant watershed sulphur sources. However, such sources are not significant for low pH ($\text{pH} < 6$) lakes in the Northeast. Also, some workers have suggested that forest growth is also responsible for acidification of soils and surface waters, but none of these models accounts for forest-growth related acidification.

Empirical equilibrium models have been developed that use steady state chemical weathering and ionic electroneutrality to calculate a steady state alkalinity given an acid deposition rate. These models are easier to apply than the dynamic models, but certain

difficulties persist. Weathering rates vary significantly in different watersheds. Empirical equilibrium models have been developed by Wright and Henriksen (1983), Schnoor et al. (1984) and others. The Henriksen-Wright model and the Schnoor model are described here as these form the basis for applications of the Direct Distribution model of Small and Sutton (1986b).

3.2.2.1. *Henriksen-Wright model*

The Henriksen-Wright model relates the equilibrium alkalinity (ANC) of a lake to the acid deposition rate, the annual rainfall, flow-through ratio and chemical weathering in the watershed (Wright and Henriksen, 1983). The model assumes that some fraction of the deposition of acid is neutralised in the watershed system. The neutralisation fraction N_F is assumed to be constant and independent of the level of acid deposition. The remaining fraction $(1-N_F)$ acts to decrease the alkalinity of the lake, as given by :

$$ANC = ANC_0 - (1 - N_F)C \quad (1)$$

where C is the acid concentration of the incoming precipitation adjusted upward to account for dry deposition and evapotranspiration.

In the Henriksen-Wright model, this neutralisation is assumed to occur entirely as a result of the exchange of base cations Ca and Mg and is measured relative to the change in the in-lake SO_4 concentration, so that :

$$N_F \approx F = \frac{\Delta(Ca^{2+} + Mg^{2+})}{\Delta(SO_4^{2-})} \quad (2)$$

As long as the base cation exchange is the primary source of neutralisation and the increase in the SO_4 concentration occurs as a result of increase in the acid deposition, F and N_F are equivalent. The value of F was typically thought to vary between 0 and 0.4 and was assumed to be constant across all lakes in a region. The early assumptions were based on highly elevated, poorly buffered Norwegian lakes. However, more recent studies have recognised the variability in F within a region. The model output for a lake is very sensitive to the assumed value of F .

The basic hypothesis here is that acidified waters are a result of a large scale acid-base titration. Bases released by the weathering of primary rock are titrated with acids deposited from the atmosphere. It is also generally accepted that other processes like cation exchange and sulphate reduction dampen the effects of acid deposition.

Small and Sutton (1986b) and Labieniec et al. (1989) discussed the use of F to represent the neutralisation fraction.

3.2.2.2. Schnoor Trickle-Down Model

Schnoor and co-workers (Schnoor et al., 1984, 1986) derive a similar acidification model based on the kinetics of weathering. In this model, the neutralisation fraction decreases as acid deposition increases, based on a non-linear relationship between the chemical weathering rate and the level of acid deposition.

$$W = \frac{(k_0 + k_h D^m)}{1000 PR} \quad (3)$$

where k_0 is the rate constant in the absence of free acidity in $\mu\text{eq m}^{-2} \text{yr}^{-1}$, k_h is the rate constant for acid hydrolysis, D is the acid deposition rate and m is a fractional order constant.

3.3. ABOUT MAGIC

This sub-section is largely summarised from the MAGIC model documentation (Sullivan and Cosby, 1995d) which is a part of the TAF documentation.

MAGIC has been the principal model used so far by NAPAP for making projections of likely future changes in surface and soil water chemistry in response to various levels of acidic deposition. The model was described in the NAPAP State of Science/ Technology Report on modelling methods (Thornton et al. 1990), and numerous model projections of future scenarios were presented in the Integrated Assessment (NAPAP 1991). Recent improvements to the model include the incorporation of an organic acid analogue (Sullivan et al., 1995c, in press), modifications to the algorithms for calculating Al dissolution (Sullivan and Cosby, 1995b, in review), modified assumptions regarding background pre-industrial sulphate concentrations (Husar et al. 1991), subregional calibration (Sullivan et al. 1994) and inclusion of nitrogen dynamics (Ferrier et al. in review). Many of the recent improvements to MAGIC were summarised by Sullivan and Cosby (1995a). The model has been tested and confirmed at a variety of sites (Jenkins et al. 1990; Wright et al. 1990; Cosby et al. 1995, in press; Sullivan et al. 1994, in press).

The Aquatics Effects and Soils Effects module of the TAF prototype described in this document includes reduced-form modelling capabilities for one region of the United

States: the Adirondack Mountains. The TAF prototype includes reduced-form models for the Adirondack lakes, based on a variant of the Direct Distribution Model of Small and colleagues, for predicting the output from MAGIC. MAGIC outputs include key elements of surface water chemistry (e.g., pH, Al, Ca concentrations) and soil solution chemistry (e.g., base saturation). Results for surface water chemistry derived from MAGIC are used to estimate fish presence/absence and acid stress indices. The objective of these reduced-form models is to estimate the results that would be simulated by the full-form model, MAGIC, under changing deposition scenarios. These estimates of chemical and biological response are then used as inputs for valuation estimation procedures.

During the past five years, the MAGIC model has been tested in a large variety of settings and under quite varying environmental conditions. This work has included comparing model hindcast simulations with diatom-inferences of historical acidification, sensitivity analyses to examine the response of the model to alternative assumptions and formulations, and detailed testing of model forecasts by comparing simulated chemistry with the results of catchment-scale and plot-scale experimental acidification and deacidification (Sullivan, 1994; Sullivan et al., 1996, in review; Cosby et al., 1996, in review). These analyses have elucidated a number of potentially-important deficiencies in model structure and method of application, and have resulted in changes to the model and its calibration procedures. The work has included in-depth evaluation of issues related to regional aggregation of soils data, background sulphur deposition, natural organic acidity, nitrogen, and aluminium mobilisation. The result has been an improved and more thoroughly-tested version of MAGIC.

3.3.1. Description of MAGIC

MAGIC is a lumped parameter model of intermediate complexity (Cosby et al. 1985) that is calibrated to the watershed of an individual lake or stream and then used to simulate the response of that system to changes in atmospheric deposition. MAGIC includes a section in which the concentration of major ions is governed by simultaneous reactions involving sulphur adsorption, cation weathering and exchange, aluminium dissolution/precipitation/speciation, and dissolution/speciation of inorganic carbon. A mass balance section of MAGIC calculates the flux of major ions to and from the soil in response to atmospheric inputs, chemical weathering inputs, net uptake in biomass and losses to runoff.

Model calibration to a specific catchment is accomplished by specifying deposition and hydrological forcing functions, setting the values of those parameters that can be measured (fixed parameters), and determining the values of the remaining parameters that cannot be measured (adjustable parameters) through an optimisation routine. The adjustable parameters are modified to give the best agreement between observed and predicted surface water and soil chemistry (Cosby et al. 1985a, b ,c).

3.3.2. Changes to the Model

3.3.2.1. Background Sulphate and Subregional Calibration

Subsequent to the MAGIC modelling that was conducted for EPA's Direct Delayed Response Project (DDRP; Church et al. 1989) and for NAPAP (1991), there was concern that Adirondack soils might differ in their chemical properties from similar soils in other areas of the Northeast, and that MAGIC projections for Adirondack watersheds might be biased because they were based on soil attributes that actually reflected conditions

elsewhere than the Adirondacks. The DDRP soils data were therefore reaggregated to characterise Adirondack watershed attributes using only soil data collected from pedons in the Adirondacks (Sullivan et al. 1991).

Modelling for the DDRP and Integrated Assessment also assumed that the deposition of sulphur in pre-industrial times was limited to sea salt contributions. Based on analyses presented by Husar et al. (1991), this assumption was modified such that pre-industrial deposition of sulphate was assumed equal to 13% of current values (Sullivan et al. 1991).

Recalibration of MAGIC to the Adirondack lakes database using the regionally corrected soils and background SO_4^{2-} data resulted in approximately $10 \mu\text{eq L}^{-1}$ lower estimates of current ANC. A substantial downward shift was also observed in predicted pre-industrial and current lakewater pH (~ 0.25 pH units) for lakes having pH greater than about 5.5. These differences were attributed to lower calibrated values for pre-industrial lakewater SO_4^{2-} concentrations and higher p_{CO_2} values estimated for Adirondack lakes, compared with the Northeast as a whole (Sullivan et al. 1991).

3.3.2.2. Organic Acids

Concern was raised subsequent to the IA regarding potential bias from the failure to include organic acids in the MAGIC model formulations used by NAPAP. MAGIC hindcasts of pre-industrial lakewater pH showed poor agreement with diatom-inferences of pre-industrial pH (Sullivan et al. 1991), and preliminary analyses suggested that these differences could be due, at least in part, to the presence of naturally-occurring organic acids in Adirondack lakewaters.

Driscoll et al. (1994) compared output from several organic acid analogue models, using data collected by the Adirondack Lakes Survey Corporation (ALSC) (Kretser et al. 1989) for 1400 lakes located in the Adirondack region. The best agreement was obtained ($r^2 = 0.92$) between predicted and observed pH values using the triprotic analogue representation, with fitted pK_a values of 2.62, 5.66, and 5.94, and a calibrated site density of 0.055 mol sites per mol C. The fitted values for pK_a and site density obtained by Driscoll et al. (1994) were used in the revised MAGIC applications reported here. Model scenarios using the original version of MAGIC without organic acids are designated MAGIC1, and those that include the triprotic organic acid analogue are designated MAGIC2.

Unmodified MAGIC1 hindcasts yielded pre-industrial pH values that were substantially higher than diatom-based estimates, and the discrepancy was greatest for those lakes in the most biologically-sensitive portion of the pH range, (pH 5.0 to 6.0). Furthermore, MAGIC1 hindcast pH estimates were greater than 6.0 for all lakes investigated, whereas diatom estimates of pre-industrial pH ranged from as low as 5.2 to above 7.0. When the organic acid model was incorporated into MAGIC2 and simulated pH values were compared with diatom-inferred pH, the comparison yielded considerably closer agreement between model estimates of pre-industrial pH than did the simulations that did not consider the effects of organic acids (Sullivan et al., 1995e, in press). The mean difference in MAGIC1 versus diatom estimates of pre-industrial pH was 0.6 pH units when organic acids were omitted from the modelling scenarios, with the greatest discrepancy being for lakes with diatom-inferred pH < 6.0. This mean difference was reduced to only 0.2 pH units when the triprotic organic acid model was included, and the agreement for individual low-pH lakes improved by as much as a full pH unit (Sullivan et al. 1995e, in press).

3.3.2.3. Aluminium

Al mobilisation is now widely believed to be one of the most important ecological effects of surface water acidification. Potential effects of Al mobilisation to surface and soil waters include alterations in nutrient cycling, pH buffering effects, toxicity to aquatic biota, and toxicity to terrestrial vegetation. The relationship between $[Al^{3+}]$ and $[H^+]$ in surface waters has generally been modelled with MAGIC and other acid-base chemistry models as being cubic, determined by an assumed solubility product (K_{so}) for gibbsite ($Al(OH)_3$). Model estimates of changes in the concentration of Al^{3+} in surface waters, using this relationship, have shown a consistent pattern of overestimating the change in Al^{3+} concentration in response to experimental treatment (Sullivan et al., 1995f, in press). This overestimate of the change in Al^{3+} concentration calculated by MAGIC is generally due to a combination of the cubic relationship between H^+ and Al^{3+} assumed in the gibbsite model and the model calibration procedure of selecting a gibbsite solubility product based on measured pre-treatment data.

Sullivan and Cosby (1995b, in review) examined a large number of data sets for lakes and streams in the north-eastern United States that contain appreciable dissolved inorganic Al concentrations (Al_i). For all data sets examined, a consistent relationship was evident between pAl_i and pH for the waters of interest (pH 4 to 6). The slope of this relationship was consistently near 1.0, ranging from 0.77 to 1.28. When plots of pAl^{3+} versus pH were examined, similar results were found. The slopes of the relationships in this case were consistently near 2.0, and ranged from 1.82 to 2.34. These results illustrate that, for the surface waters in the United States that are of interest with respect to potential aluminium mobilisation, a gibbsite-type equation to model Al_i concentration directly should

use a power term of about 1. For predicting Al^{3+} concentration, a power term of about 2 should be used. None of the data examined suggested a power term close to 3, the value currently used in model formulations.

A version of MAGIC that incorporated this change was applied to the Bear Brook, Maine, watershed acidification data. The revised MAGIC projections of Al_i concentration at West Bear Brook agreed more closely with measured values than did the previous projections based on the gibbsite solubility assumption (Sullivan and Cosby, 1995b, in review). The results of comparing simulated with measured Al_i concentrations at the Risdalsheia acid exclusion site in Norway were not so consistent. However, the majority of the annual average measured values at Risdalsheia more closely followed the MAGIC trajectory that was constructed assuming an exponent of 2, rather than 3 as in the gibbsite model. Neither formulation was completely satisfactory for predicting streamwater Al_i concentration. This is to be expected given the lumped-parameter nature of the model and the complexity of the Al hydrogeochemical response. In most cases, however, a power term of 2.0 in the model formulation for Al^{3+} provided the most reasonable projections.

A new version of the MAGIC model was produced, called MAGICAL, that allows flexibility in the way surface water Al dynamics are represented. MAGICAL allows user-specification of both the exponent and the constant (K_{so}) in the solubility relationship. In previous versions of MAGIC, the exponent was fixed at a value of 3. After calculating the concentration of Al^{3+} , the model estimates the concentration of other inorganic species of Al using thermodynamic relationships in a manner analogous to ALCHEMI (Schecher and Driscoll, 1987) and other models of Al speciation.

3.3.2.4. Nitrogen

MAGIC contains an extremely simplified representation of nitrogen dynamics within catchment soils. The model simulates net nitrogen retention as a linear process. That is, retention of either NO_3^- or NH_4^+ is assumed to be linearly proportional to the input fluxes of these ions. There are no processes controlling the details of N cycling in the model. In light of the increasing concern about N saturation in forested ecosystems, this is a serious shortcoming in the model, and is currently being addressed by considering a number of modifications for the model.

The current version of the MAGIC model is not appropriate for simulations of changes in atmospheric deposition of NO_3^- . For TAF modelling efforts, however, it is desired to make projections of lakewater pH responses assuming scenarios of increasing NO_3^- deposition. Efforts are currently underway to apply an extended version of MAGIC called MAGIC_WAND, which includes aggregated nitrogen dynamics (Ferrier et al. in review), to the regional database of Adirondack lakes. These analyses will be available for subsequent versions of TAF. In the interim, a modification to the MAGIC model was made to allow simulation of the effects of changes in NO_3^- deposition. This proposed modification is based on NO_3^- input/output budget calculations.

The majority of the Adirondack lakes in the modelling data set had lakewater NO_3^- concentrations lower than the calculated concentration that would be expected based on direct NO_3^- deposition to the lake surface. For modelling these lakes, it was therefore assumed that all NO_3^- deposited on watershed soils is taken up within the terrestrial catchment, in terms of its impact on fall index chemistry. In addition, a component of the NO_3^- deposited directly to the lake surface is taken up by in-lake biota. For those lakes that had higher concentrations of lakewater NO_3^- than would be expected based on direct NO_3^-

deposition to the lake surface, it was assumed that some amount of chronic watershed leaching of NO_3^- occurs.

From the available data, the amount of chronic NO_3^- leaching from each watershed, expressed in $\mu\text{eq L}^{-1}$ in lakewater, was estimated. This value is zero for most lakes and ranges up to $16 \mu\text{eq L}^{-1}$. The amount of in-lake NO_3^- uptake for each lake was also estimated, expressed in $\mu\text{eq L}^{-1}$. For many lakes, an estimated "average" value of $4 \mu\text{eq L}^{-1}$ was used.

For modelling the response of the lakes to future changes in NO_3^- deposition, it was assumed that 1) in-lake NO_3^- uptake will remain unchanged; 2) increased NO_3^- deposition to the lake surface will be directly reflected in increased lakewater NO_3^- concentrations; and 3) the current amount of in-watershed retention of NO_3^- ($\text{kg ha}^{-1} \text{ yr}^{-1}$) deposited on the watershed will remain constant on a percentage basis over time. In other words, for watersheds that currently do not appear to be chronically leaching NO_3^- from watershed to lake, it was assumed that changes in NO_3^- deposition will only change lakewater NO_3^- concentrations by an amount equal to the change in deposition to the lake surface. For watersheds that do appear to be chronically leaching some NO_3^- to the lakes, it is assumed that the percent terrestrial retention of incoming NO_3^- will stay constant under changing levels of NO_3^- deposition.

The approach outlined here for modelling NO_3^- is viewed as a first approximation. It allows changes in NO_3^- deposition to be included in MAGIC scenarios, which was not possible using the version of MAGIC applied for the 1990 NAPAP Integrated Assessment. It lacks, however, a process basis for determining at what point watersheds start to leak NO_3^- under increasing N deposition, the dynamics of changing NO_3^- retention in watersheds that are chronically leaching NO_3^- at the present time, and the role of NH_4^+

deposition and subsequent nitrification in the dynamics of NO_3^- leaching. Including these components in the next iteration of nitrogen modelling for TAF is anticipated, using the newly developed version of MAGIC with aggregated nitrogen dynamics, MAGIC_WAND. An on-going project will develop calibration procedures for applying MAGIC_WAND to the Adirondack lakes data set.

3.3.3. Cumulative Impacts of Changes to MAGIC

In order to evaluate the incremental and cumulative impact of the model modifications, a suite of model simulations was conducted by Sullivan and Cosby (1995a) for the Adirondack DDRP lakes. The changes were considered cumulatively. The baseline structure was that used in the DDRP and NAPAP IA studies. The changes to the model that were examined included modifying the assumption regarding background sulphur deposition, reaggregating the soils data, recalibrating the model specifically for the Adirondack subregion, adding the triprotic organic acid analogue model to the surface water compartment, and changing the aluminium/hydrogen ion relationship from cubic to quadratic. The analyses of Sullivan and Cosby (1995a) did not include examination of the effects on model output of including nitrogen dynamics in the model simulations. That work is currently in progress.

A suite of simulations was conducted based on the application of an assumed deposition scenario to derive a 50 year forecast using each model structure. The deposition scenario assumed constant sulphur deposition from 1984 (the calibration year) to 1994, followed by a 30% decrease in sulphur deposition from 1995 to 2009, with constant deposition thereafter until 2034. The modelled responses of thirty three Adirondack lakes to this deposition scenario were considered. The impacts of the changes were illustrated by

tabulating the percentage of lakes predicted to have pH, ANC or Al values in excess of commonly accepted thresholds of potential biological effects.

The overall effect of the various changes to the model structure and application procedures was an increase in the percentage of lakes exceeding various biological thresholds with respect to pH, Al, and ANC subsequent to an hypothesised 30% decrease in sulphur deposition. The largest changes were observed for pH and Al; ANC projections were less affected. The modifications to the model that caused the greatest changes in projected output were the recalibration of the model to the Adirondack subregion, modification of the assumption regarding background SO_4^{2-} , and the incorporation of the triprotic organic acid model into MAGIC. The modification of the Al algorithm caused fewer lakes to be projected to exceed Al threshold values in response to the reduced deposition scenario; this change was quantitatively less important than the previous changes.

The magnitude of effect of the cumulative modifications to the model was considerable. For example, thirty-two percent of the lakes had measured pH less than 5.5 in 1984, whereas only 8% were projected to still have pH less than 5.5 after the reduction in sulphur deposition, using the original MAGIC application. In contrast, the improved version of MAGIC projected that 32% of lakes would still have pH less than 5.5 in the year 2034. Similarly, of the 30% with measured $\text{Al}_i > 50 \mu\text{g L}^{-1}$ in 1986, the original model structure projected only 4% would still have $\text{Al}_i > 50 \mu\text{g L}^{-1}$ in 2034 compared to 30% projected to continue to have high Al_i by the improved version of MAGIC. Based on model projections using the improved version of MAGIC, little recovery of Adirondack lakes would be expected after a 30% reduction in sulphur deposition. This reduction is simply not large enough to reverse the acidification trend of lakes in the region. The number of lakes having $\text{pH} < 6$ is actually projected to increase, and the number of lakes

projected to have $\text{ANC} < 0$ only decreases slightly in response to lower deposition. These estimates are independent of any possible increases in NO_3^- leaching that might occur. The lack of recovery suggested by these model projections is attributable partly to a decrease in the modelled base saturation of watershed soils. These results may affect expectations of recovery in response to sulphur emission controls mandated by the Clean Air Act Amendments of 1990.

3.3.4. Confirmation of the MAGIC Model

MAGIC has been tested after inclusion of many of the model modifications discussed in the preceding sections. The revised model with Driscoll et al.'s (1994) triprotic organic acid analogue yielded reasonable agreement between model hindcast pH and diatom-inferred pH for the data set of 33 Adirondack lakes (Sullivan et al., 1995e, in press). Differences between diatom and MAGIC estimates of pre-industrial pH of Adirondack lakes, based on the version of MAGIC that includes a triprotic organic acid representation were well within the range of expected differences due to annual and seasonal variability, uncertainties in the algorithms used to calculate pH from major ion chemistry, and the influence of dissolved CO_2 on air-equilibrated pH measurements that were used to calibrate the diatom model (Sullivan et al. 1994). However, "successful" comparison of MAGIC with diatom hindcasts in one region does not constitute a sufficient verification to impart complete confidence in using MAGIC, or any process model, for predicting the response of surface water chemistry to changes in acidic inputs. Additional model confirmation in the form of comparison of model output with measured data, is required. This has been the focus of modelling efforts at Lake Skjervatjern, Bear Brook, and Risdalsheia.

MAGIC model projections of the response of Lake Skjervatjern to whole-catchment acid additions were close to measured values for SO_4^{2-} , NO_3^- , and NH_4^+ . Although the retention of added sulphur within the terrestrial system was considerable, the MAGIC-simulated SO_4^{2-} concentrations at Skjervatjern were within 3 to 6 $\mu\text{eq L}^{-1}$ of average measured concentrations (Cosby et al. 1995). The simulated values for NO_3^- and NH_4^+ in Lake Skjervatjern were also very close to measured values for both years, within about 1 $\mu\text{eq L}^{-1}$. It is important to note, however, that the observed success in modelling the nitrogen fluxes into Lake Skjervatjern lakewater was not a result of nitrogen processing algorithms, which are not part of the current version of MAGIC. Rather, the simulation was run assuming that the percent retention of NH_4^+ and NO_3^- within the treated watershed would equal the calculated percent retention for each ion in the control catchment, based on estimated atmospheric inputs and lakewater concentrations. The actual percent net retention for both NH_4^+ and NO_3^- during the experimental treatment was very similar to the pre-manipulation percent retention of atmospheric inputs. Therefore, the MAGIC-simulated values were in agreement with measured responses without having to manually change the inputs to match measured values. Such agreement would not routinely be expected, however, as is illustrated in the Bear Brook data, and a process-based approach to modelling N cycling and fluxes would be a desirable addition to the model.

The MAGIC model simulations of the responses of the treatment catchment at Risdalsheia to reduced acidic deposition matched measured values extremely well (Cosby et al. 1995). In particular, the observed changes in SO_4^{2-} , base cation concentrations, and ANC closely paralleled the observed trends and interannual variations. Also, despite the importance of organic acids in modifying the pH of drainage waters at this site (Wright 1989), incorporation into MAGIC of the triprotic organic acid analogue, calibrated to the Norwegian 1000 Lake Survey, resulted in good agreement between modelled and measured pH.

The results of the MAGIC model testing at Risdalsheia (Cosby et al. 1995) are particularly noteworthy in two respects. First, model simulations of pH matched measured values fairly well despite using a regional model representation for organic acids to simulate pH in a system in which organic acids provide a great deal of pH-buffering. Second, agreement was demonstrated between simulated and observed chemistry, for all major variables except perhaps Al, over an eight-year period. This is a very long period of record for a model evaluation study that involves substantial change in acidic deposition inputs.

Sullivan and Cosby (1995b, in review) modified the equations used by MAGIC to simulate Al dissolution. The modified version of MAGIC, incorporating the new equations for Al, was applied to the Risdalsheia data. In general, the revised model predicted Al concentrations that were closer to measured values at this site (Sullivan and Cosby, 1995b in review).

Modelling efforts at Bear Brook (Sullivan et al. 1994, Cosby et al., 1995, in press) provide a continuation of the MAGIC model forecasting efforts presented by Norton et al. (1992). MAGIC predicted a much larger increase in streamwater SO_4^{2-} concentration than was observed in the treated stream. The trajectory of MAGIC-simulated SO_4^{2-} is approaching the anticipated steady-state concentration of about 300 $\mu\text{eq L}^{-1}$ projected to occur within the eight-year simulation period; i.e., about 200 $\mu\text{eq L}^{-1}$ higher than pre-treatment concentrations. In contrast, the trajectory of measured values is substantially lower.

It appears that MAGIC overpredicts the increase in streamwater SO_4^{2-} concentrations at Bear Brook by nearly a factor of two. This overprediction of the increase in streamwater SO_4^{2-} concentration that resulted from the manipulation experiment was due to the high value assumed for the half saturation of sulphur adsorption. The adsorptive

behaviour of the soils was effectively removed by the model because concentrations of SO_4^{2-} never approached the half saturation value.

As a consequence of the overprediction of streamwater SO_4^{2-} concentration, other key variables (especially ANC and Al) were also predicted to respond to a greater degree to the experimental acidification than was actually observed. MAGIC predicted substantially larger changes in each of these parameters than was observed. The discrepancies between MAGIC predictions and measured values for ANC increased with each year of the treatment, and are attributable mainly to the errors in predicting the responses of SO_4^{2-} and secondarily to errors in predicting the responses of Ca^{2+} and Mg^{2+} . This latter bias, however, was due primarily to pre-treatment differences between the reference and manipulated stream chemistry. This is a reflection of the extreme difficulty of finding "paired catchments" with identical chemistry. The combined influence of the observed biases in concentration of bases (CB) and concentrations in acids (CA) resulted in relatively large errors in predicted ANC, because ANC is defined in MAGIC for this application as (CB - CA).

The original calibration of MAGIC for the Bear Brook forecast was based on four years of data from the reference stream, East Bear. In order to assess the degree to which discrepancies between predicted and observed streamwater chemistry at Bear Brook could be improved by correcting sulphur dynamics and a priori differences between treatment and control catchments, a revised calibration was conducted. The revised Bear Brook calibration corrected for the obvious large bias in effective sulphur adsorption in watershed soils and also corrected for a priori differences between the treatment and reference catchments. The resulting simulations matched measured values in West Bear Brook to a substantially greater degree than had the forecasts based on the initial calibration that was based on the behaviour of East Bear.

Projected streamwater SO_4^{2-} concentration agreed closely with measured values in West Bear Brook for the first three years of manipulation (Cosby et al., 1995, in press). There was a suggestion, however, in the measured data of a levelling off in the annual increase in streamwater SO_4^{2-} concentration, whereas the model projected a steady increase in concentration throughout the duration of the model projection (1989 through 1994). The model simulation also showed much better agreement with measured values for the sum of base cations and ANC, than had the initial MAGIC simulation. Although the effects of the drought year (1992) on CB and ANC were still not captured by the simulation, the overall agreement between predicted and observed CB and ANC was much improved.

Based on the results of extensive model testing using diatom inferences of historical acidification of Adirondack lakes and the results of experimental watershed acidification (Lake Skjervatjern, Bear Brook) and deacidification (Risdalsheia), it appears that the MAGIC model provides reasonably accurate forecasts of changes in surface water acid-base chemistry in response to changing levels of acidic deposition.

Although some uncertainties remain, particularly with respect to watershed nitrogen dynamics, it can be concluded that the MAGIC model provides a generally accurate and well-tested tool for integrated assessment modelling.

3.4. CONCLUSIONS FROM THE NAPAP 1990 INTEGRATED ASSESSMENT

The NAPAP Integrated Assessment Report (NAPAP, 1990) contains a comprehensive compilation of the best available scientific, technological and economic information relevant to the issue of acid deposition at that time. The assessment covered the

entire range of plausible causes, effects and control approaches in a credible fashion. The conclusions and findings relating to surface waters are presented here.

When the NAPAP studies began, the number and location of acidic and low-pH lakes and streams in the United States were poorly understood. A number of activities were undertaken to assess the current status of surface waters. A National Surface Water Survey (NSWS) of water chemistry in a statistical sample of almost 3000 lakes and streams representing a population of 28000 lakes and 200,000 km of streams in acid-sensitive regions of the country was carried out. Studies of watershed geochemical processes, deposition rates, fish toxicity and temporal variation in lake and stream chemistry were conducted. Finally, analyses of long-term chemical data, fishery records and lake sediments to document historical changes in surface water chemistry were done.

It was found that within acid-sensitive regions of the United States, 4% of the lakes and 8% of the streams are chronically acidic. Florida has the highest percentage of acidic surface waters (23% of the lakes and 39% of the streams). In the mid-Atlantic Highlands, mid-Atlantic Coastal Plain and the Adirondack Mountains, 6% to 14% of the lakes and streams are chronically acidic; about three times that many become temporarily (days to weeks) acidic during storms and snowmelt conditions in these regions. Virtually no (< 1%) chronically acidic surface waters are located in the South-western Highlands or the mountainous West.

Estimates were also made on the basis of lake surface area and stream length. As acidic lakes tend to be smaller than nonacidic lakes, the percentage of acidic lake area in the NSWS was a factor of 2 smaller than the percentage of acidic lakes based on numbers. Overall, 263 km² (2%) of the 12000 km² of lake area in the NSWS was acidic (ANC < 0

$\mu\text{eq/L}$), and 1310 km^2 (11%) had $\text{ANC} \leq 50 \mu\text{eq/L}$. On a length basis, 7900 km of the 211,400 km of NSWS streams were acidic and 26400 km had $\text{ANC} \leq 50 \mu\text{eq/L}$.

Acidic deposition is the dominant source of acid anions, excluding chloride, in about 75% of the acidic lakes and about 50% of the acidic streams in the NSWS. Most of these have become more acidic (i.e. declined in pH) because of acidic deposition. These acidic surface waters are found primarily in the mid-Atlantic Highlands, the Adirondacks, New England, the mid-Atlantic Coastal Plain, Florida and the eastern portion of the Upper Midwest. Natural organic acids are the dominant source of acid anions excluding chloride, in about 25% of the acidic lakes and streams in the NSWS, and these are found in Florida, the mid-Atlantic Coastal Plains, the Upper Midwest, and New England. Acid mine drainage is the major source of the acid anions in about 25% of the acidic streams in the NSWS. These acidic streams are located in the mid-Atlantic and South-western Highlands.

Analysis of lake sediments and other historical evidence indicates surface water acidification, best explained by acidic deposition, in the Adirondacks and northcentral Florida. Historical data suggest that Florida panhandle lakes have not recently acidified. Historical data from other areas are generally not adequate to assess regional trends.

Fish losses attributable to acidification have been documented using historical records for some acidic surface waters in the Adirondacks, New England, and the mid-Atlantic Highlands. Other lines of evidence, including surveys and the application of fish response models, also support this conclusion. Detrimental biological effects may be occurring in some other NSWS regions, although the available information suggests no widespread fish population losses have occurred because of acidic deposition in Florida.

4. REDUCED-FORM MODELLING OF SURFACE WATERS

This section and section 5 have been summarised from the TAF Soils-Aquatics Module documentation (Sinha et al., 1995) which is a part of the TAF documentation.

4.1. PREVIOUS REDUCED-FORM MODELS

4.1.1. The Direct Distribution Model

This model is based on the empirical probability distribution of an indicator such as ANC in a sample of lakes. The distribution is coupled with an empirical model such as the Henriksen-Wright model or the Schnoor Trickle-down model. This model can also predict distributions of other indicators like pH. It can also characterise the probability distributions of the uncertainty in the model parameters. The distribution of pH is used to obtain distributions of measures of the fishability of the population of lakes.

Regional distributions of ANC have been observed to be unimodal with large positive skew. In areas affected by acid deposition, the minimum value of ANC may extend to -100 µeq/L and upper tails may extend to 1000 µeq/L and beyond. In the Direct Distribution model of Small and Sutton (1986b), a 3-parameter lognormal function is used to describe the distribution of the ANC :

$$f_{ANC}(ANC) = \frac{1}{(ANC - \theta)\phi\sqrt{2\pi}} \exp \left[-\frac{[\ln(ANC - \theta) - \xi]^2}{2\phi^2} \right]; \text{ANC} \geq \theta \quad (4)$$

where θ (corresponding to the minimum value of ANC), ξ , and ϕ are the parameters of the distribution. These parameters can be estimated for an ANC data set using the method described in Small and Sutton (1986b).

A range of correlation coefficients between the model parameters θ , ξ and ϕ are required when characterising the uncertainty in the distribution of ANC for a region (Small and Sutton, 1986b). These are difficult to estimate.

The pH-alkalinity relationship developed by Small and Sutton (1986a) is used to transform an alkalinity distribution to the corresponding pH distribution :

$$pH = a + b \times \operatorname{arcsinh} \left[\frac{ANC - d}{c} \right] \quad (5)$$

Measured ANC is used to estimate pH using an empirical titration curve approximated by the above equation. The shape of this titration curve is assumed to be invariant. This assumption works well for regions with low-ANC lakes, such as the Adirondacks. In regions with fewer low ANC lakes, predictions are inaccurate at the extremes of the ANC distribution. Also, this model is difficult to apply to empirical distributions that are not easily parametrised.

In another study, Small et al. (1988) examined the distribution of ANC in four subregions of the Eastern Lake Survey and found that bimodal pH curves were obtained for two subregions. Results were obtained which were similar to those of Small and Sutton (1986b).

4.1.2. Atmospheric Deposition Assessment Model (ADAM)

This was a generalised modelling framework developed to analyse acid-rain issues in North America (Rubin et al., 1992). In many ways, the ADAM model can be considered the precursor to TAF. The major components of the acid deposition problem were linked in a computer environment (Demos) designed to test alternate hypotheses and analyse uncertainty. The stochastic simulation framework links analytic models of:

1. Precursor emissions aggregated at the state or subprovince level.
2. Atmospheric transport and transformation.
3. Deposition at selected receptors.
4. Regional aquatic chemistry.
5. Fish species viability measured by a presence/absence indicator.

Uncertainties in model results are expressed as probability distributions reflecting the combined effect of all uncertain input parameters, which are also expressed probabilistically.

Emissions trajectories are considered for up to 66 source regions. Atmospheric transport and deposition is modelled using linear transfer matrices determined from the Advanced Statistical Trajectory Regional Air Pollution (ASTRAP) Model. Aquatic chemistry responses were modelled using the Direct Distribution Model of Small and Sutton (1986b). The fish presence/absence model used is based on pH only and is described in Small and Sutton (1986b), Reckhow et al. (1985), Rubin et al. (1992), and Baker et al. (1990).

Given the scenario that SO₂ emissions in 1995 are reduced by 9,100,000 tons/yr below the 1980 levels, ADAM predicts an average reduction in deposition of 46 to 47% over the time period from 1980 to 2010. This reduction is predicted to result in a decrease of the number of lakes in the Adirondacks with pH ≤ 5.5 by 4 to 17% over the same time period. This, in turn, implies a 2% increase in the number of lakes in the Adirondacks able to support lake trout and a 0.6 to 6% increase in the number of lakes in the Adirondacks able to support brook trout. In this fashion, changes are propagated throughout the entire integrated modelling framework.

4.2. METHODOLOGY FOR TAF

4.2.1. Overview

Substantial development has taken place in the ability to understand and model the individual processes of the acid deposition problem. On the other hand, not much success has been achieved in combining these models to provide an integrated assessment. TAF uses the metamodelling technique to create an integrated assessment of more complex models, whereby meta or "reduced-form" models are developed for each problem component.

Lake, stream and watershed soil chemistry are predicted by reduced-form models, which are based on an approximation to the improved version of the Model of Acidification of Groundwater in Catchments (MAGIC, see Sullivan and Cosby, 1995a; Sullivan et al., 1995c). MAGIC is a state-of-the-art lumped parameter model that uses chemical equilibrium and mass balance equations to predict changes in lake and soil chemistry. It

was designed to operate on a watershed spatial scale and a temporal scale of years to decades. MAGIC was not designed to project short-term changes in chemistry such as those resulting from storm events. Furthermore, while soil and lake properties are heterogeneous within watersheds, MAGIC uses a lumped-parameter approach to represent the processes within a watershed. Parameters are calibrated or averaged so that one value may be used to represent the entire watershed. MAGIC was calibrated for NAPAP to represent the distribution of watershed conditions for selected regions (see NAPAP, 1990).

MAGIC was used because it simulates the physical and biological processes that are primarily responsible for the chemical state of the soil and surface water, yet the model requirements of input data and computer resources are small compared to other watershed or forest-stand chemistry models such as ILWAS or NuCM. This is particularly important given the region-wide application of the TAF model.

This section describes the reduced-form models developed as a simplified representation of MAGIC. The reduced-form models have been applied to lakes in the Adirondacks region of New York using a set of 33 lakes, chosen to be representative of the target population of lakes in the region. The Adirondacks region is shown in **Figure 2**, with the major lakes and streams marked on the figure. Changes in pH are grouped into 5 major ranges. The location of the Adirondacks in New York state is shown in the inset.

Figure 2. The Adirondacks region of New York showing the pH change from 1844 to 1984 (courtesy E&S Environmental Chemistry).

The aquatics module predicts the effects of acidic deposition on lake and stream chemistry and resulting impacts on fish species. The lake and stream chemistry are characterised by concentrations of acid neutralising capacity (ANC), pH, calcium and aluminium. The reduced-form models provide close approximations to MAGIC, but require much less watershed-specific input data. Data for calibrating the module were obtained from MAGIC simulations on each watershed for several input deposition

scenarios, beginning with estimated historic deposition from 1844 to 1985, then introducing a set of step deposition changes ranging from a 30% increase to a 60% decrease (**Figure 3**). The deposition changes in the aquatics calibration runs were simulated to occur as steep ramps from 1985 to 1986.

Figure 3. Illustration of MAGIC Simulations used to train the reduced-form models

The MAGIC simulations were based on the mean parameter set of the from 2 to 10 calibrations that were considered successful for each watershed (a fuller discussion of the multiple MAGIC calibrations is provided in § 4.4).

The TAF reduced-form model (see **Figure 4** and **5**) utilises a linearised approximation to the most recent version of MAGIC (Sullivan and Cosby, 1995a), assuming an exponential approach to equilibrium ANC concentrations in the soil water of each watershed in which a fraction of the incoming acid deposition is neutralised (Small et al., 1995). This equilibrium value changes as a result of cumulative deposition. A fraction of direct (i.e., un-neutralised) runoff is also assumed for each lake. Non-linear regression

is used to estimate the parameters of the TAF reduced-form ANC model from MAGIC calibration runs (see **Figure 3**). Lake calcium is modelled in a similar fashion by assuming an exponential approach to an equilibrium value, with a characteristic lag time. The pH-ANC relationship of Small and Sutton (1986a) is fit to the pH-ANC output of the MAGIC calibration runs, and subsequently used to derive the pH of each lake from the lake ANC. Lake aluminium is modelled by an empirical aluminium-pH relationship proposed by Sullivan and Cosby (1995b).

Figure 4. The Soils-Aquatics Module in TAF. Both Soils and Aquatics models are driven by MAGIC.

Figure 5. The main components of the Aquatics Module.

The effects on biota are modelled as the fraction of lakes able to support one of 3 fish species (Adirondack brook trout, Ontario lake trout and Adirondack common shiner, representative of acid-tolerant, moderately sensitive and acid-sensitive species, respectively) and the Acid Stress Index (ASI) for 3 fish species (Adirondack brook trout, Smallmouth bass and Rainbow trout), as well as a function for fish species richness for each lake (Baker et. al., 1990). The first two effects are functions of the pH, aluminium and calcium in the lakes, whereas the latter effect is also a function of the physical characteristics of the lakes. The outputs from the Soils-Aquatics Module are shown in **Figure 6**. The Analytica code which generated the influence diagrams and reduced-form models presented here is in **Appendix B**.

Figure 6. Outputs from the Soils-Aquatics Module.

4.2.1.1. Inputs required

Once the model parameters are specified for each of the 33 watersheds and for the region as a whole, the only inputs to the module from the “upstream” portions of TAF are the time series of the deposition inputs for each of the chemical species, namely wet and dry sulphur and wet and dry NO_x-nitrogen in units of $\text{kg ha}^{-1} \text{yr}^{-1}$. The module converts the annual deposition of each chemical species to an average concentration in the precipitation in units of $\mu\text{eq L}^{-1}$. The TAF Transport Module (see **Figure 1**) projects a regional mean deposition input for each chemical species. The regional input is scaled for each watershed based on the ratio of the watershed-specific deposition to the regional average for the DDRP data used to calibrate the full-form MAGIC model.

4.2.1.2. Specification Domain

The model currently makes projections only for the Adirondacks region of New York state, for the years 1990 through 2030. The Aquatics and Soils modules were calibrated with changes in the average annual deposition input of sulphur plus NO_x ranging from a 75% decrease to a 75% increase. Model projections for deposition changes outside this range may not be reliable.

4.2.1.3. Regional Representation Weighting Factors

The EPA Eastern Lake Survey (ELS: Overton et al., 1986 and Kanciruk et al., 1986) measured lake chemistry for 155 lakes in the Adirondack region. These lakes were statistically chosen to represent the target population of all lakes larger than 4 hectares in surface area. The target population was estimated to include about 1290 lakes. A subset of these lakes was modelled using MAGIC for the Direct/Delayed Response Project (DDRP) in support of the 1990 NAPAP Integrated Assessment. DDRP chose to model 38 of the 155 sampled lakes. Lakes were excluded that were judged insensitive to acidification ($\text{ANC} > 400 \mu\text{eq/L}$), difficult to measure (watersheds > 3000 ha, lake area > 2000 ha, or shallow lakes less than 1.5 m deep), or anthropogenically disturbed. MAGIC calibrations were not successful for three of the 38 DDRP Adirondack watersheds and two were not recalibrated subsequent to the 1990 NAPAP Integrated Assessment because corresponding historical diatom data were not available. TAF modules were based on the remaining 33 watersheds that represent 610 of the original ELS target population. See **Table 1** for more information related to the 33 sample watersheds.

Lake ID	Lake Name	DDRP Weight	Elevation (m)	Watershed Area (ha.)	Lake Area (ha.)
1A1-003	Hawk Pond	12.29	645.30	95.90	13.80
1A1-012	Whitney Lake	12.29	748.60	272.00	43.00
1A1-014	Wilmurt Lake	22.49	752.00	272.90	39.00
1A1-017	Constable Pond	12.29	582.20	945.10	20.60
1A1-020	Fourth Lake	12.29	608.70	259.00	23.00
1A1-028	Dry Channel Pond	12.29	497.10	209.70	27.40
1A1-029	Middle Pond	40.47	484.00	181.90	24.30
1A1-033	Kiawassa Lake	40.47	466.00	515.00	115.00
1A1-039	John Pond	12.29	545.60	36.00	6.00
1A1-046	Partlow Lake	22.49	534.30	288.40	29.90
1A1-049	Middle South Pond	12.29	603.50	132.70	19.40
1A1-057	Hitchcock Lake	12.29	566.90	115.80	14.20
1A1-061	Wolf Lake (W.C.)	12.29	791.00	187.00	4.40
1A1-064	Mt. Arab Lake	22.49	505.70	117.00	50.00
1A1-066	Woodhull lake	12.29	571.50	1821.00	443.00
1A1-073	Gull Lake	12.29	593.80	70.60	10.90
1A2-002	St. John Lake	12.29	672.70	148.00	13.00
1A2-006	Lake Frances	22.49	454.20	96.00	6.00
1A2-037	Fish Ponds (NE)	40.47	485.60	1038.70	7.40
1A2-041	Mud Lake (S.L.)	22.49	527.30	303.00	9.00
1A2-042	North Branch Lake	12.29	575.50	159.80	6.50
1A2-045	Woods Lake (S.L.)	12.29	418.50	168.00	26.00
1A2-046	Nine Corner Lake	12.29	570.00	204.60	45.00
1A2-048	Unnamed (Mud Lake)	12.29	484.60	101.00	5.00
1A2-052	Chub Lake	12.29	503.80	54.00	7.00
1A2-054	Trout Lake (P.L.)	12.29	651.10	255.90	16.70
1A3-001	Nate Pond	22.49	613.90	116.30	8.30
1A3-040	Zack Pond	22.49	565.70	202.00	36.00
1A3-042	Cheney Pond	22.49	502.90	158.00	7.00
1A3-043	Unknown Pond	40.47	496.80	497.00	14.00
1A3-046	Long Pond (K.R.)	22.49	563.90	151.30	15.40
1A3-048	Grass Pond (H.W.)	12.29	545.60	236.70	5.30
1A3-065	South Lake	12.29	615.10	1644.00	196.00

Table 1. Sample Watershed Characteristics

Some assumptions were made so that the model results for this subset of lakes could be extrapolated to the entire ELS target population of 1290 lakes. If it is assumed that lakes with ANC > 400 µeq/L will not change significantly in response to changing deposition, and that all lakes not modelled will change in the same manner as the modelled systems, estimates of the proportion of affected lakes can be made for the entire ELS target population. The factors that can be extrapolated are the fraction of lakes with pH < 5.5, the fraction of lakes supporting given fish species, and fraction of region with base saturation less than 10 percent. The fraction of affected lakes or watersheds modelled based on the DDRP weights is multiplied by the fraction of lakes in the ELS target population with ANC

< 400 $\mu\text{eq/L}$ (0.869 for the Adirondacks) to give the fraction of affected lakes in the ELS target population (Sullivan, 1995; Ryan, 1995; Cosby, 1995).

4.2.1.4. Temporal Scale

Projections are generated from the year 1985 through the year 2030 and the internal Time system variable is defined as a sequence from 1985 to 2030. The time increment for the module is 1 year, but can easily be set at 5 years. The TAF Peer Review Model has a time increment of 5 years to conserve storage. Initial lake chemistry in 1985 is determined from the Eastern Lake Survey; the reduced-form TAF modules are then applied to project changes in lake and soil chemistry from this baseline condition.

4.2.1.5. Aquatics Outputs

Output from the aquatics module can be grouped under two categories, viz. lake chemistry outputs and effects on biota.

Lake chemistry outputs are:

1. Cumulative distribution of lake pH in the region.
2. Fraction of lakes in region with pH below 5.5.
3. Acid Neutralising Capacity time series for each lake in the region.
4. Average lake aluminium time series for the region.
5. Average lake calcium time series for the region.

The effects on biota are:

1. Time series of the fraction of lakes able to support one of 3 fish species (Adirondack brook trout, Ontario lake trout and Adirondack common shiner)
2. Time series of the average Acid Stress Index in the region for 3 fish species (Adirondack brook trout, Smallmouth bass and Rainbow trout)
3. Time series of the Fish species richness.

4.2.1.6. Deposition Input

MAGIC generates projections of lake and soil chemistry from deposition scenarios that include all major ion species. The TAF Aquatics and Soils module simplifies the treatment of deposition by considering only changes in sulphur and nitrate deposition for the projections. A baseline "effective" deposition concentration was calculated for each watershed from the MAGIC projections as the sum of the acid anion equivalent concentrations minus the sum of base cation concentrations for 1985, the nominal calibration year. This is a measure of the acidity of the deposition.

The TAF Transport and Deposition Module projects deposition of sulphur and NO_x nitrogen for the Adirondack region as a whole. MAGIC calibrations were based on estimates of deposition to individual watersheds. The DDRP data used in the MAGIC calibrations showed a gradient of sulphate deposition with greater deposition to the southwest than the northeast part of the Adirondack region. To maintain this gradient in the TAF module, the regional estimate of deposition was adjusted to provide a watershed-specific estimate for each of the 33 watersheds used in the TAF module. Deposition adjustment factors were calculated for sulphur deposition and NO_x-N deposition. The adjustment factor was calculated as the watershed-specific annual wet + dry sulphate or nitrate deposition ($\text{kg ha}^{-1} \text{ yr}^{-1}$) from the 1984 DDRP data divided by the mean annual

deposition across all 33 watersheds (Ryan, 1995). The adjustment factors ranged from 0.94 to 1.11 for sulphate deposition and 0.98 to 1.02 for nitrate deposition (Table 2). The watershed-specific deposition in the TAF module was calculated as the wet+dry deposition times the adjustment factor.

Lake ID	Sulphur	NOx-Nitrogen
1A1-003	0.94	1.01
1A1-012	0.96	1.01
1A1-014	0.98	1.01
1A1-017	0.95	1.01
1A1-020	0.97	1.01
1A1-028	1.01	1.01
1A1-029	0.97	1.00
1A1-033	1.04	1.01
1A1-039	1.00	0.99
1A1-046	1.01	0.99
1A1-049	0.94	1.01
1A1-057	0.96	1.01
1A1-061	0.96	1.01
1A1-064	1.03	0.99
1A1-066	0.97	1.01
1A1-073	0.95	1.01
1A2-002	1.04	0.99
1A2-006	1.11	1.02
1A2-037	1.03	0.99
1A2-041	1.06	1.00
1A2-042	0.98	1.01
1A2-045	1.05	0.98
1A2-046	0.99	1.01
1A2-048	1.08	0.99
1A2-052	1.00	1.00
1A2-054	0.98	1.01
1A3-001	1.03	1.00
1A3-040	1.03	1.00
1A3-042	1.00	0.99
1A3-043	1.01	0.99
1A3-046	1.02	0.99
1A3-048	0.97	0.99
1A3-065	0.98	1.01

Table 2. Watershed Deposition Adjustment Factors

The change in effective deposition is the driving input of the reduced form model. As sulphate and nitrate concentrations in the deposition decrease, the acidity decreases. Cations and anions other than nitrate and sulphate are assumed to remain constant in this

implementation. Changes of equal magnitude in sulphate and nitrate would not be expected to result in the same effect on the soils or lake water. Because of biological uptake of nitrate, changes in the nitrate concentration of the deposition do not affect the acidity of the soils and surface water as much as sulphate. Factors were calculated for adjusting the change in nitrate deposition to a change in sulphate deposition that would produce the same effect.

In MAGIC, the behaviour of mobile mineral acid anions (e.g., SO_4^{2-} , NO_3^-) in runoff is functionally equivalent. Thus, for the purposes of providing input to the reduced-form aquatics module of TAF, a change in the NO_3^- concentration in runoff can be represented by an equivalent change in the SO_4^{2-} concentration in runoff.

Nitrate equivalent deposition (NED) factors were calculated for each watershed under multiple scenarios of both increasing and decreasing nitrate deposition. Each NED factor provides a basis for converting a given change in nitrate-N deposition into an "equivalent" change in sulphate-S deposition to allow incorporation into the reduced-form TAF model.

The NED factors were calculated as follows for each watershed. First, the change in surface water SO_4^{2-} concentration ($\mu\text{eq L}^{-1}$) predicted by MAGIC was determined for a given change in SO_4^{2-} -S deposition ($\text{kg ha}^{-1} \text{ yr}^{-1}$). Next, a similar relationship was calculated between assumed change in NO_3^- -N deposition and lakewater NO_3^- concentration for the steady state NO_3^- modelling approach that was adopted. Finally, the NED factors were calculated as the ratio between the sulphur and nitrogen relationships. Thus, the NED factor provides a number for each watershed by which the assumed NO_3^- -N deposition can be divided to make it functionally equivalent to an assumed SO_4^{2-} -S deposition with respect

to its effect on mobile mineral acid anion concentrations in lakewater. The NED factors were calculated from the changes in predicted chemistry over a series of 50-year MAGIC simulations. Separate NED factors were calculated for each watershed for both increasing and decreasing deposition scenarios. For a few watersheds, an hypothetical increase in NO_3^- -N deposition was functionally equivalent to an increase in SO_4^{2-} -S deposition about one-third as large (i.e., $\text{NED} = 3$). For most watersheds, however, the NED factors ranged between 5 and 10 (**Figure 4**). This implies, for example, that a change in NO_3^- -N deposition of $10 \text{ kg ha}^{-1} \text{ yr}^{-1}$ would produce in most lakes a change in mobile mineral acid anion concentration in lakewater equivalent to a 1 to 2 $\text{kg ha}^{-1} \text{ yr}^{-1}$ change in SO_4^{2-} -S deposition. If equal changes in NO_3^- -N and SO_4^{2-} -S deposition had yielded equal estimates of change in lakewater acid anion concentration (NO_3^- , SO_4^{2-}), then the NED factor would have been equal to 1. An exception to the general pattern of watershed NED factors in the range of 5 to 10 was evident for decreasing N deposition scenarios for those watersheds that exhibited base-year (1985) lakewater NO_3^- concentrations less than about $3 \text{ } \mu\text{eq L}^{-1}$ (**Figure 5**). This is because a decrease in N deposition cannot cause lakewater NO_3^- concentration to decrease below zero. Thus, a decrease in N deposition will have no effect on a lake that already contains near-zero lakewater NO_3^- under ambient deposition. The NED factors for scenarios of decreasing N deposition were therefore very high for those lakes that had low measured concentrations of lakewater NO_3^- .

For a given deposition change direction (increasing or decreasing) three NED factors were calculated for each watershed, corresponding to changes in deposition of 25%, 50%, or 75%. The influence of the magnitude of the assumed deposition change on the calculated values of NED was generally relatively small (**Figures 4, 5**). The NED values for changes in NO_3^- -N deposition of 50% (**Table 3**, solid circles on **Figures 7 and 8**) were selected to represent each watershed in the TAF modelling. For reduced-form

modelling of changes in $\text{NO}_3\text{-N}$ deposition, each watershed was therefore assigned one NED value for scenarios of increasing deposition and another NED for scenarios of decreasing deposition.

For scenarios with increasing nitrate deposition, the nitrate deposition increase from the base year to the current year is divided by the factor RATIO_I to yield the equivalent increase in sulphate deposition. This value is added to the change in sulphate deposition from the base year to give an overall change in effective deposition. For scenarios with decreasing nitrate deposition, the nitrate deposition decrease from the base year to the current year is divided by the factor RATIO_D to get the equivalent decrease in sulphur deposition, which is subtracted from the change in sulphur deposition.

Figure 7. Nitrate equivalent deposition (NED) factors calculated for the modelled set of Adirondack lakes for scenarios of increasing NO_3^- deposition. Solid circles indicate factors calculated for the +50% NO_3^- deposition scenario. Open circles indicate factors calculated for the +25% and +75% deposition scenarios (courtesy Dr. P. Ryan, ORNL)

Decreasing Deposition Scenarios

Figure 8. Nitrate equivalent deposition (NED) factors calculated for the modelled set of Adirondack lakes for scenarios of decreasing NO_3^- deposition. Solid circles indicate factors calculated for the -50% NO_3^- deposition scenario. Open circles indicate factors calculated for the -25% and -75% deposition scenarios. Many lakes show NED factors greater than 10, indicating that decreases in NO_3^- deposition will have no appreciable effect on lakewater chemistry because lakewater NO_3^- concentrations are very low (courtesy Dr. P. Ryan, ORNL).

LAKE ID	RATIO _i	RATIO _D
1A1003	3.63	4.97
1A1012	7.48	47.98
1A1014	5.48	9.64
1A1017	6.29	9.85
1A1020	7.87	14.4
1A1028	7.16	270.24
1A1029	8.11	∞
1A1033	4.97	91.51
1A1039	6.84	14.12
1A1046	3.45	6.1
1A1049	3.63	5.25
1A1057	10.15	73.14
1A1061	8.49	25.08
1A1064	2.25	142.23
1A1066	2.62	4.58
1A1073	4.98	7.17
1A2002	8.08	20.17
1A2006	5.35	10.05
1A2037	5.93	13.55
1A2041	7.28	129.38
1A2042	5.11	8.97
1A2045	6.44	108.17
1A2046	6.2	24.62
1A2048	9.85	342.92
1A2052	7.89	17.1
1A2054	7.41	32.55
1A3001	6.4	32.97
1A3040	6.03	221.74
1A3042	6.96	40.7
1A3043	6.56	163.08
1A3046	9.83	∞
1A3048	2.65	4.68
1A3065	2.26	3.2

Table 3. Nitrogen Equivalent Deposition (NED) Factors

4.2.2. Reduced-Form Model for Acid Neutralising Capacity

The lake water is represented as a mixture of a direct deposition and runoff component and a soil water component (Small et al., 1995). Therefore, the lake ANC is given by

$$ANC_t = (1 - d_f)ANC_{s,t} - d_f(D_t - D_0) \quad (6)$$

where d_f is the fraction of direct runoff without neutralisation of acid and $ANC_{s,t}$ is the soil water ANC and D is the acid deposition. The soil water ANC is assumed to exponentially approach an equilibrium value

$$ANC_{s,t+\delta t} = ANC_{s,t} + [ANC_{se,t+\delta t} - ANC_{s,t}] \times (1 - e^{-\delta t/\tau}) \quad (7)$$

where τ is the characteristic lag time and $ANC_{se,t}$ is the equilibrium value given by

$$ANC_{se,t} = ANC_{s,0} - (1 - N_{F,t})(D_t - D_0). \quad (8)$$

where $N_{F,t}$ is the fraction of acid deposition input neutralised in the watershed. The neutralisation fraction $N_{F,t}$ has been shown by Labieniec et al (1989) to be analogous to the Henriksen F-factor. Small et al. (1995) assumed $N_{F,t}$ constant for all t , but noted that this was not consistent with MAGIC, where the neutralisation fraction decreased as a result of cumulative deposition. To model this dynamic behaviour of the neutralisation fraction, the change in neutralisation fraction ΔN_F is modelled as linear with the average deposition over

a time step. The level of deposition which does not produce a change in N_F is designated as the Nominal Deposition. Thus,

$$\Delta N_{F,t} = m \times (Dep_t - DNF) \quad (9)$$

where m is a slope factor and DNF is the Nominal Deposition. Therefore, the N_F at any time t is given by

$$N_{F,t} = N_{F,0} + m \times \left(\sum_{i=1}^t Dep_i - tp \times DNF \right) \quad (10)$$

where Dep_t is the average deposition over a time interval and tp is the number of time periods elapsed. The TAF Aquatics module uses a time step δt of 5 years, causing the number of time periods elapsed to be equal to the elapsed time divided by five.

4.2.3. Reduced-Form Model for Lake Calcium

Lake calcium is modelled in a similar fashion to soil water ANC, by allowing the calcium in each watershed to approach equilibrium with a characteristic lag time

$$Ca_{e,t+\delta} = Ca_t + m \times [Ca_{e,t+\delta} - Ca_t] \times (1 - e^{-\delta/\tau}) \quad (11)$$

where $Ca_{e,t+\delta}$ is the equilibrium calcium value given by

$$Ca_{e,t} = m \times Dep_t + b \quad (12)$$

where m and b are parameters of the linear relationship between equilibrium calcium and average deposition over a time interval.

4.2.4. The pH-ANC Relationship

The pH-ANC relationship of Small and Sutton (1986) is defined by

$$pH = a + b \times \operatorname{arcsinh}\left(\frac{ANC - d}{c}\right) \quad (5)$$

where a , b , c and d are parameters obtained by non-linear regression. Lake pH and lake ANC data points for all 33 watersheds for 52 years and across all calibrations, for a total of 17160 data points, were used to estimate the relationship (see **Figure 9**). This relationship is then used to estimate the lake pH in each lake. Using the weighting factors, a cumulative distribution of lake pH can then be constructed for the region. The fraction of lakes in the region below pH 5.5 is read from this distribution.

Figure 9. pH-ANC Relationship for the Adirondacks Based on MAGIC Calibrations

The inclusion of organic acids in the new version of MAGIC tends to increase the variability of the pH-ANC distribution and lowers the estimated pH for a given value of ANC. The pH for high pH lakes is slightly underestimated by the pH-ANC relationship that is presented here.

4.2.5. The Empirical pH-Al Relationship

Lake aluminium is modelled using the empirical pH-Al relationship of Sullivan and Cosby (1995b). They analysed data from surface waters of interest in the United States with respect to Al mobilisation from catchment soils in response to acidic deposition. The Al variable of interest for model predictions is Al_t (total monomeric aluminium) rather than Al^{3+} , since Al_t includes species in addition to Al^{3+} that are also toxic to fish biota. Al_t is used in the fish viability indicators.

pAl and pH have been found to have an empirical linear relationship with a slope distributed around 1.0, ranging from 0.77 to 1.28. Assuming a value of 1.0 for the slope, the change in pAl from the base year 1985 to time t can be computed as follows:

$$pAl_t = [pH_t - pH_{1985}] + pAl_{1985} \quad (13)$$

where pAl_t is the negative common logarithm of the lake aluminium concentration at time t , pAl_{1985} is the negative common logarithm of the lake aluminium concentration in 1985, pH_t is the pH at time t and pH_{1985} is the pH in 1985. The time series of aluminium in the region is generated from this relationship.

4.3. CALIBRATION TO MAGIC

Once the reduced-form models were defined, and the ranges over which they would operate had been established, they were calibrated against MAGIC, the parent model. MAGIC was run on all calibrations for all the 33 sample watersheds, as well as on the mean calibration for each watershed. The resulting simulated data set was used to fit the reduced-form models. Data formatting and initial analysis was done on a SUN SPARCstation using the GCC C compiler. Subsequently, the data were imported into SAS version 6.10 for OS/2, running on an IBM PC 486 DX4/100 with 32 MB of RAM and 65 MB of free hard disk space for storing the data set. The reduced-form models were defined in SAS and were fit to the data. Some excerpts of the SAS program code are presented in **Appendix A, Listing A.1.**

Estimated parameters are for the change in Neutralisation Fraction (DNF), the Soil Water ANC (m, defined here as “ml”, and τ , defined here as “tau”), the Equilibrium Calcium (m, defined here as “mCae”, and b' , defined here as “iCae”) and Lake Calcium (m, defined here as “mCa”, and τ , defined here as “tCa”). These parameters were obtained by non-linear regression methods using adaptive step control. The parameters for the mean calibration data set are listed in **Table 4**. Each row in the table is for one of the 33 sample watersheds.

Lake ID	df	Soil Water ANC		DNF ($\mu\text{eq/L}$)	Equilibrium Calcium		Lake Calcium	
		ml	tau(yr)		mCae	iCae($\mu\text{eq/L}$)	mCa	tCa(yr)
1A1-003	0.34	-6.88E-04	2.82	-19.52	0.42	24.18	0.48	0.08
1A1-012	0.38	-1.04E-03	14.14	68.50	0.76	17.78	0.71	1.45
1A1-014	0.27	-9.08E-04	13.04	66.15	0.70	27.41	0.49	0.07
1A1-017	0.32	-1.31E-03	12.26	58.87	0.80	20.73	0.69	2.16
1A1-020	0.22	-4.01E-04	8.07	77.89	0.84	15.15	0.95	3.11
1A1-028	0.28	-9.86E-04	15.59	65.49	0.75	21.26	1.25	19.26
1A1-029	0.35	-1.93E-03	18.89	58.66	0.67	112.94	0.85	16.22
1A1-033	0.47	-2.49E-03	16.18	61.15	0.67	154.66	1.83	25.67
1A1-039	0.26	-2.32E-03	13.22	58.21	0.73	7.01	0.52	0.11
1A1-046	0.17	-3.26E-04	12.70	55.76	0.63	69.47	1.84	27.11
1A1-049	0.37	-6.73E-04	2.72	-47.35	0.32	20.51	0.10	0.13
1A1-057	0.23	-1.49E-03	11.09	54.82	0.72	4.80	0.77	2.04
1A1-061	0.25	-9.31E-04	3.53	2.47	0.20	12.98	0.49	0.08
1A1-064	0.19	-3.88E-04	5.75	56.35	0.69	71.38	2.80	38.35
1A1-066	0.12	1.84E-04	4.88	79.90	0.68	18.44	0.47	0.06
1A1-073	0.25	8.27E-07	4.84	34802.01	0.40	22.61	0.45	0.08
1A2-002	0.29	-2.20E-03	11.54	60.07	0.73	0.31	0.56	0.10
1A2-006	0.10	-1.63E-03	38.65	67.98	0.45	72.97	0.81	15.94
1A2-037	0.17	-1.34E-03	10.03	63.04	0.75	72.50	0.45	0.19
1A2-041	0.14	-7.11E-04	12.31	62.05	0.62	35.33	0.44	0.17
1A2-042	0.15	-8.13E-04	11.84	57.61	0.68	8.20	0.52	0.17
1A2-045	0.23	-1.14E-03	5.32	34.36	0.49	27.38	1.85	26.53
1A2-046	0.26	-2.33E-04	3.66	42.69	0.82	5.92	0.55	0.13
1A2-048	0.24	1.42E-03	6.97	88.38	0.36	18.64	0.22	0.07
1A2-052	0.26	-7.63E-04	11.19	65.92	0.80	6.49	0.54	0.15
1A2-054	0.20	-6.95E-04	4.09	13.31	0.34	18.87	0.40	0.11
1A3-001	0.38	-1.64E-03	20.55	65.03	0.51	91.92	0.81	13.04
1A3-040	0.32	-1.00E-03	8.40	70.71	0.61	63.43	0.56	0.16
1A3-042	0.22	-1.37E-03	11.06	61.28	0.69	52.91	0.43	0.11
1A3-043	0.15	-1.16E-03	19.17	61.47	0.61	255.71	0.82	16.00
1A3-046	0.21	-2.76E-03	14.60	57.92	0.45	44.43	0.08	0.15
1A3-048	0.21	-2.03E-03	21.01	60.04	0.97	8.22	0.40	0.18
1A3-065	0.30	-1.08E-03	12.98	71.55	0.70	13.49	0.70	2.24

Table 4. Parameters for Mean Calibration Data Set

The direct runoff factor (d_f) ranged from 0.098 to 0.466, with a mean of 0.251 and a standard deviation of 0.084. The soil water ANC lag factor ranged from 2.72 yr to 38.65 yr, with a mean of 11.61 yr and a standard deviation of 7.12 yr. The lake calcium lag factor ranged from 0.06 yr to 38.35 yr, with a mean of 6.41 yr and a standard deviation of 10.54 yr. These estimated values for the fraction of direct runoff and the characteristic lag times are consistent with expectations for the range of Adirondack lakes evaluated in this study.

Using these values for the parameters in the reduced-form equations, the reduced-form model outputs were compared against MAGIC. **Figures 10, 11 and 12** show the reduced-form fits to MAGIC acid neutralising capacity, lake calcium and lake pH for a typical watershed (1A1-012).

Figure 10. Reduced-Form Fit to MAGIC ANC for Watershed 1A1-012

Figure 11. Reduced-Form Fit to MAGIC Calcium for Watershed 1A1-012

Figure 12. Reduced-Form Fit to MAGIC pH for Watershed 1A1-012

The following figures (Figure 13 through 15) depict the reduced-form lake chemistry values for the entire region, generated by averaging with the weighting factors for each watershed.

Figure 13. Predicted TAF ANC for the Adirondacks

Figure 14. Predicted TAF Calcium for the Adirondacks

Figure 15. Predicted TAF pH for the Adirondacks

The root mean square errors and the mean errors for the reduced-form fits are presented in Table 5.

Lake ID	RMS Error ($\mu\text{eq/L}$)		Mean Error ($\mu\text{eq/L}$)	
	Lake ANC	Lake Calcium	Lake ANC	Lake Calcium
1A1-003	1.79	1.16	0.06	0.41
1A1-012	0.86	0.99	-0.16	0.43
1A1-014	1.14	0.65	-0.16	0.20
1A1-017	1.13	1.28	-0.25	0.63
1A1-020	0.96	1.11	-0.13	0.51
1A1-028	1.20	0.41	-0.14	0.01
1A1-029	1.36	0.39	-0.23	-0.05
1A1-033	1.48	0.69	-0.38	0.12
1A1-039	1.64	2.01	-0.39	0.85
1A1-046	1.51	0.23	-0.01	0.01
1A1-049	2.22	1.71	0.24	-0.82
1A1-057	1.27	2.01	-0.37	1.04
1A1-061	1.93	1.06	-0.72	0.29
1A1-064	1.28	0.43	-0.10	0.13
1A1-066	1.49	0.45	0.35	-0.09
1A1-073	2.59	1.31	-1.11	0.37
1A2-002	1.64	2.02	-0.40	0.88
1A2-006	1.06	0.32	-0.20	-0.02
1A2-037	1.75	1.27	-0.42	0.45
1A2-041	1.41	0.66	-0.17	0.21
1A2-042	1.24	0.75	-0.13	0.24
1A2-045	2.68	0.50	-0.15	0.10
1A2-046	0.94	0.71	-0.06	-0.05
1A2-048	4.61	0.89	1.40	-0.41
1A2-052	1.34	0.95	-0.21	0.31
1A2-054	2.41	0.65	0.20	0.21
1A3-001	1.18	0.31	-0.24	-0.02
1A3-040	1.26	1.38	-0.34	0.61
1A3-042	1.48	1.08	-0.36	0.38
1A3-043	1.20	0.40	-0.22	-0.04
1A3-046	2.10	3.33	-0.62	-1.24
1A3-048	1.50	0.84	-0.25	0.27
1A3-065	1.03	0.89	-0.17	0.44

Table 5. Root Mean Square Errors and Mean Errors of fit

The pH-ANC distribution in Figure 9 and the weighting factors were used to construct a cumulative probability distribution of pH for each year in the simulation (see § 4.5). The

pH, lake calcium and lake aluminium time series were then used to calculate the effects on fish indicators (see § 5).

4.4. MANAGEMENT OF UNCERTAINTY

The objective in developing a first characterisation of uncertainty in the TAF models for aquatics and soils is to attempt to reflect the uncertainty in the parent MAGIC model upon which the reduced-form modules are based. To date, this uncertainty has been expressed through the development of multiple MAGIC calibration data sets for each of the 33 reference lakes. These multiple calibrations reflect the uncertainty in the lake chemistry, with each calibration assumed to be equally likely. In the attempt to translate the uncertainty in the calibrations for MAGIC and in MAGIC itself into an "equivalent" uncertainty in our reduced-form model, the standard errors of the multiple MAGIC calibrations on the residuals were used to specify uncertainty. Uncertainties are small, but persist in time, since the residual differences from the mean tend to persist for a given calibration run. This uncertainty in MAGIC is, however, larger than the error in the reduced-form approximation to MAGIC described in **Table 5**.

Uncertainty was characterised for lake ANC and lake calcium. Analytica propagated uncertainty through all dependent models. The mean and the standard deviation in the change in lake chemistry outputs from MAGIC for each year were calculated (see **Figure 16**).

Figure 16. MAGIC Calibrations, Mean Calibration and TAF Fit to MAGIC for Watershed 1A1-012

The coefficient of variation (in percent) was calculated as:

$$v_{calibrations} = 100 \times \frac{\sigma_{calibrations}}{\mu_{calibrations}} \quad (14)$$

and found to be nearly constant over time (see **Figure 17** and **Table 6**). Excerpts from the SAS Code for characterising uncertainty are presented in **Appendix A, Listing A.2**.

Figure 17. Coefficient of Variation (in %) in MAGIC ANC for Watershed 1A1-012

The deviation from the mean lake chemistry output is calculated as the change in the variable of interest from the base year 1985 multiplied by the coefficient of variation:

$$\sigma_{from\ mean} = (ANC_t - ANC_0) \times v_{calibrations} \quad (15)$$

The uncertain lake chemistry output is then defined as:

$$ANC_{probabilistic} = ANC_{deterministic} + \sigma_{from\ mean} \times N(0,1) \quad (16)$$

where $N(0,1)$ is a unit normal distribution that applies to the entire time period of a given simulation. Similar relationships have been defined for lake calcium. Uncertainty is propagated throughout the reduced-form model by Analytica. A key issue, yet to be

resolved, is whether independent values of the $N(0,1)$ variate should be generated for each of the 33 watersheds in a given simulation (assuming uncertainties across lakes are independent), or whether the same $N(0,1)$ variate should be used for all watersheds in a given simulation (implying perfectly correlated uncertainty across lakes). In reality, the correlation in uncertainty is intermediate between these two cases.

Lake ID	Coefficient of Variation for ANC (%)	Coefficient of Variation for Calcium (%)
1A1-003	1.766e+1	6.890e+1
1A1-012	1.763e+1	1.082e+2
1A1-014	1.975e+1	3.713e+1
1A1-017	3.320e+1	2.844e+1
1A1-020	1.911e+1	1.422e+2
1A1-028	3.123e+1	9.547e+1
1A1-029	3.023e+1	1.988e+2
1A1-033	2.026e+1	9.593e+1
1A1-039	3.114e+1	1.134e+2
1A1-046	2.393e+1	4.284e+1
1A1-049	1.755e+1	6.511e+1
1A1-057	4.528e+1	4.653e+1
1A1-061	9.197e+0	1.806e+2
1A1-064	1.986e+1	1.452e+2
1A1-066	1.545e+1	4.735e+1
1A1-073	2.078e+1	1.138e+2
1A2-002	3.171e+1	1.309e+2
1A2-006	1.593e+2	8.273e+1
1A2-037	3.887e+1	4.140e+1
1A2-041	2.658e+1	2.931e+1
1A2-042	5.520e+1	3.797e+1
1A2-045	4.058e+1	6.016e+1
1A2-046	1.426e+1	5.324e+1
1A2-048	2.212e+2	7.349e+1
1A2-052	1.771e+1	4.748e+1
1A2-054	2.303e+1	8.479e+1
1A3-001	4.841e+1	4.501e+1
1A3-040	1.781e+1	4.515e+1
1A3-042	8.281e+1	5.109e+1
1A3-043	5.897e+1	5.733e+2
1A3-046	2.836e+1	1.121e+2
1A3-048	6.612e+1	7.347e+1
1A3-065	2.640e+1	3.709e+1

Table 6. Coefficient of Variation for ANC and Calcium

4.5. RESULTS AND DISCUSSION

The reduced-form models for ANC and calcium were fit to MAGIC. The error measures presented in **Table 5** were averaged using the weighting factors. The average error measures are presented in **Table 7**. These measures are indicative of the quality of the reduced-form fit to MAGIC.

Root Mean Square Error ($\mu\text{eq/L}$)		Mean Error ($\mu\text{eq/L}$)	
Lake ANC	Lake Calcium	Lake ANC	Lake Calcium
1.65	1.14	-0.21	0.15

Table 7. Weighted Average of the Error Measures

The reduced form models underestimate the MAGIC ANC on average by 0.21 $\mu\text{eq/L}$ and overestimate the MAGIC Calcium by 0.15 $\mu\text{eq/L}$. These errors are small compared to the uncertainty in MAGIC, which is around an order of magnitude larger in value. Therefore, the uncertainty in the outputs of ANC and calcium from the TAF Aquatics module are defined as the uncertainty in MAGIC, though the reduced-form fit errors are also presented for completeness.

For this document, a test deposition scenario of a 30% decrease in acid deposition was chosen for the purpose of illustrating the cumulative distribution of pH in 1990 and 2030. This test scenario is illustrated in **Figure 18**.

Figure 18. Test Scenario (30% Reduction)

This test scenario was used to construct the cumulative probability distribution of pH for the entire region, in the years 1990 (**Figure 19**) and 2030 (**Figure 20**).

Figure 19. Cumulative Probability Distribution of pH in 1990

Figure 20. Cumulative Distribution of pH in 2030

From **Figure 19**, it is seen that 40% of lakes in the region have pH less than 5.5 in 1990. However, in 2030 (**Figure 20**), the number of lakes with pH less than 5.5 has fallen to 30%. The CDF of predicted pH for the years 1990 and 2030 are compared in **Figure 21**.

Figure 21. Comparison of predicted pH for 1990 and 2030

The predicted effect of the deposition reduction scenario is summarised in **Figures 10 through 15**. Note that the average lake chemistry is only affected in a small way by the deposition reduction. However, a further increase in acidification is avoided. In both cases

(and for all years in between), the TAF pH closely matches the MAGIC pH. Thus, the reduced-form models are an acceptable approximation to the parent MAGIC model.

4.6. CONCLUSIONS

Simplified reduced form models were developed to mimic the performance of the more complicated MAGIC model in the Adirondacks. These models were developed for lake acid neutralising capacity and lake calcium. The models were calibrated against MAGIC, and the calibrated model outputs were shown to closely mimic MAGIC outputs of ANC, calcium and pH. Subsequently, the reduced-form models were implemented as part of the TAF Integrated Model in Analytica. These models incorporate a representation of the uncertainty in MAGIC.

Outputs from these reduced-form models were used as input to the fish viability indicators, described in the next section. The fish viability indicators were also implemented in Analytica. The TAF Benefits and Valuation Module, developed by Resources For the Future, uses one of these fish viability indicators (namely the Acid Stress Index or ASI) to assign a dollar value to recreational fishing in the Adirondack Mountains.

5. ESTIMATING EFFECTS OF LAKE CHEMISTRY CHANGES **ON FISH BIOTA**

5.1. OVERVIEW OF THE METHODS USED IN THE NAPAP 1990 ASSESSMENT

As a lake acidifies, the structure and function of its biota will change. Baker et al. (1990) describe the types of biological effects expected, procedures to estimate the magnitude and significance of these changes, potential mechanisms for observed effects, and the levels of acidity (and associated parameters) at which changes in the biological community are expected to occur.

The NAPAP 1990 IA states that fish populations have decreased in the Adirondacks due to the acidification of the lakes from anthropogenic sources. Around 20% of the lakes in the Adirondacks have an average pH less than 5.5. Decreases in the pH of lake water affect the fertility of adult fish and the survival rates of younger fish. As pH decreases further, the survival rates of adult fish also decline. The response of each species to decline in pH also varies. For example, the pH range in which common shiner populations typically experience recruitment failure is 6.0 to 5.4, whereas the corresponding range for brook trout populations is much lower at 5.2 to 4.9 (NAPAP, 1990). It has been estimated that human-induced acidification is responsible for the loss of fish populations in around 16% of 858 Adirondack lakes for which information is available (Baker et al., 1990).

Baker et al. (1990) describe three important measures related to fish viability, namely the Acid Stress Index (ASI), Probability of Fish Presence and Fish Species

Richness. All these indicators are generated by the TAF Aquatics Module. Logistic models have been used to define these indicators. Of these indicators, ASI is the one that is most important for TAF, for reasons described below.

Recreational productivity is the catch of a particular species that an average angler will make in an hour, and is referred to as the Catch Per Unit Effort (CPUE). The CPUE has been related to the skill of the angler, the characteristics of the lake and the acidic stress in the lake using multiple regression techniques (NAPAP, 1990). Thus, CPUE values can be predicted for a given lake, and a dollar value can be assigned.

As part of the TAF modelling effort, it is necessary to quantify the relationship between changes in acid-base chemistry and regional effects on fish communities. The TAF Valuation module uses Acid Stress Index outputs to assess the economic impact of the degradation of the ability of the lakes in the region to support fish species.

5.2. ACID STRESS INDEX IN LAKES

An important estimate of the degradation of fish species in an acidified lake is the Conditional fish Mortality Rate (CMR, see Baker et al., 1990), which is the increased likelihood that a fish of a given life stage will die when exposed to the specified water quality conditions, over and above the mortality expected in a circumneutral reference water. Three basic toxicity models have been developed for regional application :

- tolerant toxicity model - 21 day survival of brook trout fry
- intermediate toxicity model - 8 day survival of smallmouth bass alevins

- sensitive toxicity model - 21 day survival of rainbow trout fry

The toxicity models inputs are pH, aluminium and calcium. The outputs range between 0 and 100, with higher values indicating greater acid-induced stress (i.e. increased percent mortality, see **Figure 22**). The conditional mortality rate is often referred to as the Acid Stress Index (ASI). ASI is calculated using a logistic relationship of the form

$$ASI = \frac{100}{1 + e^x} \quad (17)$$

where x is a function of pH, calcium and aluminium as described below (Baker et. al., 1990). ASI is 0 when $pH > 8$ or calcium $> 2000 \mu\text{eq/L}$. Note that aluminium is assigned the value of 0 when $pH > 6.5$, so that aluminium toxicity is only effective below this value of pH. Calcium is in $\mu\text{eq/L}$ and aluminium is in $\mu\text{g/L}$. The Acid Stress Indices (ASI) for three fish species are modelled, each of which is representative of a broad class of species and x in **Eq. 17** is given by:

1. Tolerant species (brook trout)

$$x = -23.49 + 5.35pH + 2.97 \times 10^{-3} Ca - 1.93 \times 10^{-3} Al \quad (18)$$

2. Intermediate species (smallmouth bass)

$$x = -18.73 + 3.57pH + 1.45 \times 10^{-2} Ca - 4.37 \times 10^{-2} Al \quad (19)$$

3. Sensitive species (rainbow trout)

$$x = -8.90 + 1.56pH + 4.08 \times 10^{-3} Ca - 7.04 \times 10^{-2} Al \quad (20)$$

Figure 22. Illustration of the Acid Stress Index Function for Brook Trout. Ca is 65 $\mu\text{eq/L}$ and Al is (from L to R) 100, 600, and 1500 $\mu\text{eq/L}$ respectively.

5.3. FISH PRESENCE/ABSENCE IN LAKES

Some fish species are more sensitive to the acidification of their habitat than other species. At a specified level of acid stress, some species may achieve 100% mortality, while others may have reduced numbers. The presence or absence of a fish species has been modelled as a function of water chemistry variables (see Baker et al., 1990). Three species with a range of acid sensitivity have been selected. Acidification response of presence/absence of fish species in lakes is calculated using a logistic relationship of the form

$$P(\text{presence}) = \frac{1}{1 + e^x} \quad (21)$$

where x is a function of lake pH and lake calcium (Baker et. al., 1990). Fish Presence/Absence relationships for three species are modelled, each of which is representative of a broad class of species and x in **Eq. 21** is given by:

1. Tolerant species (Adirondack brook trout)

$$x = -16.94 + 18.34 \frac{pCa}{pH} \quad (22)$$

2. Intermediate species (Ontario lake trout)

$$x = -30.87 + 38.11 \frac{pCa}{pH} \quad (23)$$

3. Sensitive species (Adirondack common shiner)

$$x = -9.28 + 12.16 \frac{pCa}{pH} \quad (24)$$

The pH presence/absence relationship for a tolerant species at different calcium concentration is shown in **Figure 23**.

Figure 23. Illustration of the Probability of Brook Trout Presence

5.4. FISH SPECIES RICHNESS OF LAKES

Models have also been developed with the number of species per lake as the dependent variable (see Baker et al., 1990). These models estimate the change in the total number of fish populations in a region (the Fish Species Richness) due to the change in lake chemistry. As is the case for ASI and Presence/Absence, the models for fish species richness are calibrated using logistic regression analysis. Models which address baseline conditions only (Function B) and both acidification and baseline conditions (Function AB) are documented in the literature. For the purposes of the TAF modelling effort, a Function AB model with lake chemistry and physical characteristics has been implemented. For some applications it may be suitable to implement both Function B and Function AB models (Christensen, 1995).

Fish species richness for the region is modelled as a combined baseline and acidification (Function AB) logistic model (Baker et. al., 1990). The number of species in each lake is assumed to follow a random binomial process with parameters p and N . The

parameter p is the probability of colonisation success and is a function of the lake characteristics. It is calculated by the logistic relationship :

$$p = \frac{r}{1 + e^x} \quad (25)$$

where x is a function of lake pH, lake calcium, lake surface area, lake elevation and lake silica (for expressions of x see below). Parameter N is the total potential number of colonising species in the region and is set at 13. Lake area is in hectares, elevation is in m, lake calcium is in $\mu\text{eq/L}$ and silica is in mg/L .

The species richness model selected for the TAF Aquatics Module is the Function AB/ Model 10 (Baker et al., 1990) with Mean Square Error = 3.85; in this model, x and r in Eq. 25 are given by:

$$\begin{aligned} x = & -23.98 + 3.81pH + 1.26 \log_{10}(\text{area}) - 5.27 \times 10^{-3} \times \text{elevation} + 0.934 \log_{10}(\text{silica} + 1) \\ & + 10.74 \log_{10}(\text{Ca}) - 1.6 \times pH \times \log_{10}(\text{Ca}) \\ r = & 0.670 \end{aligned} \quad (26)$$

5.5. RESULTS AND DISCUSSION

For the purposes of this document, the test scenario shown in **Figure 18** has been selected to illustrate the ASI and Fish Presence/Absence outputs.

Since the inputs to the logistic model are distributions of pH and calcium, the output is also uncertain. Distributions of Species Richness can be generated in Analytica. The Acid Stress Index was calculated for the Adirondacks by computing the ASI for each lake and

averaging using the weighting factors. The average ASI is illustrated in **Figure 24**. Higher values of ASI represent higher acid stress and hence a lower CPUE. Rainbow trout has an ASI close to 35, while Brook Trout has an ASI of around 2. Thus, Rainbow Trout will be the mostly severely affected, while Brook Trout will be less susceptible, being a less sensitive species. Smallmouth Bass is a species of intermediate sensitivity.

Figure 24. Predicted Average ASI in the Adirondacks

The Probability of Fish Presence, $P(\text{Presence of Fish Species}|\text{Acidification})$ is averaged over all lakes in the same fashion, using the weighting factors, to obtain the expected probability of fish presence in the region. The probability of presence, which can be interpreted as the expected fraction of lakes in the region where the species will be present, is illustrated in **Figure 25**. Higher values represent less sensitivity.

Figure 25. Probability of Fish Presence in the Adirondacks

Brook Trout, the least sensitive species has a probability of presence of around 89%. Common Shiner on the other hand, is the most sensitive species, and has a probability of presence close to 56%. Both measures of fish viability indicate only small responses to the 30 percent deposition reduction scenario tested, with ASI slightly decreasing and the probability of fish presence slightly increasing. This is consistent with the small changes in regional lake chemistry predicted to occur as a result of the deposition reduction (Figures 13 through 15).

Figure 26 illustrates Analytica running the TAF Soils-Aquatics Module. Probability bands for the ASI in the Adirondacks for Brook Trout are displayed as a time series.

Figure 26. Analytica Probabilistic Output for ASI

Note that the ASI trend (Figure 24) and the Probability of Presence trend (Figure 25) closely mimic the Test Scenario trend (Figure 18). There is a decrease in acid deposition from 1995 to 2010, and this decrease is represented as a decrease in ASI from 1995 to 2010 and a corresponding increase in the Probability of Presence. This illustrates the ability of the reduced-form models to track predicted changes in acid deposition from year to year, and their uncertainty.

5.6. CONCLUSIONS

The reduced-form models for ANC and calcium developed and calibrated in § 4 were applied to obtaining three measures of fish viability, namely Acid Stress Index, Probability of Fish Species Presence and Fish Species Richness. The measures were tested using the test deposition scenario (30% decrease) and were found to reflect the small improvement in lake chemistry resulting from the decreasing deposition through a small improvement in the values of these measures.

Since the measures had probabilistic inputs, the outputs can also be computed in a probabilistic manner. Mean values were presented for sake of clarity. These mean values were characteristic of each of the fish species that they represented. One of these measures, namely the Acid Stress Index for the Adirondacks, is used in the TAF Valuation Module to assess the economic impact of acid deposition on anglers who use the Adirondack lakes for recreational fishing. NAPAP (1990) estimated the resulting losses in fishable acreage as 1.07 million dollars annually. Losses incurred due to additional travel costs to other fishing areas were estimated to be between \$1 million and \$13 million annually.

It is believed (NAPAP, 1990) that these estimates may understate the actual value of damages in the region. This was because only two of the brook trout anglers surveyed caught brook trout in lakes where the ASI was greater than 0, and the ASI values of these lakes were still not very much greater than 0. Therefore it was not possible to simulate increases in the Willingness-to-Pay (WTP) of brook trout anglers as water quality conditions improved. Additionally, the distribution of ASI in the lakes used to calibrate the linkage model is not the same as the distribution of lakes in the ELS data set as a whole. The mean ASI in the lakes in the calibration data set is lower than the mean ASI in the ELS

data set. Also the distribution of ASI in the calibration data set is positively skewed, such that the mean ASI in the ELS data set lies in the tail of the ASI distribution in the calibration data set (NAPAP, 1990).

6. SUMMARY

The Tracking and Analysis Framework (TAF) was developed to address the integrated assessment issues that the National Acid Precipitation Program would study under the Clean Air Act Amendments Title IV mandate. All the key components of acid deposition and its resulting environmental and economic effects were incorporated into the Framework. This document dealt with completed and ongoing work to assess the effects of acid deposition on surface waters for TAF.

The improvements to the Model for Acidification of Groundwater in Catchments (MAGIC), and how these improvements would change the response of the surface waters in the Adirondacks to acid deposition were described. Reduced-Form Models were developed as simplified approximations to MAGIC Acid Neutralising Capacity (ANC) and MAGIC Lake Calcium. A relationship between ANC and pH was used to obtain the pH. New empirical information about lake aluminium was used to obtain lake aluminium concentrations from the lake pH values for each lake. The reduced-form lake chemistry outputs were compared against MAGIC and were found to provide excellent approximations. Uncertainty in MAGIC was characterised within the reduced-form models.

The lake chemistry outputs were used to obtain three indicators of fish viability in the lakes in the Adirondacks. These indicators were the Acid Stress Index, Probability of Fish Species Presence and Fish Species Richness. The first two indicators were calculated for three fish species each. The trends in these indicators were shown to follow the acid deposition trend, with small improvement in the values of these indicators predicted to result from a 30% reduction in acid deposition.

Modifications and enhancements to the TAF Aquatics and Soil modules were planned in keeping with the overall aims and objectives of TAF. These include improvements in the full-form MAGIC model to better represent natural processes, improvements in the fit between the reduced form models and MAGIC, and the modelling of additional acid-sensitive regions.

MAGIC currently models nitrogen by assuming a fixed proportion of uptake of each nitrogen species in each model compartment. Methods of allowing dynamic nitrogen uptake in MAGIC based on watershed history and nitrogen saturation status are being studied. Sensitivity analyses are also being performed to improve the projection of changes in soil conditions based on the treatment of organic acids, aluminium solubility, and carbon dioxide concentration in the soil layers. Future versions of TAF could be calibrated to improved MAGIC projections that result from these studies.

The ability to model additional acid-sensitive regions must be added to TAF so that a more representative national assessment can be made. Regions that were modelled for the 1990 NAPAP Assessment, namely New England, Mid-Atlantic Highlands, and the Southern Blue Ridge Province, could be added after revised MAGIC projections are made. These regional models would consider the effects of acid deposition on stream chemistry and stream biota as well as lakes. New fish models for streams (Bulger, 1995) could also be incorporated.

The ability to modify the distributions of ANC, calcium and pH as and when new monitoring data become available is possible using Bayesian Monte Carlo methods. This feature could also be incorporated.

At present, uncertainty is represented as the uncertainty in MAGIC calibrations. It is proposed to derive joint probability distributions between the parameters of the reduced-form models in order to be able to better characterise the uncertainty. Such a derivation may be possible using specialised optimisation techniques.

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APPENDIX A: SAS™ CODE EXCERPTS FOR REDUCED FORM MODELS

LISTING A.1. LAKE ANC AND LAKE CALCIUM MODELS

```

%let prog=full1n;
libname tafall "U:\RSB7\TAF\";
libname tafavg "e:\rsinha\taf\";
options linesize=129 pagesize=69;
%let pathall= U:\RSB7\TAF\;
%let pathavg= e:\rsinha\taf\;
%let curr_dbs= stpavg;
/* %let wsd_id= '1A1-003' '1A1-012' '1A1-014' '1A1-017' '1A1-020' '1A1-
028'
                '1A1-029' '1A1-033' '1A1-039' '1A1-046' '1A1-049' '1A1-
057'
                '1A1-061' '1A1-064' '1A1-066' '1A1-073' '1A2-002' '1A2-
006'
                '1A2-037' '1A2-041' '1A2-042' '1A2-045' '1A2-046' '1A2-
048'
                '1A2-052' '1A2-054' '1A3-001' '1A3-040' '1A3-042' '1A3-
043'
                '1A3-046' '1A3-048' '1A3-065'; */
%let wsd_id= '1A1-073';
%let fname= '1A1061.PR1';
%let libr= tafavg;
filename plt "&pathavg&prog..plt";
filename out "&pathavg&prog..txt";

goptions gsfname=append rotate=landscape
        gsfname=plt device=os2 ftext=centx colours=(black);
/* goptions nodisplay gsfname=append noprompt rotate=landscape
        gsfname=plt device=hplj5p2 ftext=centx colours=(black); */
axis1 label=(a=90 r=0);

/* Code to estimate a constant df */
title1 'Estimation of df for watershed ';
data wsd;
    set &libr.&curr_dbs;
    where SA_WSD=&wsd_id and SCENAR NE 'CONSTANT';
    by SA_WSD Flenam;
    drop All Al2 ALT AL_Cal Ca1 Ca2 BS1 BS2 pH1 pH2 NH4 SO4 NO3 FCL0
SBC0
        NO30 NH40;
    retain ANC0 D0 ANCOp DOp ANC1844 D1844;

```

```
SO40=-Calk0;
if YEAR=1844 then
do;
    ANC1844=ANC;
    D1844=SO40;
end;
if YEAR=1986 then
do;
    ANC0p=ANC;
    D0p=SO40;
end;
delANC=ANC0-ANC0p;
delD=(D0p-D0);
if YEAR=1985 then
do;
    ANC0=ANC;
    D0=SO40;
end;
run;

proc nlin data=wsd g4singular se maxiter=100 step=100;
by SA_WSD Filenam;
parms m=1;
model delANC=m*delD;
der.m=delD;
output out=wsd
      p=ldelANC
      parms=df
run;
/*
proc gplot data=wsd;
by SA_WSD Filenam;
plot
    delANC*delD=1
    ldelANC*delD=2
    / vaxis=axis1 overlay;
run;
*/
/* Code to calculate the parameters of the regression */
title 'SANC-Dep relationship for step scenarios';
data wsd;
set wsd;
where SCENAR NE : 'C';
by SA_WSD Filenam;
retain Ca0 ANC0 D0 ANC0p D0p SANC0 Year0 Ddttmp ANC1844 SANCpr
      D1844 NF0 Depprev Caprev ANCprev A10;
SO40=-CALK0;
SANCp=SANCpr;
if YEAR=1986 then
do;
    ANC0p=ANC;
    D0p=SO40;
end;
delt=Year-Year0;
```

```

tp=delt;
if YEAR=1985 then
do;
  ANC0=ANC;
  Ca0=Ca;
  Al0=Al;
  SANC0=ANC0/(1-df);
  D0=SO40;
  Depprev=SO40;
  NF0=1-((ANC1844-ANC0)/(D0-D1844));
  Year0=YEAR;
  delt=0;
  tp=0;
  delCa=.;
  Caprev=Ca;
  ANCprev=.;
  SANC=SANC0;
  Ddttmp=0;
end;
else
  if YEAR>1985 then
  do;
    Ddttmp=Ddttmp+SO40;
    Ddt=Ddttmp;
    Dep=Ddt-D0/2-SO40/2;
    avdep=(SO40+Depprev)/2;
    if Year=1986 then avdep=.;
    Depprev=SO40;
    SANC=(ANC+df*(SO40-D0))/(1-df);
    SANCpr=SANC;
    delCa=Ca-Caprev;
    Calast=Caprev;
    Caprev=Ca;
    dANC=ANC-ANCprev;
    ANCprev=ANC;
  end;
run;

proc nlin data=wsd method=marquardt tau=0.001 g4singular maxiter=100
          se step=100;
  by SA_WSD Filenam;
/*   bounds tau>0, tau<=100; */
  parms ml=-0.1 tau=5.0 DNF=60;
  model SANC=SANCp+(1-exp(-(1)/tau))*(SANC0-SANCp-(1-NF0-ml*(Dep-
tp*DNF))
          *(Depprev-D0));
  der.tau=-exp(-(1)/tau)*(SANC0-SANCp-(1-NF0-ml*(Dep-tp*DNF))
          *(Depprev-D0))/(tau**2);
  der.ml=-(1-exp(-(1)/tau))*(tp*DNF-Dep)*(Depprev-D0);
  der.DNF=-(1-exp(-(1)/tau))*ml*tp*(Depprev-D0);
  output out=wsd
         p=lSANC
         r=rSANC
         parms=ml tau DNF

```

```
run;
/*
proc gplot data=wsd;
  by SA_WSD Filenam;
  plot
    SANC*Year=1
    lSANC*Year=2
    / vaxis=axis1 overlay;
run;
*/
/* Code to compare the MAGIC ANC with the Calculated RFM ANC */
title 'Comparison of MAGIC ANC with calculated RFM ANC time series';
data wsd;
  set wsd;
  by SA_WSD Filenam;
  retain NFprev;
  lANC=(1-df)*lSANC-df*(SO40-D0);
  if Year=1985 then
  do;
    NFprev=NF0;
    NF=NF0;
    delNF=0;
  end;
  else
    if Year>1985 then
    do;
      delNF=m1*(avdep-DNF);
      NF=NFprev+delNF;
      NFprev=NF;
    end;
  end;

run;

proc gplot data=wsd;
  by SA_WSD Filenam;
  plot
    ANC*Year=1
    lANC*Year=2
    / vaxis=axis1 overlay;
run;

title 'Empirical relationship between equilibrium Ca and avg dep.';
proc nlin data=wsd g4singular se;
  by SA_WSD Filenam;
  parms mCae=1 iCae=5;
  model Cae=mCae*avdep+iCae;
  der.mCae=avdep;
  der.iCae=1;
  output out=wsd
    p=lCae
    parms=mCae iCae
run;
/*
proc gplot data=wsd;
  by SA_WSD Filenam;
```

```
plot
  Cae*avdep=1
  lCae*avdep=2
  / vaxis=axis1 overlay;
run;
*/
title 'Exponential relationship for Ca in each watershed';
proc nlin data=wsd method=marquardt tau=0.001 g4singular maxiter=100
      se step=100;
  by SA_WSD Filenam;
  parms mCa=-1.0 tCa=10.0;
  bounds tCa>0;
  model Ca=Calast+mCa*(lCae-Calast)*(1-exp(-(1)/tCa));
  der.mCa=(lCae-Calast)*(1-exp(-(1)/tCa));
  der.tCa=-mCa*(lCae-Calast)*((1)/(tCa**2))*exp(-(1)/tCa);
  output out=wsd
    p=lCa
    r=rCa
    parms=mCa tCa
run;
data wsd; set wsd; by SA_WSD Filenam;
  ANCsq=(ANC-lANC)**2; Caesq=(Cae-lCae)**2; Casq=(Ca-lCa)**2; run;
proc means data=wsd mean; by SA_WSD Filenam;
  var ANCsq Caesq Casq;
  output out=ws mean=mANCsq mCaesq mCasq;
run;
data wsd; set wsd; merge ws wsd; by SA_WSD Filenam; run;

title 'MAGIC Ca and Pred. Ca vs. Year for step scenarios';
proc gplot data=wsd;
  by SA_WSD Filenam;
  plot
    Ca*Year=1
    lCa*Year=2
    / vaxis=axis1 overlay;
run;

title 'MAGIC pH and Pred.pH vs. Year for step scenarios';
data wsd;
  set wsd;
  by SA_WSD Filenam;
  ag=6.01241; bg=2.91910E-1; cg=1.56592E1; dg=7.34333E1;
  nancg=(lanc-dg)/cg;
  al=6.00802; bl=4.55357E-1; cl=1.53896E1; dl=4.26385E1;
  nancl=(lanc-dl)/cl;
  if lANC>50 then lpH=ag+bg*log(nancg+sqrt(nancg*nancg+1));
      else lpH=al+bl*log(nancl+sqrt(nancl*nancl+1));
run;

proc gplot data=wsd;
  by SA_WSD Filenam;
  plot
    pH*Year=1
```

```

    lpH*Year=2
    / vaxis=axis1 overlay;
run;

/* Write all the relevant parameters to a file */
data output;
    set wsd;
    where Year=1995 and SCENAR='D60S85';
    file out mod;
    put SA_WSD Filenam df ANC0 D0 A10 Ca0 ANC1844 D1844 NF0 SANCO
        ml tau DNF mANCsq mCae iCae mCaesq mCa tCa
mCasq;
run;

filename out2 "&pathavg&prog..out";
data output;
    set wsd;
    file out2 mod;
    put SA_WSD Filenam SCENAR Year ANC lANC Ca lCa pH lpH;
run;

```

LISTING A.2. UNCERTAINTY ANALYSIS CODE

```

%let prog=uncert;
libname tafall "U:\RSB7\TAF\";
libname tafavg "e:\rsinha\taf\";
options linesize=129 pagesize=69;
%let pathall= U:\RSB7\TAF\;
%let pathavg= e:\rsinha\taf\;
%let curr_dbs= stpall;
/* %let wsd_id= '1A1-003' '1A1-012' '1A1-014' '1A1-017' '1A1-020' '1A1-
028'
                '1A1-029' '1A1-033' '1A1-039' '1A1-046' '1A1-049' '1A1-
057'
                '1A1-061' '1A1-064' '1A1-066' '1A1-073' '1A2-002' '1A2-
006'
                '1A2-037' '1A2-041' '1A2-042' '1A2-045' '1A2-046' '1A2-
048'
                '1A2-052' '1A2-054' '1A3-001' '1A3-040' '1A3-042' '1A3-
043'
                '1A3-046' '1A3-048' '1A3-065'; */
%let step= 5;
%let wsd_id= '1A1-012';
%let c_sce1= 'D60S85';
%let c_sce2= 'I10S85';
%let libravg= tafavg;
%let librall= tafall;
filename plt "&pathavg&prog..plt";

```

```
filename out "&pathavg&prog..txt";

goptions gsfname=append rotate=landscape
          gsfname=plt device=os2 ftext=centx colours=(black);
/* goptions nodisplay gsfname=append noprompt rotate=landscape
          gsfname=plt device=hplj5p2 ftext=centx colours=(black); */
axis1 label=(a=90 r=0);

data wsd;
  set &librall.&curr_dbs;
  where SA_WSD=&wsd_id and
        (SCENAR=&c_sce1 or SCENAR=&c_sce2) and Year>=1985;
  by SA_WSD Filenam;
  drop Al1 Al2 ALT AL_Ca1 Ca1 Ca2 BS1 BS2 pH1 pH2 NH4 SO4 NO3 FCL0
SBC0
      NO30 NH40 Al pH Calk Calk0 Cae SO40 Qp Qs Elev Wt Lsiz Wsiz;
  retain ANC0 Ca0;
  if YEAR=1985 then
  do;
    ANC0=ANC;
    Ca0=Ca;
  end;
run;

data wsd; set wsd; by SA_WSD Filenam; if mod(Year,&step)=0; run;
data uncert; set &libravg..uncert; run;
proc sort data=uncert; by SA_WSD; run;
data wsd; set wsd; merge wsd uncert; by SA_WSD; run;

data wsd; set wsd; by SA_WSD Filenam;
  delANC=ANC-ANC0;
  delCa=Ca-Ca0;
  nANC=ANC1987+delANC;
  nCa=Ca1984+delCa;
run;

/* Organise data into proper format */
proc sort data=wsd; by SA_WSD SCENAR Year Filenam; run;
proc means noprint data=wsd cv; by SA_WSD SCENAR Year;
  var nANC delANC nCa delCa;
  output out=mvals cv=cANC cdelANC cCa cdelCa; run;
data mvals; set mvals; by SA_WSD;
  eANC=abs(cANC); edelANC=abs(cdelANC);
  eCa=abs(cCa); edelCa=abs(cdelCa);
run;
proc means noprint data=mvals mean; by SA_WSD;
  var eANC edelANC eCa edelCa;
  output out=avgvals mean=mANC mdelANC mCa mdelCa;
proc print data=avgvals; run;

title 'Coefficient of Variation in MAGIC ANC across calibrations';
proc gplot data=mvals;
  by SA_WSD;
  plot
```



```
        eANC*Year=SCENAR
    / vaxis=axis1;
run;
title 'Coefficient of Variation in MAGIC Ca across calibrations';
proc gplot data=mvals;
    by SA_WSD;
    plot
        eCa*Year=SCENAR
    / vaxis=axis1;
run;

title 'Coefficient of Variation in MAGIC delANC across calibrations';
proc gplot data=mvals;
    by SA_WSD;
    plot
        edelANC*Year=SCENAR
    / vaxis=axis1;
run;

title 'Coefficient of Variation in MAGIC delCa across calibrations';
proc gplot data=mvals;
    by SA_WSD;
    plot
        edelCa*Year=SCENAR
    / vaxis=axis1;
run;

title 'Change in ANC across calibrations (60% decrease)';
proc gplot data=wsd;
    by SA_WSD SCENAR;
    plot
        delANC*Year=SCENAR
    / vaxis=axis1;
run;

proc sort data=wsd; by SA_WSD SCENAR Filenam Year; run;
data output; set wsd; file out;
    put SA_WSD SCENAR Filenam Year delANC;
run;
```

APPENDIX B. ANALYTICA™ CODE FOR THE SOILS-

AQUATICS MODELS

{ From user RichS, Model Taf_model at Fri, Dec 29, 1995 2:05 PM}
Softwareversion 1.0a20

Attribute Reference

Attribute The

Attribute Date_bough

Model Soils_aquatics_modul

Title: Soils-Aquatics Effects

Description: The Soils-Aquatics module estimates the effect of changes~~
in S and N species deposition on natural ecosystems. The model is ba~~
sed on the MAGIC model.

Author: Soils: Patrick Ryan~

Aquatics: Mitchell Small and Rajarishi Sinha~

Other Contributors: Timothy Sullivan

Date: Tue, Jul 11, 1995 7:02 AM

Saveauthor: RichS

Savedate: Fri, Dec 29, 1995 2:05 PM

Defaultsize: 48,20

Diagstate: 1,39,79,526,267,1

Icon: (FE 00 00 0F 57 80 03 FA AA F0 0D 55 55 5C 1A AA AA AE 35 55 55 ~~
57 6A AA AA AF D5 55 55 55 AA AA AA BF 55 55 D5 63 AA AA 6B CF 55 55 E~~
F 0F FF AA 70 A0 00 D5 D8 0A 2A 6A 7F E0 84 3D AA B6 31 87 55 58 84 21~~
AF FA 31 8D 50 00 00 00 F6 F7 BC F3 80 00 00 00 FF FF FF FF FF FE EF ~~
FF FC 1F BF FF 98 03 FF FF 80 49 78 3F 80 21 E0 19 80 01 C9 01 98 07 C~~
2 01 FF FF C0 01 FF FF F8 19 FF FF FF FF)

Nodecolor: 13107,-26215,-1

Diagramcolor: -8739,-8739,-8739

Fileinfo: 0,Model Soils_aquatics_modul,1,1,-32557,:Soils_Aquatics 3.0

Getresource Pagesetup,1

Module Aquatics

Title: Aquatics Component

Description: Aquatics Portions of the TAF Soils-Aquatics Module

Author: Rajarishi Sinha

Date: Tue, Jul 11, 1995 12:46 PM

Defaultsize: 48,20

Location: 312,56

Nodesize: 48,36

Nodeinfo: 1,1,1,1,1,1,0

Diagstate: 1,41,92,527,250,1

Icon: (00 00 00 00 00 00 00 00 00 00 00 00 0E 00 00 00 37 80 00 00 37 ~~
C0 00 00 77 C0 00 00 77 E0 00 00 F3 E0 00 00 FB E0 00 00 FB F0 00 00 F~~

```

9 F0 00 00 F9 F8 00 00 F8 FC 00 00 F8 FF C0 00 FC 7F F8 00 FC 3F FF F8~~
FC 3F FF FE FE 1F FF FF FE 1F FF FF FF 07 FC 7F FF 80 00 07 FF 80 00 ~~
03 FF C0 00 07 FF F0 00 0F FF FE 00 1F FF FF F8 1F FF FF FF FF FF FF F~~
F FF FF FF FF FF FF FF FF FF FF FF FF FF )

```

Nodecolor: 13107,-26215,-1

Diagramcolor: -8739,-8739,-8739

Module Ph_anc_conversion

Title: pH-ANC conversion

Description: Conversion from Acid Neutralising Capacity to lake pH

Author: Rajarishi Sinha

Date: Wed, Jul 12, 1995 6:45 AM

Location: 176,72

Nodesize: 48,24

Nodeinfo: 1,1,1,1,1,1,0

Diagstate: 1,41,111,390,304,1

Nodecolor: 13107,-26215,-1

Variable La

Title: Lake Parameter a

Description: Parameter for lake pH - ANC relationship.~

Different values are specified above and below the cutoff of ANC.~

~

Old Def:~

if Lake_anc<=cutoff then 6.00802 else 6.10241

Definition: Table(Cut_index)(6.00802,6.10241)

Location: 56,80

Nodesize: 44,20

Valuestate: 1,120,130,416,303,1,STAT

Reformval: [Time, Statslabels]

Variable Lb

Title: Lake Parameter b

Description: Parameter for lake pH - ANC relationship.~

Different values are specified above and below the cutoff of ANC.~

~

Old Def: ~

if Lake_anc<=cutoff then 0.455357 else 0.29191

Definition: Table(Cut_index)(0.455357,0.29191)

Location: 56,128

Nodesize: 44,20

Valuestate: 1,104,114,416,303,0,STAT

Reformval: [Time, Statslabels]

Variable Lc

Title: Lake Parameter c

Units: ueq/L

Description: Parameter for lake pH - ANC relationship.~

Different values are specified above and below the cutoff of ANC.~

~

Old Def:~

if Lake_anc<=cutoff then 15.3896 else 15.6592

Definition: Table(Cut_index)(15.3896,15.6592)

Location: 56,176

```

Nodesize: 44,20
Valuestate: 1,88,98,416,303,0,STAT
Reformval: [Time, Statslabels ]

Variable Ld
Title: Lake Parameter d
Units: ueq/L
Description: Parameter for lake pH - ANC relationship.~
Different values are specified above and below the cutoff of ANC.~
~
Old Def:~
if Lake_anc<=cutoff then 42.6385 else 73.4333
Definition: Table(Cut_index)(42.6385,73.4333)
Location: 56,224
Nodesize: 44,20
Valuestate: 1,218,162,416,303,0,STAT
Reformval: [Time, Statslabels ]

Variable Phl
Title: lake pH
Description: Lake pH, from a pH-ANC relationship~
~
Old Def:~
La+Lb*Ln(Max([(Lake_anc-Ld)/Lc+sqrt(((Lake_anc-Ld)/Lc)^2+1),0.01]))+No~~
rmal(0,Sqrt(Lph_mse))
Definition: IF Lake_anc<=Cutoff THEN SLICE(Lake_ph_precursor,Cut_index~~
,1) ~
ELSE SLICE(Lake_ph_precursor,Cut_index,2)
Location: 280,144
Nodesize: 48,20
Windstate: 1,71,130
Valuestate: 1,41,130,416,303,0,STAT
Nodecolor: -26215,-13108,-1
Reformval: [Time, Statslabels ]
Reference: 1. Small, Mitchell J. and Sutton, Michael C., A Regional pH~~
-Alkalinity Relationship, Wat. Res., Vol. 20, No.3, pp.335-343, 1986.~
2. Sullivan T.J., Historical Changes in Surface Water Acid-Base Chemis~~
try in Response to Acid Deposition, NAPAP State of Science and Technol~~
ogy Report No. 11, National Acid Precipitation Assessment Program, Was~~
hington, DC.~
3. Sullivan, T.J., Cosby, B.J., Driscoll, C.T., Charles, D.F. and Hemo~~
nd, H.F., Influence of Organic Acids on Model Projections of Lake Acid~~
ification, Wat. Air Soil Pollut., Aug 1995, in press.~
4. Sullivan, T.J. and Cosby, B.J., Testing, Improvement, and Confirmat~~
ion of a Watershed Model of Acid-Base Chemistry, Wat. Air Soil Pollut~~
., 1995, in press.~
5. Thornton, Kent W., Methods for Projecting Future Changes in Surface~~
Water Acid-Base Chemistry, NAPAP State of Science and Technology Repo~~
rt No. 14, National Acid Precipitation Assessment Program, Washington,~~
DC.

Variable Cutoff
Title: ANC Cutoff
Units: ueq/L

```



```
Variable Mcae
Title: Equilibrium Ca slope factor
Description: Slope of the linear equilibrium Ca - deposition relations~~
hip.~
Indexed by watershed.~
NOT indexed by time.
Definition: Table(Ids)(
0.418001,0.761477,0.698267,0.802825,0.835045,0.746447,0.671943,0.67173~~
,0.734221,0.629053,0.316637,0.718092,0.204353,0.692946,0.680578,0.4022~~
81,0.729532,0.451837,0.749351,0.619116,0.681056,0.494246,0.815425,0.35~~
8481,0.796399,0.343432,0.513613,0.612221,0.692219,0.614819,0.449652,0.~~
971031,0.701342)
Location: 64,128
Nodesize: 48,20
```

Variable Icae
Title: Equilibrium Ca intercept factor
Units: ueq/L
Description: Intercept of the linear equilibrium Ca - deposition relationship.
Indexed by watershed.
NOT indexed by time.
Definition: Table(Ids)(
24.1826,17.7774,27.4132,20.7347,15.1481,21.2596,112.943,154.659,7.0056~
7,69.4725,20.5073,4.80484,12.9797,71.378,18.4444,22.612,0.31477,72.974~
7,72.5032,35.3283,8.20167,27.3823,5.92141,18.6392,6.48815,18.8723,91.9~
24,63.4292,52.9058,255.712,44.4327,8.22124,13.4851)
Location: 64,176
Nodesize: 48,20

114

.556701,0.807133,0.446179,0.444266,0.518739,1.85296,0.553975,0.223027,~~
0.542508,0.403285,0.808333,0.559906,0.42606,0.815103,0.082412,0.401462~~
,0.7016)

Location: 64,32

Nodesize: 48,20

Variable Tca

Title: Lake Ca lag factor

Units: 1/yr

Description: Time lag factor in the exponential Ca - deposition - time~~
relationship.~

Indexed by watershed.~

NOT indexed by time.

Definition: Table(Ids)(

0.0837467,1.45368,0.0706469,2.15941,3.10786,19.2598,16.2178,25.671,0.1~~
07635,27.1094,0.129762,2.03678,0.0761341,38.3484,0.0649915,0.0779266,0~~
.104257,15.9355,0.191868,0.16913,0.174401,26.5279,0.132693,0.0668772,0~~
.148688,0.106264,13.0361,0.163622,0.106687,15.9991,0.150362,0.183436,2~~
.24203)

Location: 64,80

Nodesize: 48,20

Variable Cae

Title: Equilibrium Ca

Units: ueq/L

Description: The Ca concentration at equilibrium, indexed by watershed~~
.

NOT indexed by time.

Definition: mCae*avdep[Emissions_Species='SOx']+iCae

Location: 176,128

Nodesize: 48,20

Valuestate: 1,264,274,416,303,0,MIDM

Reformval: [Time, Ids]

Variable Lca

Title: Lake Calcium

Units: ueq/L

Description: The calcium in each lake, indexed by watershed and time.

Definition: Dynamic(Cabase, (Lca[Time-1]+(Mca*(Cae[Time]-Lca[Time-1]))*~~
(1-Exp(Max([Min([(-Dt)/Tca),84]),-84]))))

Location: 296,128

Nodesize: 48,20

Windstate: 1,109,207

Valuestate: 1,40,50,416,303,0,MIDM

Reformval: [Time, Ids]

Variable Cabase

Title: Calcium in base year

Units: ueq/L

Description: Calcium in each lake in the base year, indexed by watersh~~
ed.~

NOT indexed by time.

Definition: Table(Ids)(

61.13,77.55,87.16,84.16,83.8,97.16,173.11,223.89,76.44,124.4,50.7,62.6~~

5,31.31,133.71,74,60.15,74.18,117.22,147.69,90.08,63.8,76.62,73.85,51.~~
 16,71.66,52.75,140.22,126.83,122.14,313.26,94.54,92.49,74.37)
 Location: 64,224
 Nodesize: 48,20

Variable Lca_mse

Title: MSE for Lake Calcium

Units: (ueq/L)^2

Description: The mean of the squares of residuals for the lake calcium~~
 .~

Indexed by watershed.~

NOT indexed by time or species.

Definition: Table(Ids)(

1.34427,0.980338,0.416287,1.63474,1.2407,0.169521,0.154988,0.481825,4.~~
 04046,0.0536752,2.93175,4.04488,1.12438,0.182927,0.203548,1.7117,4.075~~
 54,0.100011,1.61955,0.44166,0.561695,0.252578,0.504,0.788817,0.908888,~~
 0.427629,0.0945983,1.89541,1.17326,0.16172,11.0718,0.705388,0.794295)

Location: 64,280

Nodesize: 44,20

Valuestate: 1,152,162,416,303,0,MIDM

Numberformat: 1,D,6,2,0,0

Chance Uncert_lca

Title: RFM error in Lake Calcium

Description: The uncertainty in the lake calcium estimate, defined as ~~
 a normal distribution with 0 mean and variance equal to the mean squar~~
 ed error of the Lake calcium relationship.

Definition: Normal(0, sqrt(lCa_mse))

Location: 168,280

Nodesize: 44,20

Nodecolor: 0,-13108,26214

Variable Nu_dca

Title: MAGIC Calibration Uncertainty

Units: %

Description: The coefficient of variation for Change in Calcium (in %)~~
 , over the various MAGIC calibrations that are available for each lake~~
 , indexed by lake.

Definition: Table(Ids)(

68.9024,108.25,37.1271,28.4382,142.219,95.466,198.779,95.9317,113.407,~~
 42.8421,65.1139,46.5268,180.647,145.161,47.3542,113.752,130.926,82.726~~
 3,41.3982,29.3088,37.9728,60.1563,53.2369,73.4927,47.4767,84.7938,45.0~~
 089,45.1523,51.0853,573.31,112.091,73.4657,37.0892)

Location: 296,224

Nodesize: 48,20

Defnstate: 1,332,290,281,468,0,MIDM

Variable Lake_ca

Title: Lake Calcium with uncertainty

Units: ueq/L

Description: Lake Calcium, incorporating uncertainty. The uncertain la~~
 ke Calcium is defined as:~

Ca(t) = Ca_deterministic(t) + epsilon * sigma~

where epsilon is a unit normal and sigma = Change in Ca * nu

Definition: $Lca + (Lca - Cabase) * Nu_dca * (-Unit_Normal) / 100$

Location: 408,128

Nodesize: 44,24

Windstate: 1,219,311

Valuestate: 1,88,98,416,303,0,STAT

Nodecolor: -26215,-13108,-1

Reformval: [Time, Statslabels]

Close Lake_calcium_model

Variable First

Title: First Presence/Absence Parameter

Description: First parameter in the presence/absence relationship, indexed by the appropriate fish species index

Definition: $Table(Fish_species_pa)(-16.94, -30.87, -9.28)$

Location: 72,96

Nodesize: 60,24

Variable Second

Title: Second Presence/Absence Parameter

Description: First parameter in the presence/absence relationship, indexed by the appropriate fish species index

Definition: $Table(Fish_species_pa)(18.34, 38.11, 12.16)$

Location: 208,96

Nodesize: 60,24

Close Fish_biology

Module Fish_species_richnes

Title: Fish Species Richness

Description: Sub-module to calculate the species richness for each region.

Model selected is Function AB / Model 10 with MSE = 3.85

Author: Rajarishi Sinha

Date: Fri, Aug 25, 1995 11:46 AM

Location: 304,184

Nodesize: 48,20

Diagstate: 1,41,88,467,384,1

Variable Probp

Title: Probability of Number of species in each lake

Description: The number of species in each lake is assumed to follow a binomial process with parameters P (probability of colonisation) and N (total number of species).

Definition: $Comb * (P^{Number_of_species}) * (1-P)^{(N-Number_of_species)}$

Location: 320,224

Nodesize: 48,28

Valuestate: 1,150,164,416,303,1,MIDM

Nodecolor: -26215,-13108,-1

Reformval: [Time, Undefined]

Variable Beta0

Title: Intercept

Description: Intercept coefficient in the logistic relationship for species richness

Definition: -23.98

Location: 64,80

Nodesize: 48,20

Variable Beta1

Title: Lake pH coefficient

Description: Coefficient for the lake pH in the logistic relationship for species richness.

Definition: 3.81

Location: 64,128

Nodesize: 48,20

Variable Beta2

Title: Lake area coefficient

Description: Coefficient for the lake area in the logistic relationship for species richness.

Definition: 1.26

Location: 64,176

Nodesize: 48,20

Variable Beta3

Title: Lake elevation coefficient

Units: 1/m

Description: Coefficient for the lake elevation in the logistic relationship for species richness.

Definition: -5.27e-3

Location: 64,224

Nodesize: 48,20

Variable N

Title: Total number of species

Description: The total number of species in each lake. The largest number of species caught in any one lake by the ALSC was 13, so this value was selected.

Definition: 13

Location: 64,32

Nodesize: 48,20

Variable P

Title: Probability of Colonisation success

Description: The probability that the lake will be colonised by a species of fish, indexed by Watershed, Region and time.

The candidate species richness model is 10.

Definition: $(1/(1+\text{Exp}((((\text{Beta0}+(\text{Beta1}*\text{Phl}))+(\text{Beta2}*\text{Logten}(\text{Lsiz}))+(\text{Beta3}*\text{Elev}))+(\text{Beta4}*\text{Logten}((\text{Silica}+1))))+(\text{Beta5}*\text{Logten}(\text{Lake_ca}))+(\text{Beta6}*\text{Phl})*\text{Logten}(\text{Lake_ca}))))))$

Check: if ≥ 0 and ≤ 1

Location: 200,224

Nodesize: 48,24

Windstate: 1,142,82

Valuestate: 1,56,66,416,303,0,STAT

Nodecolor: -26215,-13108,-1
Reformval: [Time, Undefined]
Reference: 1. Baker, Joan P., Biological Effects of Changes in Surface Water Acid-Base Chemistry, NAPAP State of Science and Technology Report No. 13, National Acid Precipitation Assessment Program, Washington, DC.

Index Number_of_species
Title: Number of species Index
Description: An index for the number of species, from 0 to N
Definition: sequence(0,N)
Location: 304,304
Nodesize: 48,20
Nodecolor: -1,-13108,26214

Variable Comb
Title: Combinatorial coefficient
Description: The binomial combinatorial coefficient
Definition: Table(Number_of_species)(
1,13,78,286,715,1287,1716,1716,1287,715,286,78,13,1)
Location: 192,32
Nodesize: 48,20
Defnstate: 1,72,82,417,314,0,MIDM

Variable Silica
Title: Silica
Units: mg/L
Description: Silica in each lake, constant over time.
Indexed by watershed.
Definition: Table(Ids)(
0.84,1.21,2.56,2.29,1.76,0.21,2.54,1.03,0.39,3.89,0.29,1.5,4.44,0.41,1.35,0.61,1.14,0.09,5.76,4.14,4.12,1.9,1.87,1.36,3.28,1.24,3.61,0.12,2.24,5.61,1.51,7.04,2.84)
Location: 200,152
Nodesize: 44,20

Variable Beta4
Title: Lake silica coefficient
Description: Coefficient for silica in the logistic relationship for species richness.
Definition: 0.934
Location: 64,272
Nodesize: 48,20

Variable Beta5
Title: Lake calcium coefficient
Description: Coefficient for calcium in the logistic relationship for species richness.
Definition: 10.74
Location: 64,320
Nodesize: 48,20

Variable Beta6
Title: Lake pH*pCa coefficient

Description: Coefficient for pH*pCa in the logistic relationship for species richness.

Definition: -1.6

Location: 200,304

Nodesize: 48,20

Close Fish_species_richnes

Module Lake_aluminum_model

Title: Lake Aluminum Model

Description: Sub-module which calculates the aluminum concentration in each lake.

Author: Rajarishi Sinha

Date: Sun, Sep 10, 1995 1:22 PM

Location: 304,40

Nodesize: 48,24

Nodeinfo: 1,1,1,1,1,1,0

Diagstate: 1,42,110,394,144,1

Nodecolor: 13107,-26215,-1

Variable Albase

Title: Aluminum in base year

Units: ueq/L

Description: Al3+ in base year, i.e. 1985, indexed by watershed. NOT indexed by time.

Definition: Table(Ids)(

19.24,2.32,0.04,0.92,1.69,2.12,0,0,0.66,0,26.2,13.94,37.82,0,2.06,8.84,4.35,0,0,0.45,2.65,6.22,7.47,42.7,4.04,23.82,0,0,0.01,0,0.01,2.55,2.88)

Check: if >=0

Location: 56,48

Nodesize: 44,20

Reference: 1. Sullivan, Timothy J. and Cosby, B.J., Modelling the Concentration of Aluminum in Surface Waters, in review, July 1995.

Variable Palbase

Title: pAl in base year

Description: The pAl value for the aluminum in the base year, indexed by watershed.

Definition: -logten(If Albase>0 then ((1/3)*(1E-6)*Albase) else 1E-9)

Location: 168,48

Nodesize: 48,20

Variable Lake_aluminum

Title: Lake Aluminum

Units: ueq/L

Description: The aluminum in each lake, indexed by watershed and time.

~

~

Old Def:~

Dynamic(Albase,3E6*(10^((- (Phl[Time=0])-Phl[Time=1985])+Palbase)))

Definition: 3E6*(10^(Palbase-Phl-Phl[Time=1985]))

Check: if >=0

Location: 280,48

Nodesize: 48,20
Windstate: 1,120,132
Valuestate: 1,56,66,416,303,0,MIDM
Nodecolor: -26215,-13108,-1
Reformval: [Time, Ids]
Reference: 1. Sullivan, Timothy J. and Cosby, B.J., Modelling the Concentration of Aluminum in Surface Waters, in review, July 1995.

Close Lake_aluminum_model

Module Acid_stress_index_mo
Title: Acid Stress Index Model
Description: sub-module which computes the Acid Stress Index
Author: Rajarishi Sinha
Date: Tue, Sep 12, 1995 2:13 PM
Location: 304,128
Nodesize: 48,20
Nodeinfo: 1,1,1,1,1,1,0
Diagstate: 1,41,91,321,269,1
Nodecolor: 13107,-26215,-1

Variable Inorgal
Title: Inorganic Al in lake
Units: ug/L
Description: Aluminum in region, truncated at pH 6.5
Definition: $(\text{Phl} \leq 6.5) * \text{Lake_aluminum} * 9$
Check: if ≥ 0
Location: 56,32
Nodesize: 40,20
Valuestate: 1,120,130,416,303,0,MIDM
Nodecolor: -26215,-13108,-1
Reformval: [Time, Ids]

Variable X
Title: x parameter in ASI equation
Description: Parameter passed to the ASI equation~
~
Old Equation~
 $((\text{First_asi} + (\text{Second_asi} * \text{Phl})) + (\text{Third_asi} * \text{Lake_ca})) + (\text{Fourth_asi} * \text{Inorgal})$
Definition: $\text{First_asi} + (\text{Second_asi} * \text{Phl}) + \text{Third_asi} * \text{Lake_ca} + (\text{Fourth_asi} * \text{Inorgal})$
Location: 240,128
Nodesize: 48,20
Windstate: 1,149,169
Valuestate: 1,86,124,416,303,0,STAT
Nodecolor: -26215,-13108,-1
Reformval: [Time, Statslabels]
Reference: 1. Baker, Joan P., Biological Effects of Changes in Surface Water Acid-Base Chemistry, NAPAP State of Science and Technology Report No. 13, National Acid Precipitation Assessment Program, Washington, DC.

Variable First_asi

Title: ASI Parameter 1

Definition: Table(Fish_species_asi)(
-23.49,-18.73,-8.9)

Location: 56,80

Nodesize: 40,20

Variable Second_asi

Title: ASI Parameter 2

Definition: Table(Fish_species_asi)(
5.35,3.57,1.56)

Location: 56,128

Nodesize: 40,20

Variable Third_asi

Title: ASI Parameter 3

Definition: Table(Fish_species_asi)(
2.97m,0.0145,4.08m)

Location: 56,176

Nodesize: 40,20

Variable Fourth_asi

Title: ASI Parameter 4

Definition: Table(Fish_species_asi)(
-1.93m,-0.0437,-0.0704)

Location: 56,224

Nodesize: 40,20

Variable Asi_in_lake

Title: ASI in lake

Description: The Acid Stress index for each lake, indexed by watershed~~
and year. This node is output to the valuation module using the Publ~~
ic Index 'Year' instead of the System Index 'Time'.

Definition: (Phl<=8 Or Lake_ca<=2000)* (100/(1+Exp(Max([Min([X,84]),-8~~
4]))))

Check: if >=0 and <=100

Location: 240,200

Nodesize: 44,20

Windstate: 1,69,168

Valuestate: 1,72,82,416,303,0,MIDM

Aliases: Formnode Asi_in_lake1

Nodecolor: -26215,-13108,-1

Reformval: [Time, Fish_species_asi]

Reference: 1. Baker, Joan P., Biological Effects of Changes in Surface~~
Water Acid-Base Chemistry, NAPAP State of Science and Technology Repo~~
rt No. 13, National Acid Precipitation Assessment Program, Washington,~~
DC.

Index Asi_time_index

Title: ASI Time Index

Units: Year

Description: A Time index running from 1980 to 2030 in steps of Dt. Id~~
entical to Year_5, but internal to Soils/Aquatics.

Definition: Sequence(1980, 2030, Dt)

Location: 240,32

Nodesize: 44,20

Close Acid_stress_index_mo

Variable Fishresponse

Title: Fish Presence/Absence

Units: Surviving Fraction

Description: The probability that a given species of fish can survive ~
in ~
water of a given pH

Definition: $(1/(1+\text{Exp}((\text{First}+(\text{Second}*(-(\text{Logten}((500n*\text{Lake_ca}))/\text{Phl}))))))$

Location: 432,72

Nodesize: 56,20

Valuestate: 1,120,130,416,303,1,MIDM

Reference: 1. Baker, Joan P., Biological Effects of Changes in Surface~~
Water Acid-Base Chemistry, NAPAP State of Science and Technology Repo~~
rt No. 13, National Acid Precipitation Assessment Program, Washington,~~
DC.

Module Acid_neutralising_ca

Title: Acid Neutralising Capacity

Author: Kevin

Date: Fri, Sep 15, 1995 2:42 PM

Location: 56,72

Nodesize: 48,24

Diagstate: 1,41,181,598,317,17

Nodecolor: 13107,-26215,-1

Diagramcolor: -8739,-8739,-8739

Variable Ancpre

Title: Pre-Industrial Acid Neutralising Capacity

Units: ueq/L

Description: ANC at time 0 (1844, i.e. pre-industrial time), indexed b~~
y lake.~

NOT indexed by time.~

For the ANC-NF relationship

Definition: Table(Ids)(

41.5,47.46,70.18,59.27,52.53,55.45,192.17,257.09,40.47,121.09,34.26,30~~
.5,33.94,140.16,50.82,51.3,39.04,113.33,188.53,97.61,55.59,64.52,39.62~~
,38.85,58.59,48.15,175.65,136.06,121.41,327.84,101.04,59.49,41.43)

Location: 56,184

Nodesize: 52,24

Variable Ml

Title: Lake Slope Factor

Units: L/ueq

Description: Slope for the neutralisation fraction - effective deposit~~
ion relationship, indexed by lake.~

NOT indexed by time.

Definition: Table(Ids)(

-687.57u,-1.04345m,-907.97u,-1.31177m,-401.27u,-986.5u,-1.92662m,-2.49~~
363m,-2.32092m,-326.02u,-672.61u,-1.48563m,-931.36u,-388.07u,184.25u,8~~
27n,-2.19759m,-1.63186m,-1.3442m,-711.09u,-812.63u,-1.13611m,-233.35u,~~

Appendix B: Analytica Code

1.42186m,-762.62u,-695.13u,-1.64045m,-1.00265m,-1.36884m,-1.16334m,-2.~~
75911m,-2.0305m,-1.07945m)
Location: 56,80
Nodesize: 48,20
Valuestate: 1,152,162,416,303,0,MIDM

Variable Tau

Title: Lake Lag factor
Units: 1/year
Description: Lag factor in the exponential Soil Water ANC-Dep relation~~
ship.~
Indexed by watershed.~
NOT indexed by time or species
Definition: Table(Ids) (
2.81881,14.1375,13.0383,12.2625,8.0675,15.5934,18.8864,16.176,13.2248,~~
12.7007,2.72293,11.094,3.53327,5.75313,4.88076,4.83895,11.5383,38.6545~~
,10.0326,12.3121,11.8405,5.32151,3.65773,6.96562,11.1888,4.08844,20.54~~
98,8.39721,11.0588,19.172,14.5962,21.006,12.9798)
Location: 304,80
Nodesize: 44,20
Valuestate: 1,152,162,416,303,0,MIDM

Variable Dnf

Title: Effective Nominal Deposition
Units: ueq/L
Description: The effective nominal deposition, at which there is no ch~~
ange in neutralisation fraction, indexed by lake.~
NOT indexed by time.
Definition: Table(Ids) (
-19.5188,68.5023,66.1549,58.868,77.8905,65.4885,58.6646,61.1543,58.208~~
2,55.7593,-47.3464,54.8167,2.47183,56.351,79.8971,34.802K,60.0657,67.9~~
819,63.0406,62.0526,57.6097,34.3618,42.6925,88.377,65.9155,13.314,65.0~~
318,70.7131,61.2802,61.4667,57.9209,60.0413,71.5532)
Location: 56,32
Nodesize: 48,20

Variable Dpre

Title: Pre-industrial Deposition
Units: ueq/L
Description: Deposition at zero time, i.e. deposition in year 1844 (p~~
re-industrial).~
Indexed by lake.~
NOT indexed by time.
Definition: Table(Ids) (
8.39,8.51,8.69,8.41,8.64,9.02,8.64,9.2,8.89,9.01,8.38,8.51,8.54,9.17,8~~
.64,8.41,9.23,9.83,9.17,9.43,8.75,9.32,8.75,9.6,8.85,8.71,9.19,9.17,8.~~
91,8.95,9.1,8.59,8.69)
Location: 64,248
Nodesize: 48,24

Variable Tp

Title: Time periods elapsed
Description: Number of time periods elapsed since the base year, i.e. ~~
1985.

Definition: $\text{round}((\text{Time}-1985)/\text{dt})$

Location: 56,128

Nodesize: 48,20

Variable Lanc

Title: Lake ANC

Units: ueq/L

Description: ANC, indexed by time and lake.

Definition: $((1-\text{df})\text{SANC})-\text{df}*(\text{Total_Deposition-Dbase})$

Location: 416,184

Nodesize: 40,20

Nodeinfo: 1,1,1,1,1,1,0

Windstate: 1,280,290

Valuestate: 1,180,68,416,303,0,MIDM

Reformval: [Time, Ids]

Reference: 1. Small, Mitchell J., Cosby, Bernard J., Marnico, Ronald J., and Henrion, Max, Joint Application of an Empirical and Mechanistic Model for Regional Lake Acidification, Env. Monitoring and Assessment, 1995.

2. Small, Mitchell J. and Sutton, Michael C., A Direct Distribution Model for regional Aquatic Acidification, Water Resour. Res., Vol. 22, p. 1749-1758, 1986.

Variable Delnf

Title: Total Change in Neutralisation Fraction

Description: Changed in Neutralisation fraction, indexed by time and lake.

Defined as a linear relationship.

Definition: $\text{Ml}*(\text{Dep}[\text{Emissions_Species}='SOx']-\text{tp}*Dnf)$

Location: 192,80

Nodesize: 48,24

Windstate: 1,264,274

Valuestate: 1,168,178,416,303,0,MIDM

Reformval: [Time, Ids]

Variable Nf

Title: Neutralisation Fraction

Description: The neutralisation fraction, defined as a dynamic variable in the following fashion :~

Current NF = Previous NF + Change in NF~

The above sequence converges to:~

Current NF = NF in base year + Total Change in NF~

Indexed by lake and time.~

when NF in base year = $(1-((\text{Ancbase}-\text{Ancpre})/(\text{Dpre}-\text{Dbase})))$

Definition: $1-((\text{Measured_anc1987}-\text{Ancpre})/(\text{Dpre}-\text{Dbase}))+\text{Delnf}$

Location: 192,184

Nodesize: 48,20

Valuestate: 1,120,130,416,303,0,MIDM

Reformval: [Time, Ids]

Variable Sanc

Title: Soil Water ANC

Units: ueq/L

Description: The ANC of the soil water

Definition: $\text{dynamic}((\text{Measured_anc1987}/(1-\text{df})), \text{SANC}[\text{Time}-1] + (1 - \exp(-(dt \sim \tau))) * ((\text{Measured_anc1987}/(1-\text{df})) - \text{SANC}[\text{Time}-1] - (1 - \text{Nf}[\text{Time}]) * (\text{Total_De} \sim \text{position}[\text{Time}] - \text{Dbase})))$

Location: 304,184

Nodesize: 40,20

Windstate: 1,43,148

Valuestate: 1,63,71,416,303,0,MIDM

Reformval: [Time, Ids]

Variable Lanc_mse

Title: MSE for Lake ANC

Units: $(\text{ueq/L})^2$

Description: The mean of the squares of residuals for the lake ANC.

Indexed by watershed.

NOT indexed by time or species.

Definition: $\text{Table}(\text{Ids})($

3.22108,0.736311,1.30714,1.26589,0.913674,1.45046,1.84397,2.19785,2.68295,2.27803,4.94179,1.61369,3.70954,1.62821,2.20882,6.68576,2.67981;1.12268,3.05292,1.99553,1.53751,7.17211,0.874686,21.2932,1.79017,5.79813,1.38428,1.583,2.17776,1.4418,4.4308,2.23538,1.06155)

Location: 312,248

Nodesize: 44,20

Valuestate: 1,152,162,416,303,0,MIDM

Numberformat: 1,D,6,2,0,0

Chance Uncert_lanc

Title: RFM error in Lake ANC

Description: The uncertainty in the Lake ANC, defined by a Normal distribution with 0 mean and standard deviation equal to the mean square error in the Lake ANC.

Indexed by lake.

Definition: $\text{Normal}(0, \text{sqrt}(\text{Lanc_mse}))$

Location: 424,248

Nodesize: 44,20

Valuestate: 1,88,98,416,303,1,PDFP

Nodecolor: 0,-13108,26214

Variable Nu_danc

Title: MAGIC Calibration Uncertainty

Units: %

Description: The coefficient of variation for Change in ANC (in %), over the various MAGIC calibrations that are available for each lake, indexed by lake.

Definition: $\text{Table}(\text{Ids})($

17.6572,17.6328,19.7518,33.1994,19.1133,31.2253,30.2304,20.2635,31.1361,23.9261,17.5545,45.2753,9.19709,19.8559,15.4478,20.781,31.7061,159.31,38.87,26.5821,55.1985,40.5818,14.2602,221.209,17.7081,23.0315,48.4051,17.8123,82.8081,58.9678,28.3585,66.116,26.402)

Location: 408,80

Nodesize: 44,20

Defnstate: 1,583,290,255,465,0,MIDM

Variable Lake_anc

Title: Lake ANC with uncertainty

Units: ueq/L
 Description: Lake ANC, incorporating uncertainty. The uncertain lake ANC is defined as:

$$ANC(t) = ANC_{deterministic}(t) + \epsilon * \sigma$$
 where epsilon is a unit normal and sigma = Change in ANC * nu
 Definition: $Lanc + (Lanc - Measured_anc1987) * Nu_danc * Unit_normal / 100$
 Location: 528,184
 Nodesize: 44,20
 Windstate: 1,130,207
 Valuestate: 1,42,130,418,302,0,STAT
 Nodecolor: -26215,-13108,-1
 Reformval: [Time, Statslabels]

Variable Measured_anc1987
 Title: Measured Lake ANC in 1987
 Units: ueq/L
 Description: The acid neutralizing capacity of each lake from ELS I (1987) for each lake in the region.
 Definition: Table(Ids) (
 -21.7,11.4,30,-7.4,6,1.8,111.9,183.2,-1.7,56.3,-30.3,-18,-53,82.9,1.8,~-
 -28.1,1.8,33.5,161.2,22.4,6.2,7.8,12.9,-5.3,1.1,-14.7,76.9,69.2,30,238~-
 .4,18.2,7.3,0.5)
 Location: 192,248
 Nodesize: 44,20
 Defnstate: 1,40,77,416,303,0,MIDM

Close Acid_neutralising_ca

Close Aquatics

Module Depcalc
 Title: Deposition calculations
 Description: Module containing cumulative and time-period deposition calculations.
 Author: Rajarishi Sinha
 Date: Wed, Jul 19, 1995 6:07 PM
 Location: 192,120
 Nodesize: 48,20
 Diagstate: 1,40,92,567,305,1

Variable Multiplier_for_speci
 Title: Watershed Deposition Adjustment
 Description: This factor adjusts regional deposition to account for watershed-specific differences. It is expressed as a dimensionless fraction.
 Definition: Table(Emissions_species,Ids) (
 0.94,0.96,0.98,0.95,0.97,1.01,0.97,1.04,1,1.01,0.94,0.96,0.96,1.03,0.97,~
 7,0.95,1.04,1.11,1.03,1.06,0.98,1.05,0.99,1.08,1,0.98,1.03,1.03,1,1.01~-
 ,1.02,0.97,0.98,
 1.01,1.01,1.01,1.01,1.01,1.01,1,1.01,0.99,0.99,1.01,1.01,1.01,0.99,1.0~-
 1,1.01,0.99,1.02,0.99,1,1.01,0.98,1.01,0.99,1,1.01,1,1,0.99,0.99,0.99,~-
 0.99,1.01
)
 Location: 48,80

```

Nodesize: 44,24
Valuestate: 1,56,66,416,303,0,MIDM
Reformdef: [Emissions_species, Ids ]

Variable Conversion_factors
Title: Conversion Factors
Units: ueq*ha*m/L
Description: Conversion factor used to convert deposition expressed as~~
kg/ha/yr to precipitation concentration in ueq/L. The factor is 100 t~~
imes the inverse of the equivalent weight of the chemical species.
Definition: Table(Emissions_species)(
6.25,7.143)
Location: 48,144
Nodesize: 44,24
Windstate: 1,63,125
Defnstate: 1,368,166,416,303,0,MIDM

Variable Deposition
Title: Deposition Concentration in ueq/L
Units: ueq/L
Description: Chemical deposition in ueq/L, calculated from deposition ~~
expressed as kg/ha/yr by dividing by the annual precipitation amount i~~
n m/yr and multiplying by the conversion factor used to convert to pre~~
cipitation concentration.~
Indexed by time and watershed.
Definition: Conversion_factors*Multiplier_for_speci*Species_Deposition~~
[Year_5=Time]/Qp
Location: 160,112
Nodesize: 44,24
Windstate: 1,151,184
Valuestate: 1,152,162,546,305,0,MIDM
Reformval: [Time, Ids ]

Variable Ddt
Title: Cumulative Deposition
Units: ueq/L
Description: Cumulative Deposition on each lake upto time t, indexed ~~
by lake.
Definition: cumulate(Total_Deposition,Time)
Location: 496,168
Nodesize: 48,20
Windstate: 1,121,175
Valuestate: 1,264,274,416,303,0,MIDM
Reformval: [Time, Ids ]

Variable Deldep
Title: Change in Deposition
Units: ueq/L
Description: Change in deposition from base year (1985) to present.~
Indexed by watershed and time and region.
Definition: Total_Deposition-Total_Deposition[Time=1985]
Location: 496,24
Nodesize: 48,20
Valuestate: 1,200,210,416,303,0,MIDM

```

Reformval: [Time, Ids]

Variable Dep

Title: Integrated Deposition

Units: ueq/L

Description: The cumulative deposition, minus one half of the sum of the base year and current year deposition.

Equivalent to applying the trapezoidal rule of integration to the deposition vector.

Indexed by watershed, region and time.

Definition: $Ddt - 0.5 * (Dbase + Total_Deposition)$

Location: 496,120

Nodesize: 48,20

Windstate: 1,168,178

Valuestate: 1,116,145,416,303,0,MIDM

Reformval: [Time, Ids]

Variable Avdep

Title: Average deposition

Units: ueq/L

Description: The average deposition over a time period.

Indexed by watershed and time.

Definition: $Total_Deposition - (Uncumulate(Total_Deposition, Time) / 2)$

Location: 496,72

Nodesize: 48,20

Valuestate: 1,82,106,430,321,0,MIDM

Reformval: [Time, Ids]

Variable Nitrodec

Title: Nitrogen uptake factors (decreasing)

Description: Decreasing factors

Definition: Table(Ids)(

0.201207,0.020842,0.103734,0.101523,0.069444,3.7m,0,0.010928,0.070822,~
0.163934,0.190476,0.013672,0.039872,7.031m,0.218341,0.13947,0.049579,0~
.099502,0.073801,7.729m,0.111483,9.245m,0.040617,2.916m,0.05848,0.0307~
22,0.030331,4.51m,0.02457,6.132m,0,0.213675,0.3125)

Location: 264,176

Nodesize: 44,24

Variable Nitroinc

Title: Nitrogen uptake factors (increasing)

Description: Increasing factors

Definition: Table(Ids)(

0.275482,0.13369,0.182482,0.158983,0.127065,0.139665,0.123305,0.201207~
,0.146199,0.289855,0.275482,0.098522,0.117786,0.444444,0.381679,0.2008~
03,0.123762,0.186916,0.168634,0.137363,0.195695,0.15528,0.16129,0.1015~
23,0.126743,0.134953,0.15625,0.165837,0.143678,0.152439,0.101729,0.377~
358,0.442478)

Location: 264,232

Nodesize: 44,24

Variable Total_deposition

Title: Total Deposition

Units: ueq/L

Description: The total deposition, incorporating the sulfate deposition and the nitrogen deposition converted to an equivalent sulfate deposition.~

Indexed by watershed and time.~

~

The deposition of an equivalent amount of sulfur is converted from nitrogen deposition by multiplying by a factor which depends on whether the change in nitrogen deposition is less than or more than zero.

Definition: If (Delns[Emissions_species='NOx']<0) ~

then (Delns[Emissions_species='SOx'] + Delns[Emissions_species='NOx']*Nitrodec+Dbase) ~

Else (Delns[Emissions_species='SOx'] + Delns[Emissions_species='NOx']*Nitroinc+Dbase)

Location: 376,104

Nodesize: 44,20

Windstate: 1,142,180

Valuestate: 1,85,44,435,416,1,MIDM

Reformval: [Time, Ids]

Variable Delns

Title: Change in Nitrogen and Sulfur Deposition

Units: ueq/L

Description: The change in the nitrogen and sulfur deposition from the base year.

Definition: Deposition-Deposition[Time=1985]

Location: 264,104

Nodesize: 44,32

Close Depcalc

Module Soils

Title: Soils Component

Description: The soils portion of the TAF Soils-Aquatics Module

Author: Rajarishi Sinha; mathematical models provided by Patrick Ryan

Date: Wed, Jul 19, 1995 6:07 PM

Location: 312,184

Nodesize: 48,36

Nodeinfo: 1,1,1,1,1,1,0

Diagstate: 1,40,92,495,292,1

Icon: (00 0F FF 80 00 08 00 E0 00 10 00 30 00 30 10 18 00 20 10 08 00 ~
20 10 48 00 24 10 C8 00 22 31 08 00 23 22 08 80 31 2C 18 E0 11 38 30 F~
C 19 F0 60 FF 0F F3 C0 FF C0 FE 00 FF E0 E0 00 1F F8 E0 00 CF FE E0 00~
E1 FF FC 00 FC FF FF 80 FE 3F FF E0 FF 9F FF FC FF C0 3F FF 1F FF 81 ~
FF CF FF FC 7F E1 FF FF 1F FC FF FF C3 FE 3F FF F8 FF 9F FF FF FF C0 3~
F FF FF FF 81 FF FF FF FC 7F FF FF FF 1F)

Nodecolor: 13107,-26215,-1

Variable Bsbases

Title: BS in base Year

Units: %

Description: Base year base saturation, indexed by lake.~

NOT indexed by time.

Definition: Table(Ids)(

10.86,9.72,11.46,8.78,8.54,5.86,10.75,11.21,6.92,8.96,9.37,5.11,6.29,9~

.36,12.41,7.97,6.51,14.08,7.45,8.94,9.1,8.54,4.93,10.46,5.13,10.09,11.~~
5,9.25,6.56,13.23,4.27,8.73,10.78)
Location: 56,32
Nodesize: 48,20
Nodecolor: -26215,-13108,-1

Variable Mi

Title: BS intercept factor
Units: %
Description: The intercept in the linear change in deposition - base s~~
aturation relationship, indexed by watershed.~
NOT indexed by time.
Definition: Table(Ids)(
-0.16311,-0.5256,-0.50639,-0.4865,-0.52942,-0.2833,-0.47017,-0.36623,~~~
0.38951,-0.50468,-0.1404,-0.34076,-0.07791,-0.44386,-0.67487,-0.12411,~~
-0.36135,-0.20351,-0.34013,-0.42444,-0.4888,-0.12059,-0.36149,-0.12668~~
, -0.37789,-0.11468,-0.37445,-0.37214,-0.27303,-0.44761,-0.25875,-0.478~~
2,-0.61798)
Location: 56,88
Nodesize: 48,24
Nodecolor: -26215,-13108,-1

Variable Ms

Title: BS Slope Factor
Units: L/ueq
Description: Slope in the base saturation - effective deposition relat~~
ionship, indexed by lake.~
NOT indexed by time.
Definition: Table(Ids)(
-3.64m,-9.3m,-8.2m,-8.87m,-8.59m,-3.82m,-7.14m,-6.03m,-5.8m,-8.01m,-3.~~
52m,-5.57m,-3m,-7.6m,-9.99m,-3.29m,-5.27m,-1.82m,-6.26m,-6.84m,-8.1m,~~~
2.66m,-4.24m,-2.94m,-4.98m,-2.39m,-5.43m,-7.02m,-4.8m,-6.99m,-5.63m,-6~~
.71m,-8.12m)
Location: 56,144
Nodesize: 48,20
Nodecolor: -26215,-13108,-1

Variable Bs

Title: Base Saturation
Units: %
Description: Base saturation in %.~
Regression parameters from a (possibly) non-linear relationship
Definition: Dynamic(Bsbase,(Bs[Time-1]+delBS[Time]))
Location: 296,88
Nodesize: 48,20
Valuestate: 1,56,66,416,303,1,MIDM
Nodecolor: -26215,-13108,-1
Reformval: [Time, Undefined]
Reference: 1. Ryan, P., personal communications, May 1995-Sep 1995, Oa~~
k Ridge, TN.

Variable Delbs

Title: Change in Base Saturation
Units: %

Description: Change in base saturation, defined as linear with the change in deposition.~

Indexed by watershed and time.

Definition: $\text{Deldep} * \text{Ms} + \text{Mi} + \text{uncert_BS1}$

Location: 176,88

Nodesize: 48,20

Valuestate: 1,168,178,416,303,0,MIDM

Nodecolor: -26215,-13108,-1

Reformval: [Time, Ids]

Variable Tbs

Title: Truncated base saturation

Units: %

Description: Base saturation, truncated at 0.1

Definition: If $\text{BS} < 0.1$ then 0.1 else BS

Location: 408,88

Nodesize: 48,20

Valuestate: 1,39,39,632,434,1,CDFP

Nodecolor: -26215,-13108,-1

Reformval: [Time, Probindex]

Variable Bsl_rmse

Title: Root Mean Square Error in Change in BS

Description: The RMS error in delBS, indexed by watershed. This is used to characterize the uncertainty.

Definition: $\text{Table}(\text{Ids}) ($

0.040644,0.104456,0.127042,0.145797,0.153968,0.07408,0.134643,0.094014~~
 ,0.103762,0.131336,0.04626,0.130159,0.026136,0.094434,0.143413,0.04062~~
 5,0.078764,0.037577,0.103394,0.099403,0.089651,0.04257,0.132284,0.0354~~
 85,0.148612,0.031304,0.084972,0.111167,0.101748,0.085271,0.108819,0.07~~
 985,0.147479)

Location: 176,216

Nodesize: 44,32

Nodecolor: -26215,-13108,-1

Chance Uncert_bsl

Title: Uncertainty in the Change in BS

Description: The uncertainty in the Change in soil base saturation, defined as a normal distribution with 0 mean and standard deviation equal to the root mean square error.

Definition: $\text{Unit_normal} * \text{BS1_rmse}$

Location: 176,144

Nodesize: 44,24

Valuestate: 1,72,82,416,303,1,PDFP

Nodecolor: 0,-13108,26214

Close Soils

Module Watershed_informatio

Title: Watershed Information

Description: This sub-module contains information specific to each of the 33 sample watersheds in the Adirondacks, viz.:~

Indexes based on Lake ID and Lake name.~

DDRP weights for each watershed.~

Watershed area.~
Lake area.~
Watershed elevation.
Author: Rajarishi Sinha
Date: Wed, Aug 2, 1995 3:05 PM
Location: 64,120
Nodesize: 48,20
Diagstate: 1,40,91,374,322,1

Constant Dt
Title: Time increment
Units: years
Description: Time increment for model, in years.~
Applicable to BOTH Aquatics and Soils.
Definition: 5
Check: if >=1
Location: 56,256
Nodesize: 48,20
Nodecolor: -1,-13108,26214

Chance Unit_normal
Title: Unit Normal
Description: Unit Normal function needed to keep Lake Ca and Lake ANC --
uncorrelated.~
Note: With this formulation, the same unit normal is used for all 33 --
lakes at each time step, yielding perfect correlation in the uncertain--
ty for each lake. To check the case where the uncertainties are uncor--
related, change this definition to an array of Normal(0,1) functions, --
indexed by Lake IDs (Ids).
Definition: Normal(0,1)
Location: 296,32
Nodesize: 44,20
Nodecolor: 0,-13108,26214

Variable Lake_prob
Title: Lake Probabilities
Description: Normalized DDRP weights that sum to 1. Used in cumulativ--
e probability calculations to properly weight each lake's representati--
on.~
Indexed by Lake ID.
Definition: wts/SUM(wts)
Location: 296,200
Nodesize: 44,20
Nodecolor: -26215,-13108,-1

Variable Dbase
Title: Deposition in base year
Units: ueq/L
Description: Deposition in the base year for NF (i.e. 1985), indexed b--
y lake.~
NOT indexed by time.
Definition: Table(Ids)(
64.56,65.48,66.81,64.67,66.46,69.37,66.44,70.8,68.42,69.27,64.5,65.46,~~
65.71,70.52,66.48,64.68,71.02,75.61,70.5,72.56,67.3,71.66,67.34,73.84,~~

68.1,66.99,70.67,70.53,68.51,68.81,70,66.08,66.88)

Location: 56,144

Nodesize: 48,20

Variable Qp

Title: Precipitation

Units: m

Description: Long-term (1950-1980) Annual average precipitation to each watershed, indexed by lake.

NOT indexed by time.

Precipitation is ALWAYS MORE THAN Runoff.

Definition: Table(Ids)(

1.3,1.3,1.3,1.3,1.3,0.98,1.07,0.98,1.06,1.06,1.3,1.3,1.3,0.98,1.3,1.3,1.01,0.84,1.01,1.01,1.3,1.07,1.3,1.04,1.26,1.3,0.98,0.98,1.01,1.01,1.01,1.34,1.3)

Check: if >=0

Location: 56,88

Nodesize: 48,20

Index Ids

Title: Region Lake IDs

Description: Lake IDs for the representative lakes in the region. Only region modelled is the Adirondacks.

Lake IDs for the representative 33 lakes in the Adirondacks.

Definition: ['1A1-003','1A1-012','1A1-014','1A1-017','1A1-020','1A1-028','1A1-029','1A1-033','1A1-039','1A1-046','1A1-049','1A1-057','1A1-061','1A1-064','1A1-066','1A1-073','1A2-002','1A2-006','1A2-037','1A2-041','1A2-042','1A2-045','1A2-046','1A2-048','1A2-052','1A2-054','1A3-001','1A3-040','1A3-042','1A3-043','1A3-046','1A3-048','1A3-065']

Location: 64,32

Nodesize: 48,20

Nodecolor: -1,-13108,26214

Index Names

Title: Region Lake Names

Description: Names of the representative lakes in the region. Only region modelled is the Adirondacks.

Names of the representative 33 lakes in the Adirondacks.

Definition: ['Hawk P.','Whitney L.','Wilmurt L.','Constable P.','Fourth L.','Dry Channel P.','Middle P.','Kiwassa L.','John P.','Partlow L.','Middle South P.','Hitchcock L.','Wolf L. (W.C.)','Mt. Arab L.','Woodhull L.','Gull L.','St. John L.','Lake Frances','Fish Ponds (NE)','Mud L. (S.L.)','North Branch L.','Woods L. (S.L.)','Nine Corner L.','Unnamed (Mud L.)','Chub L.','Trout L. (P.L.)','Nate P.','Zack P.','Cheney P.','Unknown P.','Long P. (K.R.)','Grass P. (H.W.)','South L.']

Location: 176,32

Nodesize: 48,20

Windstate: 1,88,98

Nodecolor: -1,-13108,26214

Variable Wts

Title: DDRP Weights

Description: The DDRP weights for each watershed. The weight is indicative of the number of watershed which fall in each watershed class. The

e weights are based on the stratified sampling scheme used in the Eastern Lake Survey (EPA, 1986) and the National Surface Water Survey (EPA~~).~

Indexed by Lake.

Definition: Table(Ids)(

12.285,12.285,22.4929,24.58,12.285,12.285,40.4692,40.4692,24.58,22.492~~
9,12.285,12.285,12.285,22.4929,12.285,12.285,12.285,22.4929,40.4692,22~~
.4929,12.285,12.285,12.285,12.285,12.285,12.285,22.4929,22.4929,22.492~~
9,40.4692,22.4929,12.285,12.285)

Indexvals: ['item 1']

Location: 176,200

Nodesize: 44,20

Windstate: 1,120,130

Variable Lsiz

Title: Lake area

Units: ha.

Description: The area of the lake, in hectares.~

Indexed by lake.

Definition: Table(Ids)(

13.8,43,39,20.6,23,27.4,24.3,115,6,29.9,19.4,14.2,4.4,50,443,10.9,13,6~~
,7.4,9,6.5,26,45,5,7,16.7,8.3,36,7,14,15.4,5.3,196)

Check: if >=0

Location: 176,88

Nodesize: 48,20

Valuestate: 1,72,82,416,303,0,MIDM

Variable Elev

Title: Watershed elevation

Units: m

Description: The elevation of the watershed, in metres.~

Indexed by lake.

Definition: Table(Ids)(

645.3,748.6,752,582.2,608.7,497.1,484,466,545.6,534.3,603.5,566.9,791,~~
505.7,571.5,593.8,672.7,454.2,485.6,527.3,575.5,418.5,570,484.6,503.8,~~
651.1,613.9,565.7,502.9,496.8,563.9,545.6,615.1)

Check: if >=0

Location: 296,88

Nodesize: 48,20

Variable Df

Title: Direct Runoff Fraction

Description: The fraction of runoff that enters the surface water with~~
out significant soil contact and therefore the fraction not affected b~~
y acid neutralisation processes in the soil, indexed by watershed.~

NOT indexed by time or by deposition species

Definition: Table(Ids)(

0.338926,0.381027,0.27288,0.324854,0.22036,0.278124,0.352403,0.466127,~~
0.262911,0.16756,0.368157,0.234048,0.250057,0.187246,0.121444,0.247494~~
,0.286715,0.0986202,0.165124,0.143809,0.149484,0.226847,0.264053,0.238~~
512,0.255095,0.197591,0.377856,0.321328,0.223771,0.154287,0.205428,0.2~~
05432,0.304516)

Location: 56,200

Nodesize: 48,20

Variable Totlakes

Title: Total Lakes in region

Description: The total number of lakes in the region.~

Currently, only region is the Adirondacks.

Definition: 1290

Location: 176,144

Nodesize: 44,20

Variable Fudge

Title: Lakes with ANC<400 ueq/L

Description: The number of lakes with ANC < 400 ueq/L, i.e. the lakes ~
for which acid deposition matters.

Definition: 1121

Check: if >0

Location: 296,144

Nodesize: 44,24

Valuestate: 1,152,162,416,303,0,MIDM

Close Watershed_informatio

Variable Species_deposition

Title: Chemical Deposition

Description: Chemical species that are deposited on watersheds from th~
e atmosphere.~

Indexed by time.

Definition: sum(Annual_snoxn_dep[TAF_receptors='Adirondacks']*Emission~~
s_species_conv,deposition_species)

Location: 192,192

Nodesize: 48,20

Windstate: 1,427,102

Defnstate: 1,42,183,954,145,0,MIDM

Valuestate: 1,168,178,634,249,0,MIDM

Reformval: [Year_5, Chosen_policies]

Module Other_outputs

Title: Other~

Outputs

Description: Other Soils and Aquatics outputs of interest, but not uti~~
lized by other modules of the TAF Model.

Author: Kevin

Date: Wed, Nov 22, 1995 10:21 AM

Location: 440,120

Nodesize: 48,20

Diagstate: 1,40,72,384,272,17

Nodecolor: 13107,-26215,-1

Variable Wca

Title: Weighted Ca by region

Units: ueq/L

Description: Lake calcium for the entire region, calculated using the ~~
DDRP weights.~

Indexed by time.

Definition: (Sum((Lake_ca*Wts),Ids)/Sum(Wts))

Location: 304,32
Nodesize: 44,20
Valuestate: 1,136,146,416,303,1,MIDM
Aliases: Formnode Weighted_ca_by_regio
Nodecolor: -26215,-13108,-1

Variable Wphl

Title: Weighted pH by region
Description: The lake pH for the entire region, weighted by watershed --
weight.~
Indexed by region and time.
Definition: $\text{sum}(\text{pHl} * \text{Wts}, \text{Ids}) / \text{sum}(\text{Wts})$
Location: 64,200
Nodesize: 48,20
Valuestate: 1,40,50,416,303,1,MIDM
Aliases: Formnode Weighted_ph_by_regio
Nodecolor: -26215,-13108,-1
Reformval: [Time, Ids]

Chance Cdfphl

Title: CDF of Lake pH
Description: CDF of pH, indexed by region and year.
Definition: $\text{Chancedist}(\text{Lake_prob}, \text{Phl}, \text{Ids})$
Location: 192,200
Nodesize: 48,20
Valuestate: 1,213,134,416,303,1,CDFP
Aliases: Formnode Cdf_of_lake_ph
Nodecolor: 0,-13108,26214

Chance Base_saturation_dist

Title: Base Saturation Distribution
Definition: $\text{Chancedist}(\text{Lake_prob}, \text{Tbs}, \text{Ids})$
Location: 64,144
Nodesize: 44,24
Windstate: 1,40,111
Valuestate: 1,206,146,416,303,1,CDFP
Aliases: Formnode Base_saturation_dis1
Nodecolor: 0,-13108,26214
Graphsetup: Distresol:4~
Diststeps:1~
Cdfresol:4~
Cdfsteps:1~
Symbolsize:6~
Linestyle:1~
Frame:1~
Grid:1~
Ticks:1~
Mesh:1~
Scales:1~
Rotation:0~
Tilt:0~
Depth:70~
Frameauto:1~
Xminimum:0~

Xmaximum:15~
Yminimum:0~
Ymaximum:1~
Zminimum:1~
Zmaximum:2~
Xintervals:0~
Yintervals:4~
Includexzero:0~
Includeyzero:0~
Includezzero:0~

Reformval: [Chosen_policies, Time]

Variable Wbs

Title: Weighted Base Saturation by region

Units: %

Description: The weighted base saturation for the entire region, indexed by time.

Definition: $\text{sum}(\text{TBS} * \text{Wts}, \text{Ids}) / \text{sum}(\text{Wts})$

Location: 64,32

Nodesize: 48,24

Windstate: 1,90,250

Valuestate: 1,120,130,416,303,1,CONF

Aliases: Formnode Weighted_base_satura

Nodecolor: -26215,-13108,-1

Reformval: [Time, Probindex]

Variable Fraction_of_lakes

Title: % of lakes supporting each fish species

Description: Percentage of lakes in the region that support fish by fish species.

Indexed by region and time.

Definition: $\text{Sum}((\text{Fishresponse} * \text{Wts}), \text{Ids}) * \text{fudge} / (\text{sum}(\text{Wts}) * \text{totlakes})$

Check: if ≥ 0 and ≤ 1

Location: 192,32

Nodesize: 48,24

Valuestate: 1,88,98,416,303,1,CONF

Aliases: Formnode A_of_lakes_supporti

Nodecolor: -26215,-13108,-1

Reformval: [Time, Probindex]

Reference: 1. Baker, Joan P., Biological Effects of Changes in Surface Water Acid-Base Chemistry, NAPAP State of Science and Technology Report No. 13, National Acid Precipitation Assessment Program, Washington, DC.

Variable Fraction_of_lakes_wi

Title: % of lakes with pH<5.5

Description: Fraction of lakes in the region with a pH less than 5.5.

Indexed by region.

Time must be chosen from the current time popup node.

~

Old Def:~

Linearinterp(mid(Sorted_lake_ph),Cumphl,5.5)

Definition: $\text{Sum}((\text{Phl} < 5.5) * \text{Wts}, \text{Ids}) * (\text{fudge} / \text{totlakes}) * (100 / \text{sum}(\text{Wts}))$

```

Check: if >=0 and <=1
Location: 192,88
Nodesize: 48,24
Windstate: 1,149,281
Valuestate: 1,294,141,416,303,0,MIDM
Aliases: Formnode A__of_lakes_with_ph_
Nodecolor: -26215,-13108,-1

```

Variable Bstree

```

Title: % region with Base Saturation < 10%
Description: Fraction of the region which has a base saturation less t~~
han a cutoff value of 10%, resulting in potentially reduced forest gro~~
wth.~
Indexed by region and time.~
~

```

Old Def:~

```

linearinterp(mid(sortedbs),cumbs,10)*fudge/Totlakes
Definition: Sum((Tbs<10)*Wts,Ids)*(fudge/Totlakes)*(100/sum(Wts))
Check: if >=0 and <=1
Location: 64,88
Nodesize: 48,24
Windstate: 1,110,130
Valuestate: 1,56,66,416,303,1,DEFA
Aliases: Formnode A__region_with_base_
Nodecolor: -26215,-13108,-1
Graphsetup: Distresol:4~
Diststeps:1~
Cdfresol:4~
Cdfsteps:1~
Symbolsize:6~
Linestyle:1~
Frame:1~
Grid:1~
Ticks:1~
Mesh:1~
Scales:1~
Rotation:0~
Tilt:0~
Depth:70~
Frameauto:1~
Xminimum:1980~
Xmaximum:2030~
Yminimum:50~
Ymaximum:100~
Zminimum:1~
Zmaximum:2~
Xintervals:0~
Yintervals:5~
Includexzero:0~
Includeyzero:0~
Includezzero:0~

```

```

Reformval: [Time, Chosen_policies ]

```

```
Variable Aluminum_in_region
Title: Aluminum in region
Units: ueq/L
Description: The aluminum in the region, indexed by time
Definition: sum(Lake_aluminum*Wts,Ids)/sum(Wts)
Location: 192,144
Nodesize: 48,24
Valuestate: 1,41,49,416,303,1,CDFP
Aliases: Formnode Aluminum_in_region1
Nodecolor: -26215,-13108,-1
```

Close Other_outputs

```
Variable Emissions_species_co
Title: Emissions Species Conversion
Description: Matrix used to reduce the Deposition Species (Wet & Dry Sulfur and Nitrogen) down to Emission Species (SOx & NOx)
Definition: Table(Emissions_species,Deposition_species)(
1,1,0,0,
0,0,1,1
)
Location: 64,192
Nodesize: 48,20
Reformdef: [Emissions_species, Deposition_species ]
```

```
Variable Time_remapped_asl_in
Title: Time Remapped ASI in Lake
Description: The ASI in each lake, remapped to a time-esque index running from 1980 to 2030 in steps of Dt.
Definition: Table(Year_5)(
Asl_in_lake[Time=1985],Asl_in_lake[Time=1985],Asl_in_lake[Time=1990],Asl_in_lake[Time=1995],Asl_in_lake[Time=2000],Asl_in_lake[Time=2005],Asl_in_lake[Time=2010],Asl_in_lake[Time=2015],Asl_in_lake[Time=2020],Asl_in_lake[Time=2025],Asl_in_lake[Time=2030])
Location: 440,56
Nodesize: 48,20
Valuestate: 1,88,98,416,303,0,MIDM
Reformval: [Year_5, Chosen_policies ]
```

Close Soils_aquatics_modul