SWAP

MODELLING WORKSHOP REPORT

edited by

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PREFACE

This report describes a workshop on modelling surface water acidification processes organized within the SWAP programme and held at the Institute of Hydrology, March 25-28, 1985. We would like to acknowledge the support of the Director of IH, Dr J G McCulloch, for his encouragement and provision of the IH conference rooms and computing facilities.

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1. INTRODUCTION AND LIST OF PARTICIPANTS

At this early stage in the Surface Water Acidification Programme it is necessary to coordinate research in the area of modelling by the exchange of information on data and model techniques and by the planning of future collaborative research. In order to achieve this it was decided to hold a short workshop at the Institute of Hydrology. The meeting was held between 25th and 28th March 1985 with 19 scientists participating from the UK, Norway, Sweden, Germany, Finland and the United States. Several scientists not directly supported by SWAP were invited to the meeting to provide a broad spectrum of experience and ideas and to ensure that the SWAP modelling activities were closely coordinated with other groups working in the area.

The workshop participants included:

N Christophersen		Center for Industrial Research, Norway
P G Whitehead	)	Institute of Hydrology, UK
R Neale	)	" " " "
R Williams	)	" " " "
C Neal	)	" " " "
K Beven	)	" " " "
S Bird	)	University of Swansea, UK
I Littlewood	)	" " " "
S Bergstrom	)	Swedish Meteorological and Hydrological Institute, Sweden
P E Jansson	)	University of Uppsala, Sweden
U M Calles	)	" " " "
J Kamari		National Board of Water, Finland
M Haus		University of Gothingen, FRG, currently NIVA, Norway
J Cosby	)	University of Virginia, USA
G Hornberger	)	" " "
M B Beck	)	Imperial College, UK
H Wheater	)	" " "
K Bishop	)	" " "
D Drummond	)	" " "

Additional support staff were available at IH to set up data and models brought by participants on the IH computer system.

2. SWAP MODELLING OBJECTIVES

The findings of the workshop should be viewed in light of the overall SWAP modelling objectives which are summarised here:

a) An unltimate goal is to develop models capable of predicting both short and long term changes in freshwater chemistry following changes in deposition and/or management practices. To this end emphasis should be placed on identification and quantification of key processes controlling freshwater chemistry. Available modelling tools such as time series analysis (Whitehead et al., 1984), the Birkenes model (Christophersen et al., 1982, 1984) and the MAGIC model (Crosby et al., 1985) will form the initial basis for the work and be utilised or improved as necessary.

b) Another major objective of the SWAP modelling effort is to interact with other subprojects performing field and/or laboratory work and integrate the information from these projects.

3. WORKSHOP OBJECTIVES AND PROGRESS

The objectives of the workshop comprise information exchange between SWAP Participants and invited scientists, assessment of recently assembled data and models at I.H., detailed planning of SWAP modelling work for 1985, and recommendations for data collection at SWAP field sites and other sites for which data are used.

On the first day of the workshop the participants presented a summary of their current and future research interests. The following topics were presented:

An Overview of IH Catchment Studies and Modelling Research	-	P G Whitehead
Hydrochemical Studies at Plynlimon, Wales	-	C Neal
Land Use and Management Studies at Brianne, Wales	-	S Bird
Imperial College Proposals	-	B Beck

Swedish Catchment Studies and Modelling Research	-	S Bergstrom
Catchment Modelling Research at Uppsala University	-	P E Jansson
Forest Catchment and Modelling studies in Germany	-	M Haus
A Model of Acidification of Groundwater In Catchments (MAGIC)	-	J Cosby
Distributed Hydrological Models (TOPMODEL)	-	K Beven
Extensions to TOPMODEL using MAGIC chemistry	-	G Hornberger
Finnish Research and the Rains Project	-	J Kamari
The Birkenes Model and extensions to Harp Lake	-	N Chistophersen

These presentations were followed by a discussion of research needs and the formation of working groups to discuss chemical and hydrological process models, problems of parameter uncertainty, extension of laboratory and plot scale results to the catchment scale and data needs.

Demonstrations of various models available on the IH computer system were given including CAPTAIN (times series analysis applied to Loch Dee data), BIRKENES model (applied to Loch Dee and Harp Lake data), TOPMODEL (applied to Birkenes, Loch Dee and the Plynlimon data) and MAGIC (applied to White Oak Run and Loch Dee data).

Research was initiated applying these techniques to the German Lange catchment data and the other catchment data available at IH.

On the last day of the workshop a meeting was held to discuss research plans for 1985 and for the various working groups to report.

4. WORKING GROUP DISCUSSION NOTES

4.1 Catchment data and modelling exchange

All participants agreed for the need to exchange data and models. IH offered to act as a clearing house, establishing data bases and providing copies of data and models as required. This was accepted and IH has already obtained data for the following catchments:

Birkenes, Southern Norway
Lange, Harz Mountains, West Germany
Llyn Brianne, South Wales

Loch Dee, South-West Scotland

Gardsjon, Sweden

Harp Lake, Canada

Plynlimon, Mid-Wales

Storgama, Norway.

A more detailed description of the data available is given in appendix 1.

With regard to exchange of models, several models and modelling techniques have already been established at IH. These include CAPTAIN (Computer Aided Package for Time Series Analysis and the Identification of Noisy Systems, Venn and Day, 1977, Whitehead et al., 1984), MIV (Multivariable time series model, Young and Whitehead, 1977), the BIRKENES model (Chistophersen et al., 1982), MAGIC (Cosby et al., 1985), EKF (Extended Kalman Filter, Beck and Young, 1976) TOPMODEL (Beven, 1982) and IHDM (Institute of Hydrology Distributed Model, Morris, 1980). Other models may be added to this list as they become available.

4.2 A Comparison of the Birkenes and Magic Chemistry

A particulary important aspect of the workshop was to assess the chemical process models (Birkenes and Magic) currently available and identify similarities and differences between these two principal approaches.

MAGIC (Model of Acidification of Groundwater In Catchments) is explicitly designed to perform long term simulations of changes in soilwater and streamwater chemistry in response to changes in acidic deposition. The processes on which the model is based are:

- anion retention by catchment soils (e.g. sulphate adsorption);
- adsorption and exchange of base cations and aluminium by soils;
- alkalinity generation by dissociation of carbonic acid (at high CO_2 partial pressures in the soil) with subsequent exchange of hydrogen ions for base cations;
- weathering of minerals in the soil to provide a source of base cations;
- control of Al^{3+} concentrations by an assumed equilibrium with a solid phase of $Al(OH)_3$.

There are several manuscripts awaiting publication describing in detail the mathematical and conceptual structure of MAGIC. Only one of them has been published to date (Cosby et al., 1985). A brief summary is given here.

MAGIC presently operates using yearly or monthly time steps. The data requirements for the model are therefore annual or monthly average values of streamwater pH, alkalinity and concentrations of base cations and inorganic anions. MAGIC also models the variations of soil and soil water chemistry at the same temporal resolution. Additional data on the base saturation of the soil, exchangeable fractions of each base cation and aluminium on the soil and the physical characteristics of the soil are required to implement the model. Data from lysimeters giving variations in soil water pH, alkalinity and base cation concentrations are helpful in selecting values for the parameters in the model.

MAGIC is driven by an assumed sequence of atmospheric deposition and mineral weathering. Current deposition levels of base cations, sulphate, nitrate and chloride are needed along with some estimate of how these levels had varied historically. Historical deposition variations may be scaled to emissions records or may be taken from other modelling studies of atmospheric transport into a region. Weathering estimates for base cations are extremely difficult to obtain. Nonetheless, it is the weathering process that controls the long term response and recovery of catchments to acidic deposition and some estimate is required.

The MAGIC and Birkenes models have may similarities. Both models are based on the same chemical processes in the soil, although the details of mathematical representations of those processes vary between the two models. They treat the effects of elevated CO_2 partial pressure in the soil and contain terms for an equilibrium with a solid phase of $Al(OH)_3$ and for complexation or hydrolysis of Al^{3+} in solution. This aspect probably needs improvement in both models. Both models treat base cation exchange between soil water and the soil matrix as an equilibrium process. The Birkenes model treats this exchange by considering divalent cations lumped together (M^{2+}) while MAGIC treats all four major base cations (Na, K, Mg, Ca) individually. ?

$S_{CaNa} = S_{MgNa}$ for WOR ?

eg $S_{CaNa} = \frac{\{Na^+\}^2 E_{Ca}}{\{Ca^{2+}\} E_{Na}^2}$ $Ca^{2+} + \ldots = 2Na^+ + CaX_2$

The major differences between the Birkenes and MAGIC models arise from the different applications for which the models were designed. The Birkenes model was intended for short term (daily time steps) modelling while MAGIC was intended for long term (yearly time steps) modelling. As a result, the hydrological component of the Birkenes model is more complex (to reproduce observed daily variations in flow) than the lumped hydrology component currently included in MAGIC (based on annual average water fluxes). Another major difference is the treatment of soil properties. For instance, base saturation is considered constant over a simulation run and is treated as a parameter in the Birkenes model, while MAGIC treats base saturation as a variable and estimates its temporal changes.

The modelling of long term catchment responses is beset by many difficulties, most of which arise due to a lack of sufficient time series of data for long term calibration and validation. Nonetheless, an implicit goal in any modelling study is to be able to make long term predictions. MAGIC can be most useful, perhaps, as an heuristic tool. Used in a speculative simulation exercise, the model provides a framework for examining various hypotheses about the long term acidification response of catchments. Coupled with shorter term modelling studies (eg daily variations as in the Birkenes model or hourly variations as in the CAPTAIN time series models), MAGIC becomes a compementary tool for integrating and understanding our observations on responses to acidic deposition.

In general therefore it appears that the MAGIC and Birkenes model chemistry is very similar although modifications would be required to consider special factors such as sea salts, differing aluminium speciation, enhanced biological activity and the effects of changing soil characteristics. There is however a broad concensus on the main chemical processes operating which is encouraging from the modelling viewpoint.

4.3 Interpretation of Plot Experiments

There was substantial discussion at the workshop on the value of plot experiments and the information that can be derived to assist modelling studies in a variety of ways. These include the generation of appropriate hypotheses for model development, the identification of ranges of parameter values to assist in parameter identification at catchment scale, the testing of model hypotheses, and the observations of fluxes and states to assist in model verification. It was the feeling of the meeting that these data are of particular importance in modelling long term effects although there was doubt that parameters from plot studies can be used directly in catchment scale models.

In this context, it should be noted that Imperial College has agreed collaboration with the Macaulay Institute to enhance selected plot experiments with a view to identifying hydrological pathways and measuring corresponding fluxes of water and solute. On the basis of this data, Imperial College will examine the extent to which existing hydrological and hydrochemical model structures are compatible with the plot observations and investigate the application of the plot results to catchment scale modelling.

4.4 Parameters Uncertainty and Estimation

A most pressing problem in surface water quality modelling, both short and long term, relates to the uncertainty in model structure and parameter estimation. Abundant data from past studies indicate that a major portion of the uncertainty is due to actual variability in the landscape and not to experimental or measurement errors. It is extremely unlikely that such variability can be directly included in a model. Such a model would be difficult to implement in any case. We are therefore forced to rely on a lumped representation and must find other ways to deal with uncertainty.

Lumped models are difficult to verify statistically on a single catchment. Confidence in the models must therefore come by applying them to several different types of catchment.

Evaluation of the effects of model uncertainties on predictions of future response is closely allied to the process of model development and calibration against field data. There is a common dilemma in using models for prediction. On the one hand the more complicated models contain a larger number of parameters, for which uniquely "best" estimates may not be identified from the field data. Such uncertainties will propogate with the prediction, making the predictions not only uncertain but possibly even ambiguous or contradictory. The simple models, on the other hand, may be too simple and may not be able to predict the variety of catchment responses that could occur. Since the ultimate objective of all the modelling studies is to extrapolate likely behaviour into the future and from one catchment to another, it is essential that the uncertainties associated with predictions be exhaustively examined.

The application of time series analysis techniques to streamwater chemistry data to infer interrelationships amongst variables has not been explored extensively and these techniques may have great value in the interpretation of data relating to acidification of surface waters. However, we would recommend that this work be defined more tightly to interface with the conceptual modelling work. For example, work could be done analysing model-generated time series (from the Birkenes model) with the aim of exposing typical dynamic patterns associated with the model. These could then be compared with patterns evident in actual data sets to see areas of agreement and disagreement. It may even prove possible to relate time series parameters to conceptual model parameters and thereby estimate parameter uncertainty. This would have obvious implications for more exhaustive uncertainty analyses. In addition there are already sufficient data for the application of some of the more advanced methods of recursive estimation (such as the extended Kalman filter) to the indentification of the conceptual lumped-parameter catchment models. In particular, these methods should be used for the identification of significant discrepancies between the performance of the current models and the observed time series. It is also important to quantify the residual uncertainties of the models and their parameter estimates.

5. RESEARCH PROGRAMME FOR 1985

i) The time series analysis techniques will be used to investigate streamwater dynamics and long term trends. The technique has already been used to quantify the effects of liming on stream quality in the Loch Dee catchment and could provide a useful method of analysing the longer data series from Norway and Sweden, especially if use is made of the recursive estimation techniques to investigate long term trends in soil properties and deposition rates. The technique will also be applied to simulation data to investigate model dynamics and problems of parameter estimation.

ii) An important part of the work will be modelling of streamwater chemistry for new catchments on a day to day and seasonal basis. The key hydrochemical processes incorporated into the Birkenes model have proved able to describe streamwater chemistry in three quite different catchments. To check the generality of these process descriptions the Birkenes model will be applied to the Loch Dee and Plynlimon sites and also to data sets from the Storgama area in Norway hitherto unused in a modelling context. Modifications to the chemistry may be necessary to take into account sea-salt effects and Al minerals other than gibbsite.

+ Brånne.

iii) The hydrological pathways may have a significant effect on streamwater chemistry. Chemistry may be controlled by the pathways rather than merely residence times in particular compartments and hence a clearer understanding of catchment hydrology is required.

The hydrological submodel in the Birkenes model is rather simplified and improvements are desirable. Based on recent ^{18}O data in precipitation, soil water and runoff from Birkenes the hydrological submodel will be subject for revision. In this context other suggested hydrological model formulations will be reviewed.

TOPMODEL represents an alternative hydrological modelling approach where the important concept of the variable source area is explicitly quantified. TOPMODEL will be set up for Birkenes, Plynlimon and Loch Dee sites and chemical submodels added.

Finite difference/element models are being developed to investigate plot scale behaviour as part of the proposal from Imperial College.

iv) The work on long term prediction will proceed in parallel with the above activities. MAGIC will be set up for Loch Dee initially, although it would be possible to investigate many catchments using the technique, and extend the work on a regional basis.

Tentative simulations applying the Birkenes model for predictions of changes in episode streamwater chemistry for selected changes in deposition and soil properties have been carried out. This work will be presented to the Muskoka conference in September.

One last activity should be mentioned in this context. For Muskoka we will also present a comparison of empirical (Henriksen, 1980) and process-oriented models for freshwater acidification. The empirical approach is rather different and a comparison of predictions resulting from the two approaches is of interest.

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APPENDIX 1 CATCHMENT DATA AVAILABLE AT IH

Birkenes, Norway

Daily Rainfall, Flow measurements and Streamwater Chemistry
Daily Temperature and Sulphate in the rainfall

These data are available for the following periods:

May - Nov 1973, May - Nov 1974, May - Nov 1975
May - Nov 1976, July - Nov 1977, July - Nov 1978
May - Nov 1980.

Streamwater Chemistry and discharge for 1972-1983 will soon be available.

Lange, Germany

Lysimeter data: Soil water flux and chemistry taken at variable time intervals from 1977 to 1985.

Stream data: Streamflow and stream chemistry with a variable sampling interval during 1977 to 1985.

Llyn Brianne, Wales

Daily rainfall, stage and stream chemistry from three sub-catchments for a 45 day sampling period during September and October 1984. Further data being collected by Welsh Water Authority and Swansea Univeristy.

Loch Dee, Scotland

White Laggan sub-catchment

Daily rainfall, flow and temperature data from January 1930 to September 1984.

Rainfall and stream chemistry sampled at a frequency varying from weekly to monthly. The data are available for the period Jan 1980 - May 1984.

Dargall Lane sub-catchment) rainfall and stream chemistry as above
Green Burn sub-catchment)
)

Gardsjon Catchment, Sweden

Daily values of rainfall, temperature, flow, sulphate in runoff, sulphate in rainfall and M^{2+} in runoff.

Variable period collection of chloride in rainfall and runoff, and sodium, aluminium and pH in runoff.

All data available for the period January 1979 to December 1981.

Harp Lake, Canada

Daily rainfall, temperature, flow and sulphate in the rainfall from May 1977 - May 1982.

Weekly stream chemistry from May 1977 - May 1982.

Plynlimon, Wales

Rainfall and flow data at 15 minute intervals.
Weekly rainfall and stream chemistry.

Data available for the period 25 May 1984 - April, 1985.

Storgama, Norway

Daily rainfall, temperature, flow and sulphate in the rainfall for the period May 1975 - November 1978. Streamwater chemistry and discharge for 1974 - 1984.

APPENDIX 2 MODEL DATA REQUIREMENTS

The following data are required for the various modelling activities:

i) Time series analysis

This technique is planned to be used mainly on observed and simulated time series of streamwater chemistry and discharge. Preferably the chemistry data should have a time resolution comparable to the discharge data.

ii) TOPMODEL - Catchment details required together with daily (or more frequent) rainfall, evapotranspiration and discharge data.

iii) The Birkenes model

A minimum data set comprises daily precipitation amount and mean daily temperature. Daily, weekly or even monthly concentrations of sulphate in precipitation combined with sulphur dry deposition estimates. Discharge is required on a daily basis and streamwater chemistry should preferably have a resolution covering major changes in the hydrograph. Aluminium speciation is desirable. Soil chemistry data including representative data for base saturation or lime potential and pCO_2 are helpful and should be collected in future studies. For prediction estimates of weathering rates are necessary.

iv) MAGIC

Estimates of present soil geology and chemistry are necessary for the approach together with information on acid deposition.