This paper has been presented to the

Summer Computer Simulation Conference

July 28-30, 1986, Reno, Nevada for publication

and the contents are subject to change.

This copy is to provide information

prior to publication.

COMPUTER SIMULATION OF WATERSHED ACIDIFICATION

by

D.C.L. Lam

Environmental Simulation Section
National Water Research Institute
Burlington, Ontario
NWRI Contribution No. 86-12

COMPUTER SIMULATION OF WATERSHED ACIDIFICATION

DAVID C. L. LAM
Environmental Simulation Section
National Water Research Institute
Burlington, Ontario, Canada L7R 4A6

ABSTRACT

Two new approaches are presented for the computer analysis of watershed acidification. The one approach is to develop simulation models to generate simple and general knowledge bases for use in an expert system. The other approach is to develop such an expert system in which data analysis can be carried out with simulation models and the knowledge bases they generate. Results from a prototype of this framework have demonstrated the feasibility of linking the two approaches. In particular, the temporal and spatial perspectives of the changes in terrestial characteristics and aquatic chemistry are represented in the new system. Spatially, the watersheds are treated as geographical elements, each of which is linked to the time series data bases through the use of microcomputer technologies. Examples of simulated and observed results are presented and the application of the modeling approaches is discussed.

INTRODUCTION

The long range transport of airborne pollutants such as sulfur and nitrogen oxides from industrial emission sites has become a major environmental concern. These pollutants eventually reach the ground as dry deposits or, when mixed with the precipitation, as "acid rain." Unless the soil contains sufficient alkaline materials to neutralize the acid, the streams and lakes will turn acidic. As the acidity increases, many fish and plankton species may perish and the aquatic ecology may be greatly disturbed.

Computer simulation models (1,2,3) of watershed acidification processes must be designed to integrate the complex hydrological and hydrogeochemical components. Specifically, the models have to link up chemical reactions that occur in the order of microseconds to soil contact times in the order of days and months and then to groundwater flow times in the order of years and decades. As well, depending on the physical and chemical characteristics of the watershed, responses to the acid deposition could be short-term episodes lasting for weeks or longterm changes lasting for decades. In addition to these time scale problems, the spatial heterogeneity of the terrestial characteristics greatly complicates the assessment of the watershed responses and resources at risk resulting from the acid loadings. To apply simulation models over a long term to all the watersheds in a large geographical area of concern is inefficient and uneconomical and, even if it can be achieved, it is impractical to analyse the vast volume of simulated results.

Therefore, new approaches are needed to circumvent these complications. In particular, it is important at the outset to establish the linkage between the terrestial component and the aquatic component, at least on a watershed basis. This linkage, along with other investigations, can be approached from two directions: simulation and expert system. The simulation approach is to provide simple, general knowledge bases from computer models for extrapolation into other watersheds of similar characteristics. The expert system approach is to provide analysis and processing of data with the assistance of the knowledge bases. These two approaches are in a "parallel" mode, according to the current taxonomy (4), in which the modeler mainly deals with the simulation models and the user is referred to an intelligent front end in the expert system (Fig. 1).

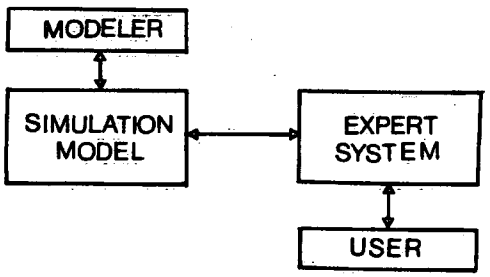

Figure 1. Simulation framework.

The purpose of this paper is to discuss the two approaches and their possible linkages, with examples of results from the simulation models, an expert system prototype and observations from field and monitoring programs.

SIMULATION MODELS

The major anions contributing to the acidity in the precipitation are sulfate and nitrate (forming sulfuric and nitric acids). A small part of these ions enters the lakes and streams directly, if the precipitation or dry deposit falls onto the surface waters. The main bulk, however, follows complicated pathways through forest canopies, organic layers, soil horizons and groundwater aquifers. As the ions go through these hydrological regimes, they take part in many chemical and biological reactions and undergo substantial changes before they join the surface waters. This concept of mobile ions is the basis for constructing a number of simulation models (1,2).

Hydrological Submodel

The key model component required is a hydrological submodel which can accurately predicts the water contents and pathways in each of the hydrological regimes. Unfortunately, most of the existing hydrological models are not adequate for such purposes, since they were developed mainly for flooding forecasts in which the short-term changes in the total runoff were emphasized. Many of them do not have the simulation capability

covering a time span of years or decades; some do not even satisfy the mass conservation principles.

New models are therefore required. An example is the one by Lam and Bobba (1) which is based on a model structure with one snow layer and three soil reservoirs. The three soil reservoirs are made to coincide with the processes of humus formation, cation exchange and soil weathering, respectively from top to bottom layer. This model is simple, portable and yet sufficiently robust to include mass balance computations for snow accumulation and melting, soil moisture bugets, runoff generation and evapotranspiration. These mechanisms are simulated by a set of governing differential equations. The inputs are the precipitation and air temperature and the outputs are the snowpack thickness, meltwater, inflow and outflow of each soil layer and its moisture content and the total runoff.

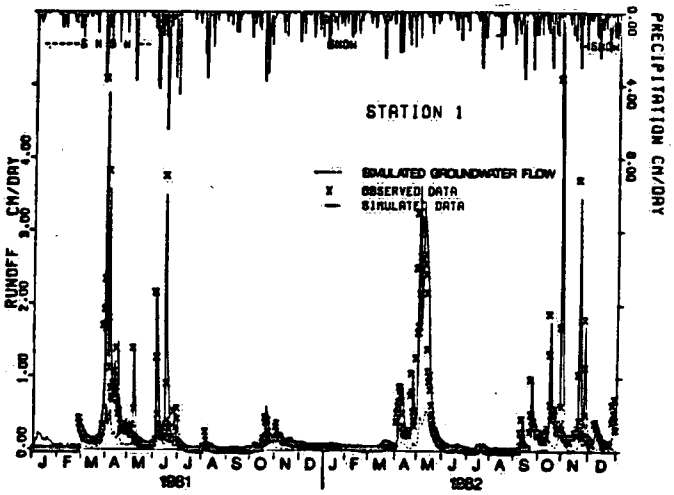

Figure 2. Simulated and observed runoff at the Turkey Lakes watershed, Ontario.

The model uses a daily time step so that numerical integration for a period of five years requires about 15 minutes of computation with a CDC Cyberg 171. Figure 2 shows an axample of simulated and observed stream runoff at a Canadian watershed. Typically, the data from the first year are used in model calibration and data from subsequent years, for model verification. At this point of development, model calibration and verification have been applied to 15 different catchments at various sites in Eastern Canada and for simulation times ranging from 3 to 8 years (5). In these cases, not only are the simulated results compared to the total runoff data but also compared to the observed groundwater and snowpack data, whenever available. In general, the model is able to simulate 75 to 80% of the variance in the observed data.

Hydrogechemical Submodel

The next step in implementing the mobile ion concept is to use the computed hydrological flows in the computation of the pathways and reactions of the chemical variables. An outline on the linkage of the hydrological model with the hydrogeochemical model is given in Lam and Bobba (1). The major variables considered include sulfate, aluminum, bicarbonate, pH, alkalinity, calcium and magnesium (nitrate is to be included only when it becomes important). Again, the hydrogeochemical submodel is described by a set of differential equations, with most of the chemical kinetics incorporated as equilibrium constraint conditions. Specifically, the mass balance computation for sulfate is carried out first for all the layers, taking into account the wet and dry deposition, adsorption and desorption, oxidation and reduction mechanisms. Then, the concentration of the major ions is evaluated following charge balance and chemical equilibrium conditions. Some of the equilibrium constants are assumed to be fixed; other model constants such as sulfate adsorption coeffient and soil weathering rates are allowed to change during model calibration from watershed to watershed.

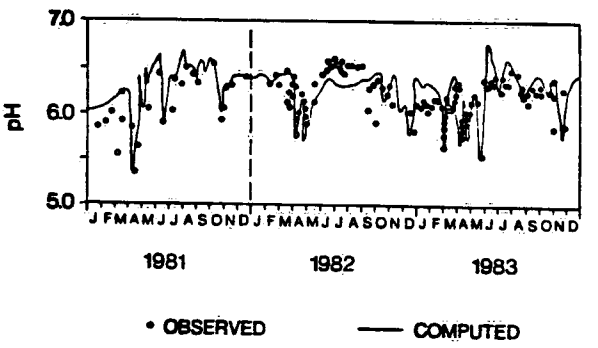

Figure 3. Simulated and observed pH at the Turkey Lakes watershed, Ontario.

Figure 3 shows an example of simulated and observed pH for the same watershed as given in Fig. 2. Comparison of the two figures provides some insight into the relationship between the hydrology and the hydrogeochemistry. For example, as shown in Fig. 2, the highest runoff in 1981 occurred in early April, as a result of snowmelt. Correspondingly, the pH experienced a substantial drop of about one unit at that time (Fig. 3). This drop in pH was due to the release of the sulfate ions previously accumulated in the snowpack. Subsequently, the pH rose to its normal level at about 6.5 and then dropped again in mid-June. This second drop in pH was associated with heavy rainfalls during that month, as the stream runoff would then contain a high groundwater portion (Fig. 2) which had been displaced by the rainwater infiltration and thus carried a substantial supply of dissolved CO_2 to the stream as carbonic acid. On the other hand, since snowfall was less in 1982 than in 1981, the snowmelt runoff which again occurred in the month of April was smaller in 1982 and the pH drop was correspondingly less (Fig. 3). Moreover, there were little variations in the stream pH in June and the rest of that summer of 1982 (Fig. 3), because no major rain events occurred (Fig. 2).

Clearly, these mechanistic models have been advanced to a stage where many detailed processes and episodes can be accurately simulated, provided that sufficient data are available for calibration and the model assumptions are valid. This linked hydrological-hydrogeochemical model has also been applied successfully to a number of watersheds in Canada (6). The computational time step is one day and the computer time required for a typical simulation of five years is about 1.5 minutes for running the hydrogeochemical submodel on the CDC Cyberg 171, an order of magnitude faster than its hydrological counterpart.

SIMULATION RESULTS FOR KNOWLEDGE-BASED SYSTEM

The mechanistic simulation models require a comprehensive set of data for calibration and verification. Indeed, only those data that are sampled at least on a weekly basis from a limited number of intense study watersheds meet the requirements. The majority of the watershed acidification data are from monitoring sites where the sampling frequencies are at monthly or yearly intervals. As indicated in the proposed simulation framework (Fig. 1), this main bulk of data is to be processed and analysed by utilizing the knowledge bases generated by the models. For example, the models can be used for prediction of the pH depression during snowmelt at a watershed with similar soil and geological characteristics. Of particular interest is the occurrence of pH threshold levels below which some fish such as brook trout cannot subsist. The occurence of such pH levels is, however, probabilistic in the sense that the sulfate ions which originate from the atmospheric load have to be accumulated for a sufficiently long time in the snowpack before they eventually enter the stream with the meltwater. There may well be meteorological conditions, e.g. insufficient snowfall or rapid thawing sequences, that eliminate or reduce the impact of the acid shock.

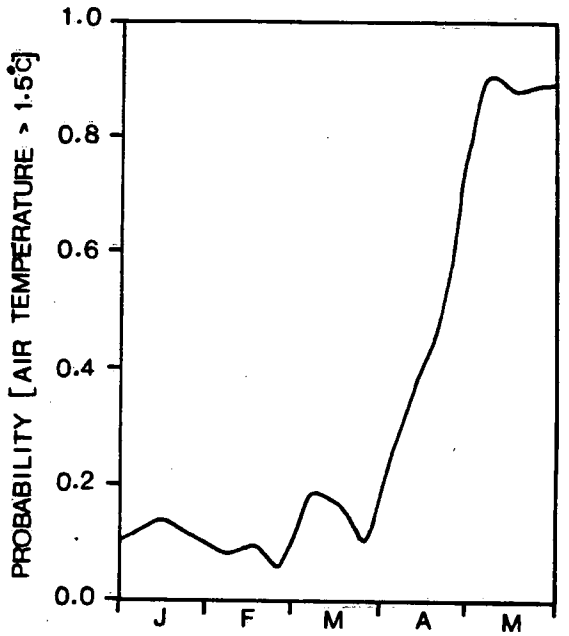

Figure 4. Probability for air temperature to be more than 1.5 °C at the Northeast Pond River watershed, Newfoundland.

Figure 4 shows the probability for the air temperature to exceed 1.5 °C, i.e. a condition conducive to snowmelt, computed from a meteorological record of thirty years (1954-1983) at a Newfoundland watershed. There is , for example, about 30% chance that snowmelt would occur in early April of any year in that watershed, about 65% in late April and more than 90% chance in May if there is still some snow accumulated. Computations using this information can be made with the simulation models to derive the probability distributions of the occurrence of episodic pH depressions.

Another important application that can be made from the simulation models is the knowledge surrounding the groundwater flow. During winter and summer drought periods, the total runoff is reduced to its lowest level and almost all of it originates from the soil reservoirs. Since the flow is slow, much of the dissolved CO_2 has been degassed and the effects of cations such as Ca^{++} and Mg^{++} become important. In fact, the pH usually peaks at this time (Fig. 3), because of the predominance of these ions. Since these periods are free of the episodic influences, the $Ca^{++}$and Mg^{++} concentrations are a good indicator of the buffering capacity left in the watershed to neutralize the acid rain.

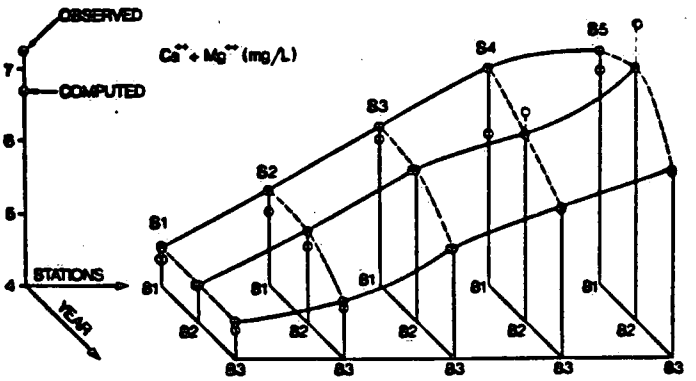

Figure 5. Simulated and observed Ca^{++} + Mg^{++} concentrations at winter drought period at Turkey Lakes Watershed,Ontario.

Figure 5 shows the simulated and observed Ca^{++}+ Mg^{++} concentrations at winter time for three consecutive years at five sampling stations (S1-S5) arranged in downstream order at the Turkey Lakes watershed in Ontario. The concentrations form a time-space surface in which there is a strong spatial gradient of increasing cation exchange activities in the downstream direction but a weaker, decreasing trend in time. The spatial gradient is related to the increase in soil depth in the downstream direction. Time-space surfaces for other major ions have also been constructed (6)

During the calibration of the hydrological model for 15 catchments, model coefficients such as the infiltration constants for different soil layers have been related to the soil type and soil porosity. The residence times in each of the soil reservoirs have also been computed and again related to the soil information in a table lookup format (5). These tables, time-space surfaces and probability distributions are part of the knowledge generated by the simulation models. Similar pieces of information on sulfate adsorption and organic acidity can be made as summary tables. As the simulation models develop , for example, to include longterm effects such as dependency of weathering rate on pH and nonlinear formulation of lime potentials (7), this body of knowledge will increase and be used to analyse the monitoring data.

KNOWLEDGE-BASED SYSTEM

A new knowledge-based system, acronymed RAISON-MICRO, for the regional acidification analysis by intelligent systems on a microcomputer has been developed (8). Essentially it is a data processing workstation which provides a user friendly environment for the creation, update, assess, retrieval and

analysis of data bases that originate from survey and monitoring programs. The system in its final form would provide three levels of decision support. The first level involves simple data analyses including statistical trends and cluster analysis. The second level supports and utilizes mass balance computations, sulfate simulation models and the knowledge bases these model generate. The three level aims at the implementation of an expert system to investigate model scenarios,including resources-at-risk assessment, to establish the usefulness of remedial measures, with particular emphasis on confidence levels and model uncertainties.

At this point of development, a prototype of the system has been implemented for the IBM PC/XT or PC/AT microcomputer with color graphics, hard dic and full memory (640K). The software is primarily written in Lattice C and Microsoft C with support from the Halo Graphics package; some specific programs use BASICA and LOGO. The source data are of two types: terrestial and aquatic. The terrestial data are mainly stored as digitized maps for such soil chemistry information as cation exchange capacity and for such soil characteristics as soil type, soil depth, geology and vegetation. The basic geographical unit for these data is a subcatchment, but area-weighted averages for catchments and watersheds can be computed. The aquatic data, which consist mainly of measurements of flows and major ions, are collected at stream and lake stations also at the subcatchment level. Unlike the terrestial data, however, they are updated more frequently in time, e.g. monthly or yearly. In summary, therefore, the design of the data bases must take into account a strong geographical component and a time series component.

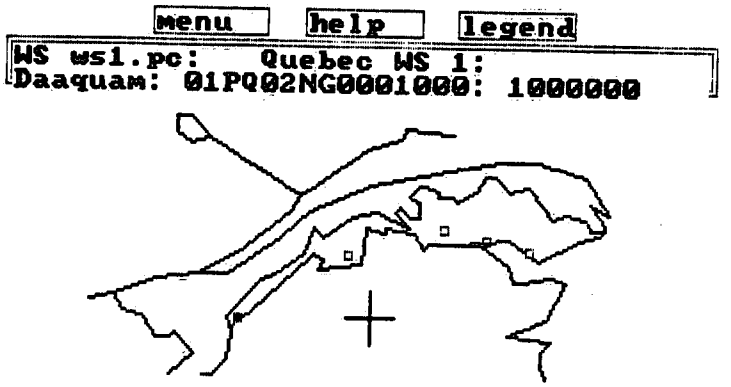

Figure 6. Watershed selection using RAISON-MICRO for the St. Lawrence Region, Quebec.

In the prototype, the data query language is featured as part of an intelligent front end, starting with a map of the main geographical area of interest, for example, the Province of Quebec. At the center of the map, the user is supplied with a cross-hair which can be moved with the cursor key or a mouse to any selected region (e.g., the St. Lawrence Region). Hitting the select key or the mouse button would replace the map by a large scale of the region (Fig.6). Further telescoping to the watershed is made by repeating the above procedure on the regional map. At the watershed level, the positions of the stations are displayed. Access to the data files at any particular station can be made by moving the cross-hair to that station. The digitized boundaries of the regions and watersheds can be entered via the PC or read from the mainframe computer. The format of the data base can be specified by schemas which are sufficiently general to suit the requirements for subsequent data analyses. Depending on the size of the records, the data can be entered through the PC or read from the mainframe computer files.

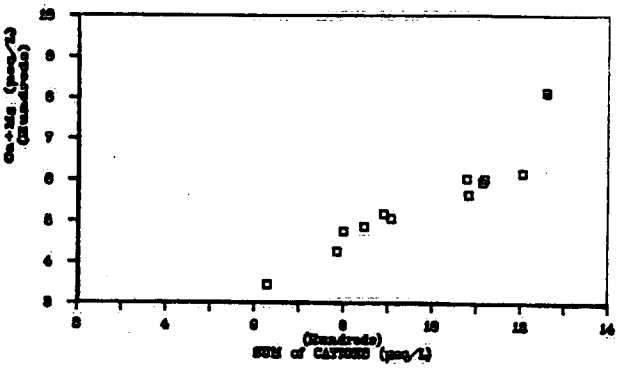

Figure 7. Observed $Ca^{++} + Mg^{++}$ versus sum of cations concentration at a Quebec watershed.

For operations with the data bases, the cross-hair is moved to the box labelled menu (Fig. 6) and a pull-down menu will be provided. Statistical analysis and some simple simulation model such as the cation denudation model by Thompson (9) can be performed directly with the data. These mathematical operations are executed using the spread sheet feature in the system, with a graphical option for displaying the results. Figure 7 shows a plot of the $Ca^{++} + Mg^{++}$ versus the sum of cations concentrations at a Quebec watershed, as an example of data display. This figure essentially shows that there is a linear relationship between $Ca^{++} + Mg^{++}$ and sum of cations so that the former, which originates mainly from cation exchange sites in the soil, is consistent with the latter, which is the pool of all positively charged ions in the stream water. Knowledge on the $Ca^{++} + Mg^{++}$ in space and time such as that shown in Fig. 4 can be utilized for further analysis of this data set. For example, the rate at which these ions are released from the soil can be related to the soil types, soil depths, residences times and the sulfate loading (5,6).

These relationships, once computed, can be entered as part of the data base and subject to more analysis. For instance, the computed cation exchange rates at all the stations of a particular watershed can be lumped into an areally weighted average for that watershed. This average value, together with the statistical information such as standard deviation, is entered into the data base of that watershed. Subsequently, the averaged cation exchange rates for all the watersheds can be retrieved and compared with, say, the data on soil sensitivity index. In particular, the spatial patterns of these two attributes can be compared at one glance, if a color coding schme is carefully chosen to represent them by a range of colors for each watershed on the regional map (Fig. 6). Of course, at that point, the patterns may or may not match, but RAISON-MICRO would have already provided

an efficient way of deciding quickly which idea or conceptual model works and which one does not. It is proposed (8) that such intellectual decision making processes can be either maintained by the user using RAISON-MICRO as a tool or, at the third level of implementation, by an expert system within RAISON-MICRO with capability of inference, pattern recognition and uncertainty analysis.

CONCLUSIONS

Results from a prototype show that the expert system approach can be applied to a number of practical problems in watershed acidification studies. Its main strength lies in the direct utilization of existing microcomputer technologies, particularly data base and computer graphics methodologies, in segregating the geographical attribute in the organization of the data base. The monitoring data can now be accessed and analysed and the results can be included as part of the data on the watershed level. This approach also facilitates the development of the linkage between the terrestial component and the aquatic component in the data.

However, there is the need to continue with the simulation modeling approach which has met with success in a number of intense studies of watersheds. Much still needs to be done to improve the models and to extract and summarize simulation results for building up the knowledge bases required for the expert system. The exact linkage of the two approaches has not been worked out, but it would emerge more clearly as the expert system is developed to a more mature level.

ACKNOWLEDGEMENT

The author is thankful to D.A. Swayne, A. S. Fraser, A.G. Bobba , D. S. Jeffries and F. C. Elder for useful discussions.

REFERENCES

1. Lam, D.C.L. and A.G. Bobba, "Modelling watershed runoffs and basin acidification", Hydrological and hydrogeochemical mechanisms and model approaches to the acidification of ecological systems, I. Johansson (ed.), Nordic Hydrological Programme, NHP-Report No. 10, Stockholm, Sweden, 1985,pp 205-215.
2. Christophersen,N.,H.M. Seip and R.F. Wright,"A model of stream chemistry at Birkenes, Norway",Water Resources Res.,18,1982,pp 977-996.
3. Gherini,S.A.,L.Mok,R.J.M. Hudson,G.F. Davis,C.W.Chen and R.A. Goldstein,"The ILWAS model: formulation and application", Water,Air, and Soil Pollution, 26, 1985, pp 425-460.
4. O'Keefe,R.,"Simulation and expert systems - a taxonomy and some examples", Simulation, 46, 1986, pp 10-16.
5. Bobba,A.G.,D.C.L. Lam,D.S.Jeffries,D.Bottomley,J.Y. Charette,P.J.Dillon and L. Logan,"Modelling the hydrological regimes in acidified watersheds", Water, Air, and Soil Pollution, 1986 (submitted). 9 p.
6. Lam, D.C.L., S. Boregowda, A.G. Bobba, D.S. Jeffries and G.G. Patry,"Interfacing hydrological and hydrogeochemical models for simulating acidification effects in Canadian watersheds", Water, Air, and Soil Pollution, 1986, (submitted) 10p.
7. Cosby,B.J.,G.M.Hornberger,J.N.Galloway and R.F. Wright,"Modeling the effects of acid deposition: assessment of a lumped parameter model and soil water and streamwater chemistry",Water Resources Res., 21, 1985, pp 51-63.
8. Swayne,D.A., A.S. Fraser, D.C.L. Lam and L. White, "Microcomputer analysis of aquatic effects due to acid precipitation: Part 1. Development of user software", Manuscript report, Dept. of Computer and Information Sciences,U. of Guelph, Guelph, Ontario, Canada, 1986, 7p.
9. Thompson,M.E.,"The cation denudation rate as a quantitative index of sensitivity of Eastern Canadian rivers to acidic atmospheric precipitation", Water, Air, and Soil Pollution, 18, 1982, pp 215-226.