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**MICRO-COMPUTER ANALYSIS OF AQUATIC
EFFECTS DUE TO ACID PRECIPITATION:
PART II. APPLICATIONS TO EASTERN CANADA DATA**

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MICRO-COMPUTER ANALYSIS OF AQUATIC EFFECTS
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ABSTRACT

Considerable progress has been made on the regional acidification analysis by intelligent systems on a microcomputer, acronymed RAISON-MICRO, particularly in the area of storage, manipulation and display of watershed data. The RAISON-MICRO system is designed to examine the relationships between terrain sensitivity indexes which assess susceptibility to acid deposition according to geologic and soil factors, and resultant aquatic chemistry. Interactive procedures making use of geographic indicators for region, watershed, and sampling site permit fast and concise data retrieval and data base editing. External computer systems including mainframes can be accessed for data transfer via menu driven protocols. Statistical analysis including frequency distributions and step-wise multiple regression analysis as well as mean, median, standard deviation and standard error can be produced on any of the data variables through a menu driven analysis package. The system is also able to seed data for specified watersheds to a programmable function library.

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RÉSUMÉ

Grâce au système d'information sur micro-ordinateur RAISON-MICRO, on a fait des progrès considérables dans l'analyse des données sur l'acidification selon les régions, surtout dans le domaine du stockage, de la manipulation et de l'affichage des données relatives aux bassins versants. Le système RAISON-MICRO est conçu pour étudier les relations entre les indices de sensibilité des sols, c'est-à-dire l'évaluation de la sensibilité des sols aux dépôts acides selon les caractéristiques géologiques et la composition de ces sols, et les réactions chimiques résultantes. La procédure d'interaction appliquée aux indicateurs géographiques sur les régions, les bassins versants et les sites d'échantillonnage accélère et condense les opérations d'extraction et de mise en forme des données. On peut accéder aux systèmes d'ordinateurs externes, y compris aux ordinateurs à grande puissance, grâce à des protocoles pilotés par menu. Grâce au progiciel d'analyse piloté par menu, on peut procéder à des analyses statistiques de toutes les variables, notamment les distributions de fréquence et les analyses à régressions multiples par étape, et calculer des moyennes, des médianes, des écarts-types ainsi que des erreurs-types. Le système peut également classer des données relatives à des bassins versants spécifiques dans une bibliothèque programmable.

INTRODUCTION

Acidification of the waters in eastern Canada has been identified as a priority in federal water policy research. One of the major obstacles to overcome in the analysis of the aquatic effects of acid deposition is the lack of geographical spatial representation for the aquatic chemistry component. This shortfall can be offset by linking the terrestrial database on land sensitivity to acid deposition with the aquatic chemistry in sampled regions.

The computer system, RAISON-MICRO has been developed to facilitate the analytical and linking phases of this analysis by providing both database and statistical interaction with a programmable function library. Various model functions of sensitivity can be programmed into the library. The first functional model to be implemented is the Cation Denudation Rate (CDR) model developed by Thompson (1982). RAISON-MICRO computes CDR values directly from the schema based database in spreadsheet form appending values to unused rows and columns.

Statistical analysis is accomplished in two modes, by direct application calls from the spreadsheet and by indirect calls to the statistical library. Further details on the technical aspects of this application are presented by Swayne et al. (1986).

The establishment of quantitative estimates for resources at risk due to the long range transport of atmospheric pollution is an exercise required as a prelude to governmental policy formulation. Only as confidence levels are assigned to the actual or to the perceived threat of ecological damage can realistic control measures be evaluated.

APPLICATION

The Province of Quebec has been segmented into hydrometric regions and watershed areas by the Water Survey of Canada. This application makes use of the segmentation as detailed in the hydrometric station maps produced by the Inland Waters Directorate (1978). Watershed areas represent the smallest unit of scale for analysis where each watershed represents the drainage basin for one major river. Additional rivers may be included within a watershed and where possible sampling is maintained on all major systems. The database for each watershed is composed of both lake and river data identified separately by station code. Our analysis includes both the lake and river component.

Access to the data base for a specific watershed is through a hierarchical procedure of map segments. The upper level entrance to the database presents a map of the Province of Quebec with hydrometric regions segmented (Fig. 1a). Selection of a particular region accesses the secondary level and presents a detailed map of the region with watersheds segmented (Fig. 1b). By selection with a cursor a specific watershed can be obtained at the third level. The depiction of the watershed displays the locations of the sampling points available in the database projected in position based upon the latitude and longitude of the site (Fig. 1c). An individual sampling station can be selected in like manner presenting the name and station identification number for the NAQUADAT data system (Demayo, 1970). When final selection is made, a call to the local database is made using pointer information from the geographic hierarchy into the bitree database selecting all data with the identified parameters.

Retrieval presents working data in a spreadsheet form by chemical compound or element. Each parameter has a row/column position and units identifier to facilitate manipulation and computation. Access to the statistical functions and library routines is by cursor selection from the spreadsheet. An example with test data is presented in Table 1.

Table 1 RAISON-MICRO spreadsheet format with CDR calculated and displayed. Asterisk (*) represents missing data.

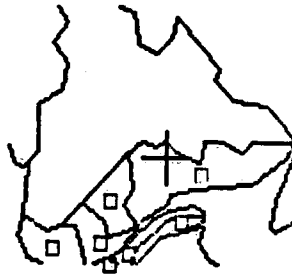
CDR	Runoff	Excess	Bases	Xchange	Std.Dev	Average	Log10	Antilog	Exit
									AVG. CDR: 11.86000
DATE	CDR	NA	K	CA	MG	CL	SO4	ALK	PH
85/08/14	11.9925	14.0000	8.00000	36.7145	3.00000	34.0000	4.00000	5.00000	7.00000
85/08/15	*	5.00000	8.00000	19.9053	6.90000	9.00000	10.0000	11.0000	7.00000
85/08/16	21.2416	18.2000	9.70000	23.4051	7.10000	9.00000	10.0000	11.0000	7.60000
85/08/17	4.38085	0.80000	7.90000	11.0000	6.50000	9.00000	10.0000	11.0000	6.80000
85/08/18	*	*	*	8.50000	3.00000	9.00000	10.0000	11.0000	7.00000
85/08/19	*	12.0000	*	7.50000	5.60000	9.00000	0.00000	1.00000	7.00000

Evaluation of the CDR model entails the computation of the following function.

$$CDR = \frac{ECAT \times \text{Discharge}}{\text{Basin Area}} \quad [1]$$

where: ECAT is the sum of the cations Na⁺, K⁺, Ca⁺², Mg⁺² in equivalent units.

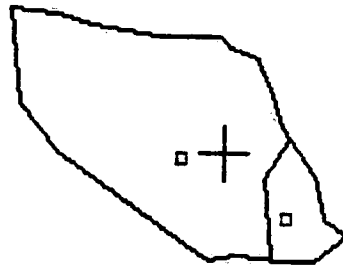
menu help legend
Map of Quebec



Choose the desired Region...

FIGURE 1 a): UPPER LEVEL HIERARCHICAL ENTRANCE TO RAISON-MICRO DATABASE

menu help legend
Quebec Region 4



Choose the desired Watershed...

FIGURE 1 b): SECONDARY LEVEL, REGIONAL SCALE IDENTIFIER TO RAISON - MICRO DATABASE

menu help legend
MS 2LC.pc: MS 2LC
2LC: 01QU02LC0027000:

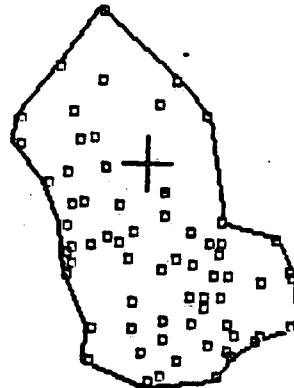


FIGURE 1 c): TERTIARY LEVEL, WATERSHED SCALE IDENTIFIER WITH STATION DISTRIBUTION POINTER TO DATABASE

The significance of the CDR function is that a measure of the rate of flow of cations out of a basin via discharge can be related to the flux of excess sulphate within the basin. Thus as the sulphate flux corrected for marine influence increases with the CDR remaining constant the pH range observed in a watershed will decrease. Stoichiometrically the relationship between excess sulphate and the CDR is derived from the relationship between the pH and the bicarbonate ion (HCO_3^-) expressed in terms of the partial pressure of carbon dioxide in surface waters.

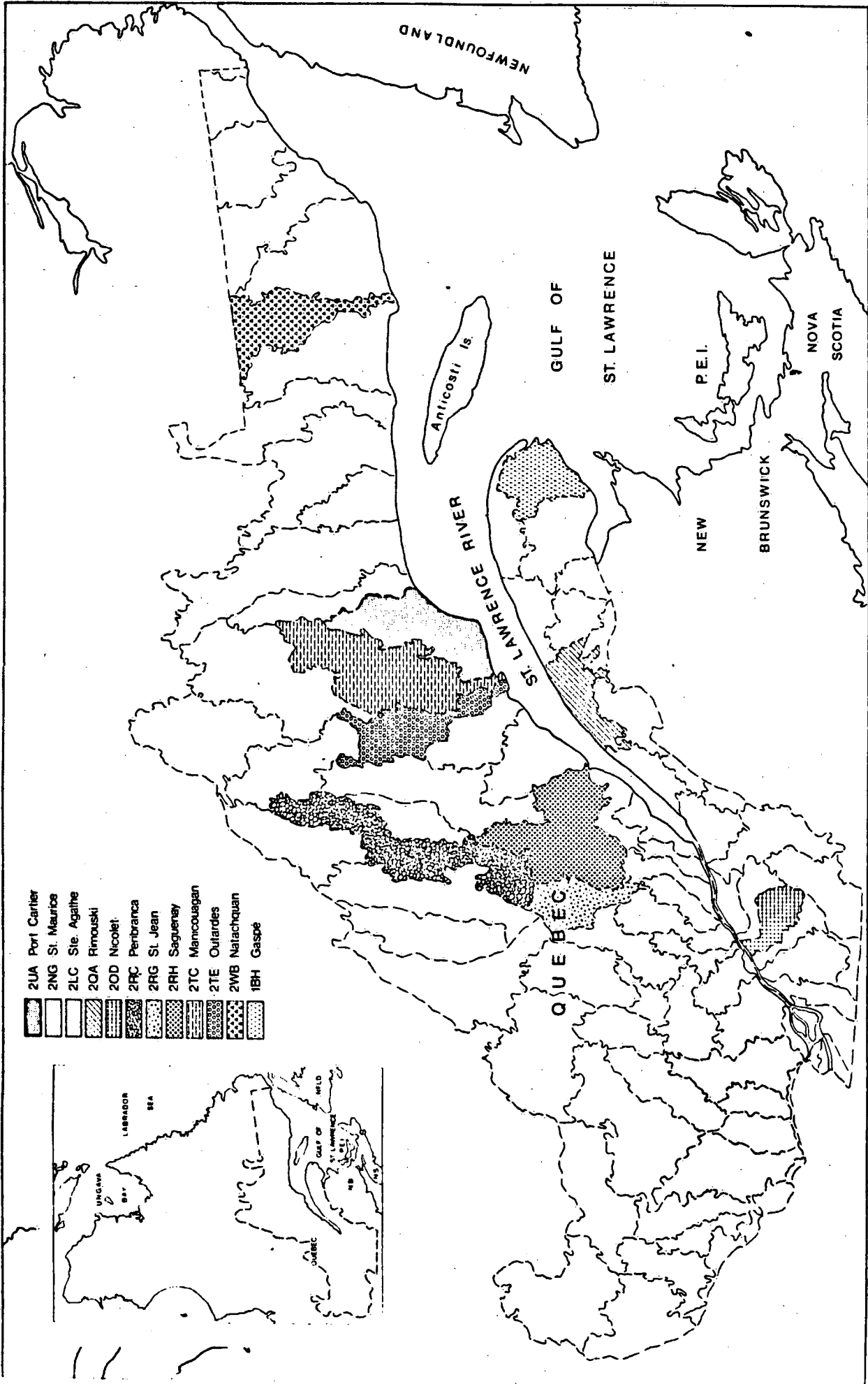
$$\text{pH} = \text{pK} + \text{pP}_{\text{CO}_2} - \text{pHCO}_3^- \quad [2]$$

It has been found that P_{CO_2} values for typical surface waters in southern Quebec are approximately ten times higher than atmospheric P_{CO_2} i.e. $10^{-2.5}$ atm in surface waters, $10^{-3.5}$ atm for the atmosphere (Fraser 1986). If the P_{CO_2} value of $10^{-2.5}$ atm is used to define the CDR model, equation [2] can be rewritten in a simpler manner

$$\text{pH} = 10.3 - \text{pHCO}_3^- \quad [3]$$

With this constraint the CDR model will predict acidic and alkaline fields divided by a 45° line from the origin at a pH of 5.1. The region below the 45° origin line represents the acidic field and above the line, the alkaline field. Based on this relationship, the nature of the CDR function should be a constant for a given watershed. Deviations from constancy are attributable to variations in basin geology where differing buffering conditions exist within the same regional watershed. Investigation has been undertaken in small individual basins to determine the constancy of the CDR in Nova Scotia rivers with favourable results (Thompson, 1985). On the regional scale, the possibility of deviations in the CDR are also related to cation exchange processes within the soils that regulate the relationship between deposited sulphate and the solution of calcium and magnesium in surface and groundwater. The "F-Ratio" (Wright 1983; Henriksen 1982) which describes this relationship will be evaluated using the RAISON system when the terrestrial sensitivity data is merged with the aquatic chemistry database.

Evaluation of chemical data related to acidification processes necessarily involves an analysis of all of the basin components. For the purposes of this study, 12 regions in southern Quebec have been identified as major sites (Fig. 2). For the purposes of discussion, region 2LC (Ste. Agathe) located north of Montreal will be used for detailed evaluation.



WATERSHED AREAS OF SOUTHERN QUEBEC

FIGURE 2: WATERSHED AREAS OF SOUTHERN QUEBEC, REGION 2LC (STE. AGATHE) IS TARGETED FOR DISCUSSION PURPOSES

Average discharge records for the Ste. Agathe watershed show the importance of the snowmelt episode in the spring. Average discharges of 2200 cfs rise to 12,800 cfs for short duration episodes (Fig. 3). The melting snow pack carries with it a large acid pulse into receiving waters. The importance of the acid shock upon the watershed ecosystem has been described by Lam et al. (1986). Elevated chemical concentrations and depressed pH levels in snowmelt water play a significant role in producing ecological stress on biological systems.

Sulphate is used in surface waters as a surrogate indicator of the acid loading from all sources. In the Ste. Agathe region a plot of calcium plus magnesium vs. alkalinity (Fig. 4) shows a clear excess of cations over anions. The anionic deficit is attributed to the presence of sulphate. A one to one relationship between calcium plus magnesium and alkalinity would indicate a system with little acid stress from depositional sulphate and negligible natural sources of sulphur such as pyrite in the basin.

CDR values estimated for the Ste. Agathe region show a nearly vertical distribution (Fig. 5). A distribution of this type may be interpreted as showing that the pH of the region is influenced by divergent geological types of mixed composition. Samples taken from the southern portion of the region are well buffered and have pH's above 6.6. The more sensitive region on the Laurentian Shield which is comprised primarily of granite and gneiss in the northern part of the region yields lower pH values and CDR's.

DISCUSSION

Application of the RAISON-MICRO system is contributing to our understanding of the chemical relationships at work between basin geology and water chemistry. As more information on soil sensitivity and terrain factors such as soil depth, texture and chemical composition become available, it will be possible to directly derive numerical relationships. At the present time, our analysis estimates that approximately 15% of the lakes studied in southern Quebec have alkalinity ratings of less than zero $\mu\text{eq/L}$. Negative alkalinities are indicative of acid stressed lakes and river systems (Henriksen and Kirkusmo 1982). Similarly, an additional 35% of lakes studied fall in the range for alkalinity between 0-50 $\mu\text{eq/L}$. This range represents systems that are strongly susceptible to acid deposition and must be carefully watched for signs of acid damage. The derivation of relational coefficients between water chemistry and land sensitivity for use in model development is the next area for activity under the RAISON system. Relational coefficients will be obtained to identify the time dependent parameterization of the F-factor in a predictive model of lake and watershed sensitivity.

DISCHARGE

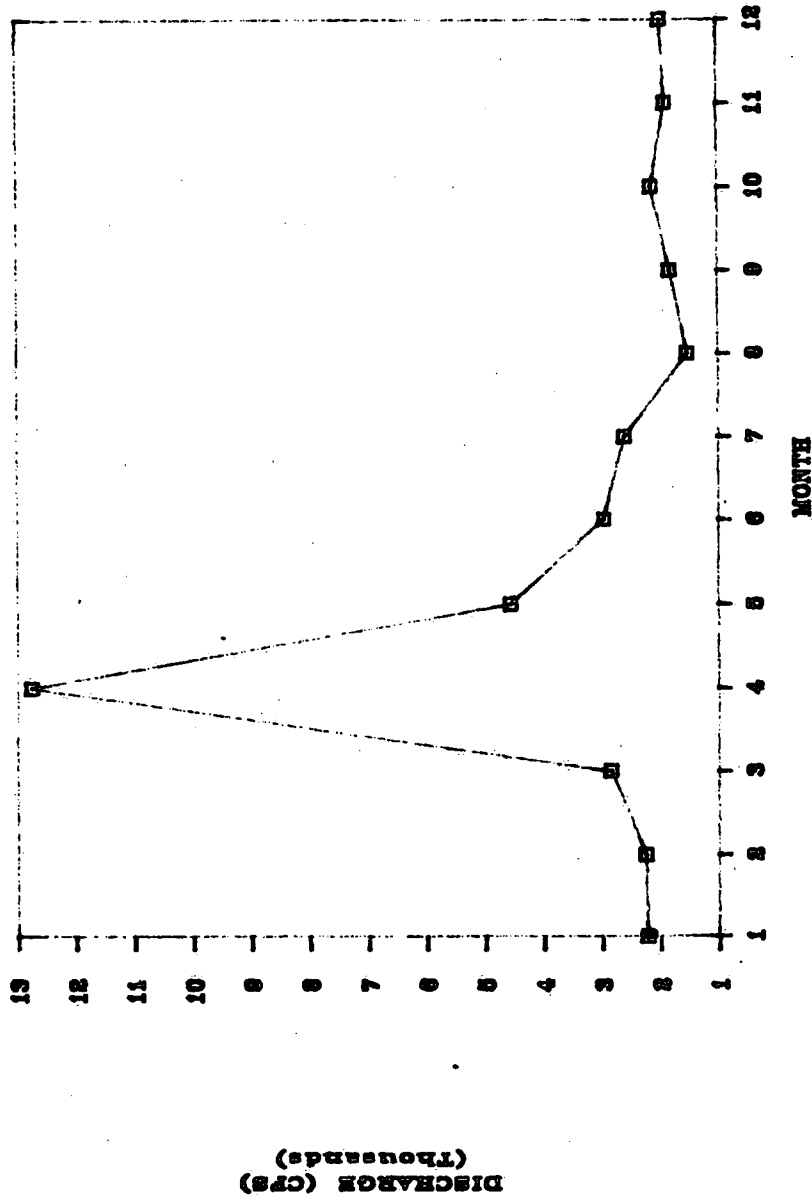


FIGURE 3: AVERAGE MONTHLY DISCHARGE FOR THE SITE. AGATHE WATERSHED

Ca+Mg VS.ALKALINITY

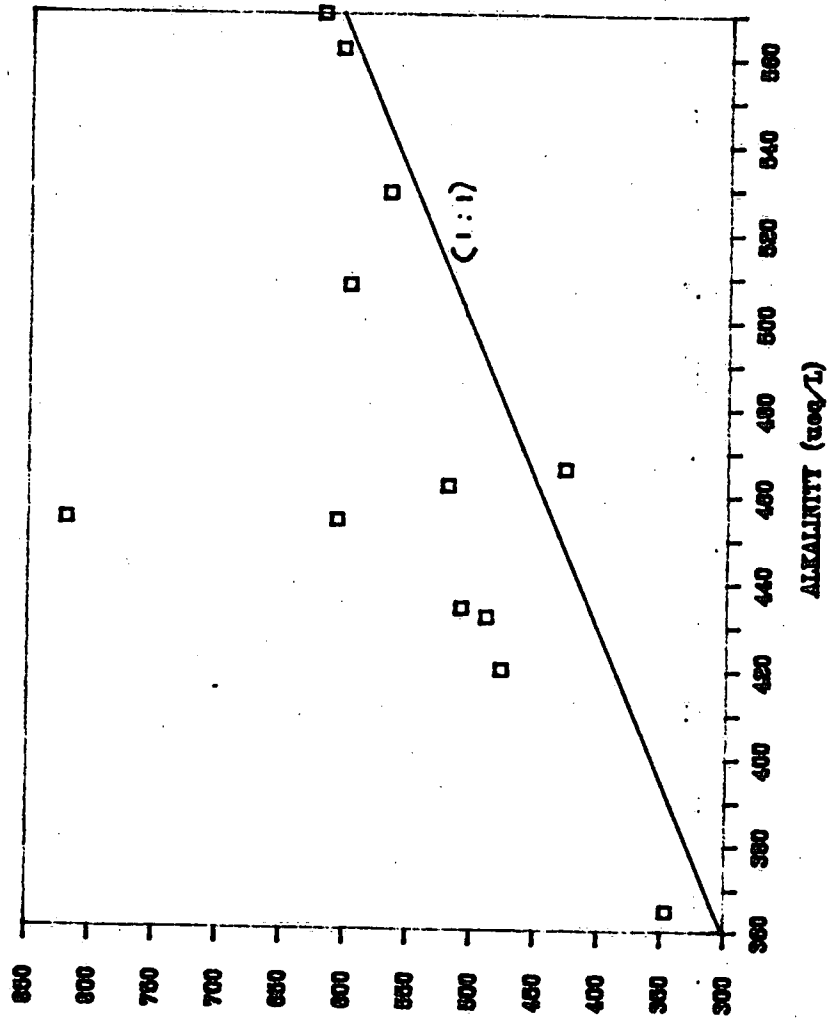


FIGURE 4: CALCIUM + MAGNESIUM vs ALKALINITY FOR THE STE. AGATHE REGION

CALCIUM + MAGNESIUM (useq/L)

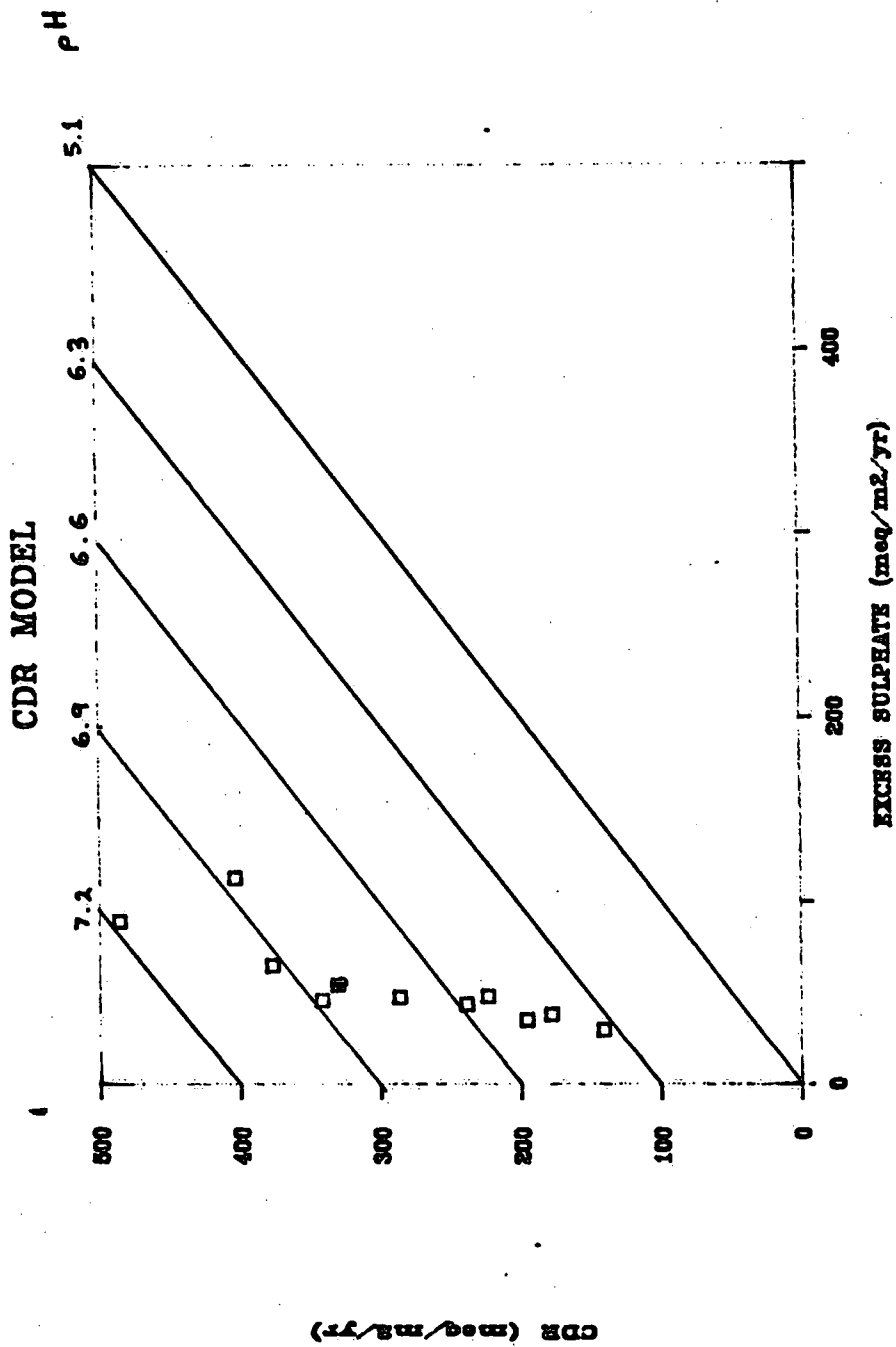


FIGURE 5: CDR MODEL PLOT FOR THE STE. AGATHE WATERSHED

As the RAISON system is able to enter new database information and to create a new knowledge base (i.e. CDR values), more computer memory is required when such data files expand. In terms of computing speed and read/write efficiency, it is more convenient to run RAISON on the IBM PC/AT than on the IBM PC/XT.

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