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THE DIGITAL GEOCHEMICAL ATLAS OF NEWFOUNDLAND

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ABSTRACT

A digital atlas is being prepared to operate as a 'turn-key' system on a personal computer that will extend the uses of the regional lake-sediment geochemical survey data for the Island of Newfoundland. The digital geochemical atlas runs in ArcView™, a software package that permits the display of the geochemical data at any scale and for any part of the island in several formats; element concentrations at individual sites as values or as proportional symbols, and interpolated geochemical surfaces as colour raster images or as line contours. Complete field and analytical data for each site, contained in a database file, can be displayed as symbols whose shape, size and colour can be controlled by the user. This database file can also be accessed through on-screen windows to display the complete geochemical profile of any sample site. Digital topography, solid and surficial geology and mineral-occurrence data are also included, allowing a user to query these databases from within the atlas and display specific selections of mineral occurrence, geological and topographic data with the geochemical data.

The digital geochemical atlas is envisaged as the first module of a comprehensive digital Geoscientific Atlas of Newfoundland and Labrador from the databases of the Geological Survey Branch and the Geological Survey of Canada. More detailed data from mineral-assessment files and university research projects also could be incorporated within such a system. The geoscientific database, when organized in this way, would be exportable to other Geographic Information Systems.

INTRODUCTION

Several geochemical atlases have been published over the past 20 years that present the results of systematic geochemical mapping over large areas (> 50 000 km²). The Geochemical Atlas of England and Wales (Webb, 1978) was perhaps the prototype of these folios of single-element distribution maps, which find application in mineral exploration, and mineral-resource and environmental assessment. Their utility is limited, however, by the choices that have to be made in order to produce them; selection of scale, amount of detail to be included, manner of presentation, etc. Although all have been produced from digital datafiles through computer-based cartographic techniques, the flexibility of application inherent in the digital data is lost once a final printed map is produced.

Geographic Information Systems (GIS) have been used for thorough analysis and interpretation of regional geochemical data, typically in large organizations. These start with 'raw' digital geochemical data to build what might be considered a digital geochemical atlas (usually with other geological and geophysical data as well). To be built successfully, this requires considerable computer resources and knowledge, one or both of which are commonly lacking in smaller organizations. Although more and more data are becoming available in digital form, their use is restricted to a relatively small number of GIS-capable groups.

Recently, some software companies have started to develop products that are specifically designed to query, manipulate and display spatial images and associated database information that have been pre-organized in a GIS. Moreover, some of these products are designed for personal computers and run in readily learned 'point-and-click' user-environments. The availability of this type of software, and of the necessary computer hardware, both at prices that are affordable to small organizations and individual professionals, offers geological surveys a new way to release the results of their geoscientific surveys. Also, it will provide these users with a powerful new tool to thoroughly interrogate the province's geoscientific database in pursuit of their own objectives. The development of widely available techniques for data analysis and integration, i.e., better use of existing data, is regarded by many explorationists as the next major breakthrough in exploration technology (Thompson, 1992). The regional geochemical data for Newfoundland has been chosen for the prototype for this new, publically available digital atlas format.

Geochemical mapping of the Island of Newfoundland (area 112,000 km²) is complete for 31 elements (Ag, As, Au,

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Table 1. Open files of gold and related elements in lake sediment from regional geochemical surveys of insular Newfoundland containing site-specific field observations and geochemical analyses

NTS AREA(S)	AUTHORS	YEAR	OPEN FILE No.
NTS 11O Port aux Basques	Davenport, P.H. and Nolan, L.W.	1987	NFLD/1582
NTS 2E Botwood	Davenport, P.H. and Nolan, L.W.	1988	2E/563
NTS 2D Gander Lake	Davenport, P.H., Nolan, L.W. and Hayes, J.P.	1988	2D/175
NTS 11P Burgeo	Davenport, P.H., Nolan, L.W. and Hayes, J.P.	1989a	11P/137
NTS 12H Sandy Lake	Davenport, P.H., Nolan, L.W., Hayes, J.P. and Liverman, D.G.E.	1989b	12H/1012
NTS 1M Belleoram	Davenport, P.H., Nolan, L.W., O'Brien, S.J. and Honarvar, P.	1990a	1M/312
NTS 12A Red Indian Lake	Davenport, P.H., Nolan, L.W., Honarvar, P. and Hogan, A.P.	1990b	12A/561
NTS 1N St. John's	Davenport, P.H., Nolan, L.W., Hayes, J.P. and Honarvar, P.	1990c	1N/499
NTS 1K Trepassey	Davenport, P.H. and Nolan, L.W.	1991a	1K/25
NTS 1L St. Lawrence	Davenport, P.H. and Nolan, L.W.	1991b	1L/136
NTS 2C & 2F Bonavista and Wesleyville	Davenport, P.H., Honarvar, P. and Bruce, P.A.	1993a	NFLD/2273
NTS 12B & 12G Stephenville and Bay of Islands	Davenport, P.H., Honarvar, P. and Bruce, P.A.	1993b	NFLD/2274
NTS 12I & 2L Port Saunders	Davenport, P.H., Honarvar, P. and Bruce, P.A.	1994a	NFLD/2275
NTS 2M & 12P St. Anthony and Blanc Sablon	Davenport, P.H., Honarvar, P. and Bruce, P.A.	1994b	NFLD/2276

Ba, Br, Ce, Co, Cr, Cs, Cu, Eu, F, Fe, Hf, La, Mn, Mo, Na, Ni, Pb, Rb, Sb, Sc, Sm, Ta, Tb, Th, U, W, Yb and Zn). Organic lake-sediment was employed as the sample medium because of its widespread availability and effectiveness for geochemical mapping as demonstrated in orientation studies (Hornbrook *et al.*, 1975). Collection of samples from over 17 000 sites was carried out using float-equipped helicopters between 1973 and 1981 by the Newfoundland Department of Mines and Energy. A survey of the St. John's area in 1990 (Christopher, 1991) completed the regional coverage in the province's principal urban region, leaving the National Parks as the only remaining unsampled tracts of any significant size.

The geochemical data are available in summary form as a set of colour single-element geochemical maps at 1:1 000 000 scale (Davenport *et al.*, 1994). The complete dataset can be obtained as sets of maps at 1:250 000 scale with explanatory notes and complete listings of field and analytical data in a series of 14 open files (Table 1).

SURVEY METHODS

Sampling

Grab samples of organic-rich sediment from the central basins of lakes were obtained with a tubular steel corer that was allowed to free-fall from the water surface. A sediment

Table 2. Nominal detection limits compared with observed medians and ranges in Newfoundland lake-sediment samples; for explanation of numerical superscripts to element abbreviations, see section on Preparation and Analysis

Element	Units	Nominal Det. limit	Median	Minimum	Maximum	Number
Ag[6]	ppm	0.2	<0.2	<0.2	5.6	18827
As[1]	ppm	0.5	5.2	<0.5	7460	17943
Au[1]	ppb	2	<2	<2	160	17943
Ba[1]	ppm	50	130	<50	5160	17943
Br[1]	ppm	1	39	<1	820	17943
Ce[1]	ppm	2	50	<2	1530	17943
Co[1]	ppm	2	8	<2	558	17943
Co[3]	ppm	2	8	<2	400	18827
Cr[1]	ppm	15	24	<15	6120	17943
Cs[1]	ppm	0.5	0.9	<0.5	31.3	17943
Cu[3]	ppm	2	12	<2	12380	18827
Eu[1]	ppm	0.5	0.6	<0.5	18.0	17943
F[9]	ppm	40	98	<40	135160	18827
Fe[1]	%	0.1	2.2	<0.1	53.5	17943
Fe[3]	%	0.01	2.1	<0.01	45.7	18827
Hf[1]	ppm	0.5	1.3	<0.5	71.9	17943
La[1]	ppm	1	22	<1	599	17943
Mn[3]	ppm	2	400	3	267000	18827
Mo[1]	ppm	5	<5	<5	661	17943
Mo[5]	ppm	2	4	<2	826	18624
Na[1]	%	0.05	0.2	<0.05	7.2	17943
Ni[1]	ppm	10	<10	<10	4250	17943
Ni[3]	ppm	2	8	<2	4980	18827
Pb[3]	ppm	2	7	<2	1290	18827
Rb[1]	ppm	5	10	<5	308	17943
Sb[1]	ppm	0.05	0.15	<0.05	22.1	17943
Sc[1]	ppm	0.1	4.3	<0.1	59.7	17943
Se[1]	ppm	3	<3	<3	48	17943
Sm[1]	ppm	0.1	4.4	<0.1	178	17943
Ta[1]	ppm	0.2	0.26	<0.2	3.1	17943
Tb[1]	ppm	0.5	0.69	<0.5	9.3	17943
Th[1]	ppm	0.1	3.7	<0.1	149.0	17943
U[8]	ppm	0.1	2.8	<0.1	2060	18686
U[1]	ppm	0.1	2.5	<0.1	2200	17943
W[1]	ppm	2	<2	<2	122	17943
Yb[1]	ppm	0.5	1.5	<0.5	77.5	17943
Zn[1]	ppm	50	<50	<50	22300	17943
Zn[3]	ppm	2	57	<2	19010	18827
LOI	%	0.01	33	0.1	99.9	18827

core, 10 to 20 cm long, was typically obtained from a depth of about 20 to 120 cm below the sediment-water boundary (the depth depending on the penetrability of the sediment and the water depth at the sample site). After discarding the top few centimetres, the remaining material was placed in a prenumbered, kraft-paper sample bag.

Preparation and Analysis

Samples were oven-dried at 40°C, disaggregated with a porcelain mortar and pestle and screened through a 180-μm stainless-steel sieve. Samples were analyzed by several techniques, some elements by two methods. To allow ready distinction between the different analytical methods, when data for an element are referred to, a numerical superscript is associated with the standard element abbreviation. These superscripts are explained below. The nominal detection limits for each element by each method are given in Table 2 together with their medians and ranges in the total sample set.

Atomic Absorption Methods (AAS)

These are based on methods developed for Canada's National Geochemical Reconnaissance program (Friske and Hornbrook, 1991). The analyses were carried out at the Geochemical Laboratory of the Department of Mines and Energy in St. John's.

Manganese, iron, cobalt, nickel, copper, zinc and lead (Mn^3, Fe^3, Co^3, Ni^3, Cu^3, Zn^3 and Pb^3) were determined on 1 g aliquots of sediment following digestion in 6 mL of a 4M HNO_3, 1M HCl mixture in a water bath at 90°C for 2 hours. For typical organic lake-sediment this digestion yields values that are > 80 percent of total content (Davenport *et al.*, 1993).

Molybdenum (Mo^5) was determined on 0.5 g aliquots of sample following digestion in 1.5 mL of hot, concentrated HNO_3 overnight at room temperature, and then in a water bath at 90°C for 30 minutes (Wagenbauer *et al.*, 1983). For typical organic lake-sediment this digestion yields Mo values that are close to its total content.

Silver (Ag^6) was determined on 0.5 g aliquots of sample following digestion in 2 mL of hot, concentrated HNO_3 in a water bath at 90°C for 2 hours (Wagenbauer *et al.*, 1983). For typical organic lake-sediment, this digestion yields Ag values that are close to its total content.

Gravimetric Analysis

Organic carbon content was estimated from the weight loss-on-ignition (LOI) during a controlled combustion, in which 1 g aliquots of sample were gradually heated to 500°C in air over a 3 hour period.

Potentiometric Analysis

Fluorine (F^9) content (total) was determined by fluoride ion-selective electrode (Wagenbauer *et al.*, 1983). The sample (0.25 g) was fused with 1 g of a 2:1 mixture of a Na_2CO_3-KNO_3 flux for 10 minutes in a nickel crucible, and the residue dissolved in 1 percent citric acid.

Neutron Activation, Delayed Neutron Counting (DNA)

Uranium (U^8) content (total) was determined on 1 g aliquots of samples at Atomic Energy of Canada Limited, Ottawa (1975 to 1978 and 1981), and at Nuclear Activation Services Limited, Hamilton (1979 and 1980). The samples were weighed and encapsulated in the Geochemical Laboratory of the Department of Mines and Energy in St. John's.

Instrumental Neutron Activation Analysis (INAA)

These analyses were carried out at Becquerel Laboratories Inc., Mississauga, Ontario (Davenport, 1988). Typically, about 10 g of sample were used for analysis, and the samples were weighed and encapsulated in the Geochemical Laboratory of the Department of Mines and Energy in St. John's. Total contents of the following elements were determined:

> *sodium, scandium, chromium, iron, cobalt, nickel, zinc, arsenic, bromine, rubidium, molybdenum, antimony, cesium, barium, lanthanum, cerium, samarium, europium, terbium, ytterbium, hafnium, tantalum, tungsten, gold, thorium and uranium* (Na^1, Sc^1, Cr^1, Fe^1, Co^1, Ni^1, Zn^1, As^1, Br^1, Rb^1, Mo^1, Sb^1, Cs^1, Ba^1, La^1, Ce^1, Sm^1, Eu^1, Tb^1, Yb^1, Hf^1, Ta^1, W^1, Au^1, Th^1 and U^1).

Quality Control

Data quality was monitored through the collection of site-duplicate samples at a frequency of 5 percent of the lakes sampled, the splitting of 1 sample in 20 during sample preparation to give laboratory duplicates, and the inclusion of bulk controls (both internal and national reference materials) also at a frequency of 5 percent throughout the analytical program. The controls measure the consistency of the calibration thoughout the extended period of analysis (1978 to 1992) and, from national reference materials, the accuracy of reported element levels. From the laboratory and site duplicates the analytical variance, and the combined sampling and analytical variance, respectively, have been estimated using the procedure of Garrett (1973). It is the relative size of the combined sampling and analytical errors with respect to the overall data variance that is important in assessing data quality. Table 3 presents the proportions of these combined errors as a percentage of total data variance for each element (and by each analytical method where more than one was employed). The proportion of combined errors should not exceed 20 to 25 percent for geochemical features to be well defined (Ramsey *et al.*, 1992; Garrett, 1969). Elements whose quality is rated as 'poor' in Table 3 are those where the analytical detection limit is close to or above the median level for the whole dataset (Table 2). In regions where these elements are locally above the overall background, however, their reproducibility is much better and their spatial distribution is adequately defined. These variance estimates are presented as 'data-quality' pie-charts with each colour-element-distribution image in the atlas.

ATLAS DESIGN

The digital atlas was conceived as a way to provide ready access to the extensive regional geochemical database for Newfoundland to all users, both geochemists and non-specialists. The large size and amount of detailed information in the database made it essential to employ a computer system that provides both database management and high-quality graphical display. The digital atlas was designed to allow data selection, manipulation and on-screen display at any scale in a variety of cartographic styles, as well as to enable the screen displays to be printed at useful scales as colour maps. Finally, the need to make the atlas widely available dictated that it be designed to operate on personal computers, ideally of both IBM compatible and Macintosh design, as well as being transportable to larger systems.

To a degree the organization of the geochemical data in this atlas is determined by the design of the computer system employed as the user-interface, but it is also strongly influenced by the structure and characteristics of the data themselves and the limits these impose on the meaningful presentation of the data. Data organization and the computer system are discussed here separately.

Table 3. Combined sampling and analytical errors as a percentage of overall data variance

Element	Sampling & analytical errors as percentage of overall data variance	'Quality rating'
Ag[6]	47	poor
As[1]	8	good
Au[1]	85	v. poor
Ba[1]	20	fair
Br[1]	10	good
Ce[1]	12	fair
Co[1]	15	fair
Co[3]	12	fair
Cr[1]	23	fair
Cs[1]	13	fair
Cu[3]	7	good
Eu[1]	45	poor
F[9]	12	fair
Fe[1]	9	good
Fe[3]	9	good
Hf[1]	25	fair
La[1]	7	good
Mn[3]	12	fair
Mo[1]	12	fair
Mo[5]	16	fair
Na[1]	7	good
Ni[1]	24	fair
Ni[3]	8	good
Pb[3]	14	fair
Rb[1]	21	fair
Sb[1]	19	fair
Sc[1]	7	good
Sm[1]	8	good
Ta[1]	30	poor
Tb[1]	12	fair
Th[1]	6	good
U[8]	10	good
U[1]	6	good
W[1]	20	fair
Yb[1]	23	fair
Zn[1]	25	fair
Zn[3]	9	good
LOI	15	fair

DATA

For convenience of description, the data contained in the atlas are broken down by source discipline (geochemical, geological, topographic, etc.), and then discussed by their attributes within a GIS. The emphasis of the atlas being geochemical, these data are discussed in some detail, and the geological and topographic information more briefly.

Geochemical Data

The characteristics and extent of the regional lake-sediment geochemical database were described in the previous section on Survey Methods. These are included in the atlas in four formats; 1) individual site values (together with UTM coordinates and field observations) in a database file, and interpolated geochemical surfaces derived from the site data as 2) colour raster images, 3) colour raster shaded-relief images and, 4) as line contours. The inclusion of the data in four ways significantly increases the size of the complete atlas, but is necessary to allow sufficiently flexible presentation at a variety of scales and in different layouts. Incidentally, it also permits the display of three elements at once.

Data Selection. There is some data redundancy because six elements were determined by two different methods having generally similar results, so to minimize the overall data size for the atlas, determinations by only one method per element are used for the colour raster and line-contoured data display formats. For these, the INAA data for Co, Fe, Mo, Ni, U and Zn are omitted because the AAS data (DNA data for U[8]) are available for more sites (Table 2) and, in most cases, have a better signal to noise ratio (Table 3). All determinations are included in the database file.

Database File of Site Data. The variables in this database (Table 4) include all analytical data as well as field observations and coordinates for all sample sites, together with the identity of the solid and surficial geological unit at each site from Colman-Sadd *et al.* (1990) and Liverman and Taylor (1990), respectively. Site and laboratory duplicates have been removed to minimize file size.

Colour Raster Images. These display the variation of each element as a continuously variable surface interpolated from the individual site values, where colour change from blue through green and yellow to red reflects increasing concentration levels.

For the elements whose 'quality' (Table 3) was rated as fair or good, the colour surface was created in following four steps.

1) Individual values (log-transformed) were interpolated to an initial grid with 1.5 by 1.5 km cells from the irregularly distributed sample sites using an iterative, minimum-curvature, surface-fitting technique (Geosoft, 1991).

2) A 3 by 3 cell (4.5 by 4.5 km) moving adapted trimmed mean (ATM) filter was then applied to smooth the grid and remove extreme values (Chork and Mazzucchelli, 1989; Davenport *et al.*, 1991).

3) The ATM grid was smoothed further by applying a 'Hanning' filter (a 3 by 3 weighted moving average filter).

4) The smoothed 1.5 by 1.5 km grid was interpolated to a 0.6 by 0.6 km grid for final plotting using the Geosoft (1991) routine 'BIGRID'.

Table 4. Variables included in database file of geochemical data, digital geochemical atlas of Newfoundland

1. Sample ID	2. NTS sheet (1:50 000)
3. Solid geological unit	4. Surficial geological unit
5. Ag[6], Silver, ppm, by AAS	6. As[1], Arsenic, ppm, by INAA
7. Au[1], Gold, ppb, by INAA	8. Ba[1], Barium, ppm, by INAA
9. Br[1], Bromine, ppm, by INAA	10. Ce[1], Cerium, ppm, by INAA
11. Co[1], Cobalt, ppm, by INAA	12. Co[3], Cobalt, ppm, by AAS
13. Cr[1], Chromium, ppm, by INAA	14. Cs[1], Cesium, ppm, by INAA
15. Cu[3], Copper, ppm, by AAS	16. Eu[1], Europium, ppm, by INAA
17. F[9], Fluorine, ppm, by ISE	18. Fe[1], Iron, %, by INAA
19. Fe[3], Iron, %, by AAS	20. Hf[1], Hafnium, ppm, by INAA
21. La[1], Lanthanum, ppm, by INAA	22. Mn[3], Manganese, ppm, by AAS
23. Mo[1], Molybdenum, ppm, by INAA	24. Mo[5], Molybdenum, ppm, by AAS
25. Na[1], Sodium, %, by INAA	26. Ni[1], Nickel, ppm, by INAA
27. Ni[3], Nickel, ppm, by AAS	28. Pb[3], Lead, ppm, by AAS
29. Rb[1], Rubidium, ppm, by INAA	30. Sb[1], Antimony, ppm, by INAA
31. Sc[1], Scandium, ppm, by INAA	32. Sm[1], Samarium, ppm, by INAA
33. Ta[1], Tantalum, ppm, by INAA	34. Tb[1], Terbium, ppm, by INAA
35. Th[1], Thorium, ppm, by INAA	36. U[8], Uranium, ppm, by DNA
37. U[1], Uranium, ppm, by INAA	38. W[1], Tungsten, ppm, by INAA
39. Yb[1], Ytterbium, ppm, by INAA	40. Zn[1], Zinc, ppm, by INAA
41. Zn[3], Zinc, ppm, by AAS	42. LOI, Loss-on-ignition, %, GRAV
43. Lake area, ha	44. Lake depth, m
45. Vegetation type	46. Water level
47. Sediment colour	48. Sediment composition
49. Site contamination	50. UTM easting, m (all zone 21)
51. UTM northing, m (all zone 21)	52. Solid geology, code
53. Surficial geology unit	

For the elements whose 'quality' (Table 3) was assessed as poor or very poor the colour surface was created in a similar manner, but a greater degree of smoothing was applied at Step 2, where a 5 by 5 cell (7.5 by 7.5 km) moving ATM filter was used rather than the 3 by 3 cell. The larger filter window results in averaging over a 56 km² cell rather than a 20 km² cell, giving a much more generalized interpolated surface. For these elements in particular, a further problem is the significant degree of truncation of the data by the analytical detection limit. Values less than detection were arbitrarily assigned a value of half of the detection limit prior to interpolation. For ATM windows containing cells with these assigned values, the resulting 'means' can no longer be considered fully rational measures of concentration. The deviation from a rational scale of measurement increases as the proportion of assigned values to measured values in the filter window increases, but the computed 'means' will maintain at least an ordinal relationship. Contour intervals have been continued below the detection limit of several elements for the colour images because information can be extracted even at these low levels, but the images in this range should be treated as showing only relative or semi-quantitative variations.

To emphasize the geochemical relief in these colour surfaces, a second set of shaded-relief images was created by adding shadows computed as if the geochemical surfaces were landscapes illuminated by the sun shining from the northwest. This was accomplished using a program CS_bil (Kilfoil, *this volume*). The shaded-relief images are more generalized than the unshaded colour images because of the use of a 5 by 5 cell (7.5 by 7.5 km) moving ATM filter at Step 2. Local detail is downplayed whereas larger spatial trends are emphasized, especially northeast-oriented regional features with illumination from the northwest.

Line Contours (Isopleths). The continously variable concentration surfaces for each element have been prepared for display also as line contours. The surface interpolation was as described in the previous section for the colour images, with an additional smoothing step involving one pass of a Hanning filter over the 0.6 by 0.6 km grid following step 4. Up to 21 contours at the 98th, 95th, 90th, 85th, 80th, 75th, 70th, 65th, 60th, 55th, 50th, 45th, 40th, 35th, 30th, 25th, 20th, 15th, 10th and 5th percentiles were drawn. The actual number of contours drawn depends on the degree of truncation of the data by the analytical detection limit; no contours are drawn below an element's detection limit.

Geological Data

Interpretation of geochemical data is much more incisive when it is done within a geological framework. As a solid geology base for the atlas, the 1:1 000 000-scale geological map of Newfoundland (Colman-Sadd *et al.*, 1990) was digitized and included. Surficial geology in digital format was taken from the compilation of Liverman (unpublished data), based on the 1:500 000-scale map by Liverman and Taylor

(1990). Finally, the database from MODS/PC version 1.1 (Stapleton and Parsons, 1993) is used as the source of mineral-occurrence data for the atlas.

Topographic Data

The Universal Transverse Mercator topographic base for the atlas is from the 1:1 000 000-scale International Map of the World series sheets NK/NL-21/22 (St. John's) and NM-21/22 (Corner Brook) obtained in digital form from the Surveys and Mapping Division, Newfoundland Department of Environment and Lands. Three separate layers are included for streams and rivers, lakes, and coastline. A reference grid of 1:50 000-scale National Topographic System (NTS) sheets is also provided.

In addition, a digital terrain model (Nolan and Bruce, *this volume*) is included as shaded-relief raster images in both colour and greytones. This model was computed from the digital topographic contour data from 1:250 000-scale National Topographic System maps from the Surveys and Mapping Branch, federal Department of Natural Resources.

THE DISPLAY SYSTEM

The display system for the geochemical atlas comprises a commercial computer software package installed on a suitably equipped computer. Together, they can be termed a Geographic Information System (GIS) that provides a tool to explore the databases of the geochemical atlas, display all or part of its contents, ask questions, display or save the results and pass information or graphics to other applications.

Software

The software package ArcView™, developed by ESRI® (Environmental Systems Research Institute Inc., California), has been chosen as the 'display engine' for the geochemical atlas. ArcView™ displays combinations of spatially related data organized in ARC/INFO® format. ARC/INFO®, also an ESRI® product, is a fully fledged GIS, which can accept data in a wide variety of input formats, whereas for ArcView™ the data must be already organized and formatted to be usable. Once organized, however, ArcView™ is a very flexible tool for screen displays of almost every conceivable combination of the different data types included in a geochemical atlas, and for on-screen querying of the related database files. The main characteristics that led us to choose ArcView™ were as follows:

1) it runs on personal computers (IBM compatible or Macintosh) and has an intuitive 'point-and-click' style;

2) it embraces well the design functions of the geochemical atlas in allowing very flexible data selection and a wide range of options for customizing the display of selected information to meet the user's objectives and personal preferences;

3) it promises to allow (in version 2) the user to print, as custom colour maps at standard scales, the selected geochemical and related data; and

4) it costs less than $1000, which puts it within reach of most potential users of the geochemical atlas.

Hardware

ArcView™ operates on IBM-compatible computers under Microsoft® Windows™, and although it will operate on computers with an Intel® 386 CPU, a 486DX33 or equivalent CPU with 16 Mbytes of RAM and an SVGA colour monitor is recommended as the minimum practical configuration. Because it is intended to release the atlas as a CD-ROM, a CD-ROM drive should also be part of the basic system hardware. The files of the graphical layers are typically 1 to 5 Mbytes in size, so a fast computer having a large hard-disc drive is recommended. ArcView™ versions are also available for Macintosh computers and for computers with UNIX operating systems.

Data Organization and Structure

Not only must the data be in ARC/INFO® format to be usable in ArcView™, careful thought must be given to their organization to allow the full flexibility of the system to be utilized. From an operational viewpoint, there are two main data formats:

1) raster images such as satellite imagery or, in this atlas, the colour raster images of element distributions; and

2) points, lines and closed polygons that have not only geographic coordinates but also associated data that are stored in a linked database file.

Raster Images (Figures 1 and 2) can be displayed only one at a time in each window, as adding a second image obscures the first. Operations in ArcView™ for raster images are restricted to choice of window and scale selection though zoom functions. Table 5 gives a list of the raster images included in the initial version (1.0) of the atlas.

Data Layers with Associated Database Files can be superimposed on raster images or on one another. The number displayed at once is limited practically by the display becoming too cluttered to be legible. From a data-organization and display standpoint, the data layers in the geochemical atlas in this category will be considered under the headings of point datasets, line datasets, and polygon datasets.

Point Datasets. There are two database files of point data included in the atlas, the complete geochemical database (Table 4) and the MODS/PC database (Stapleton and Parsons, 1993). Site locations and associated data can be displayed (Figure 3) using a wide selection of symbol shapes, sizes and colours. All data at a site can be displayed by pointing to it

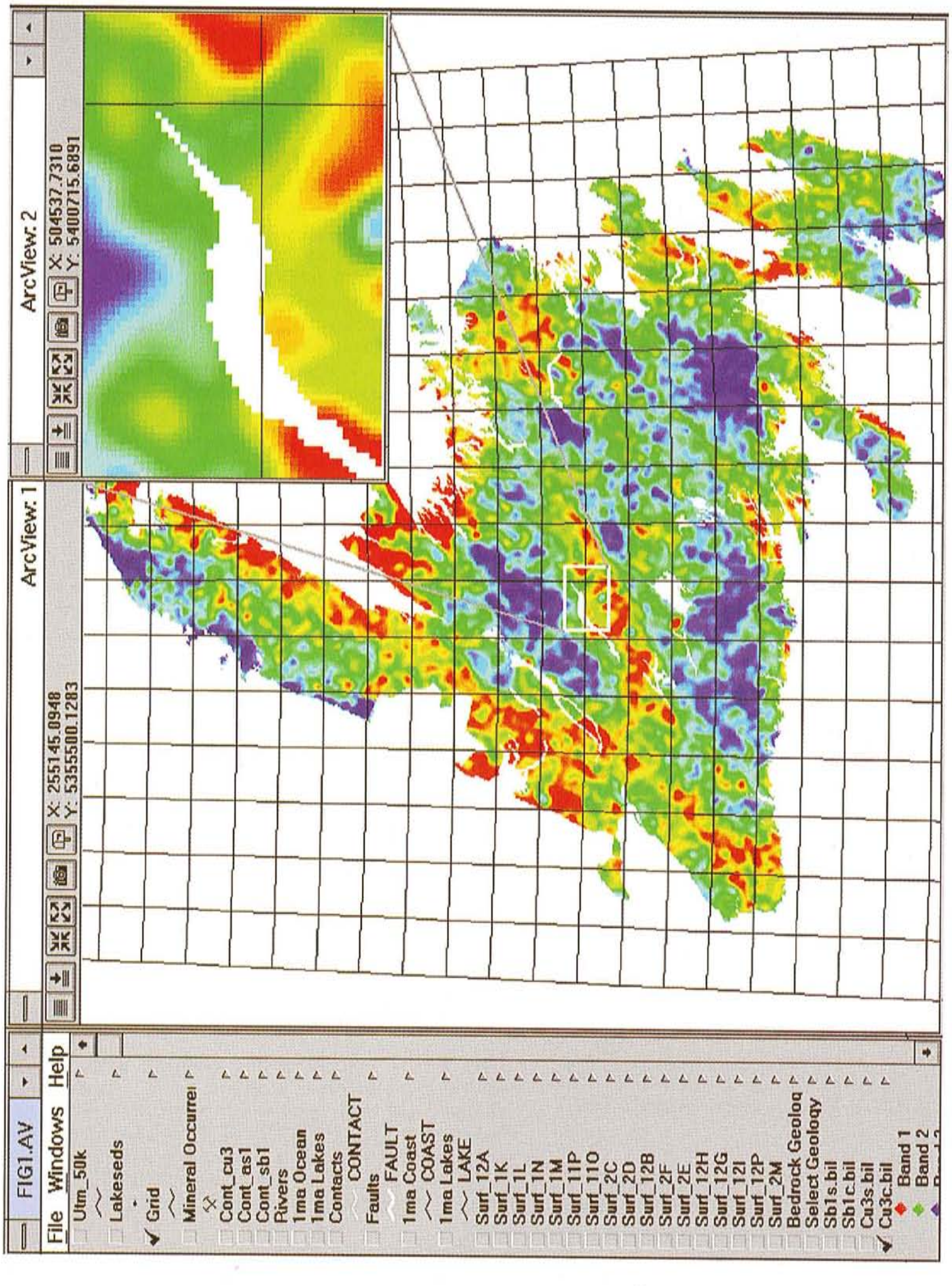

Figure 1. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu^3) in lake sediment as a colour contour image (raster image); right window shows a zoom of the area outlined in the complete image. Left window is a menu of the data layers included in the Atlas and is used to select layers for display (the tick next to 'Cu3s.bil' indicates that this layer only is being displayed).*

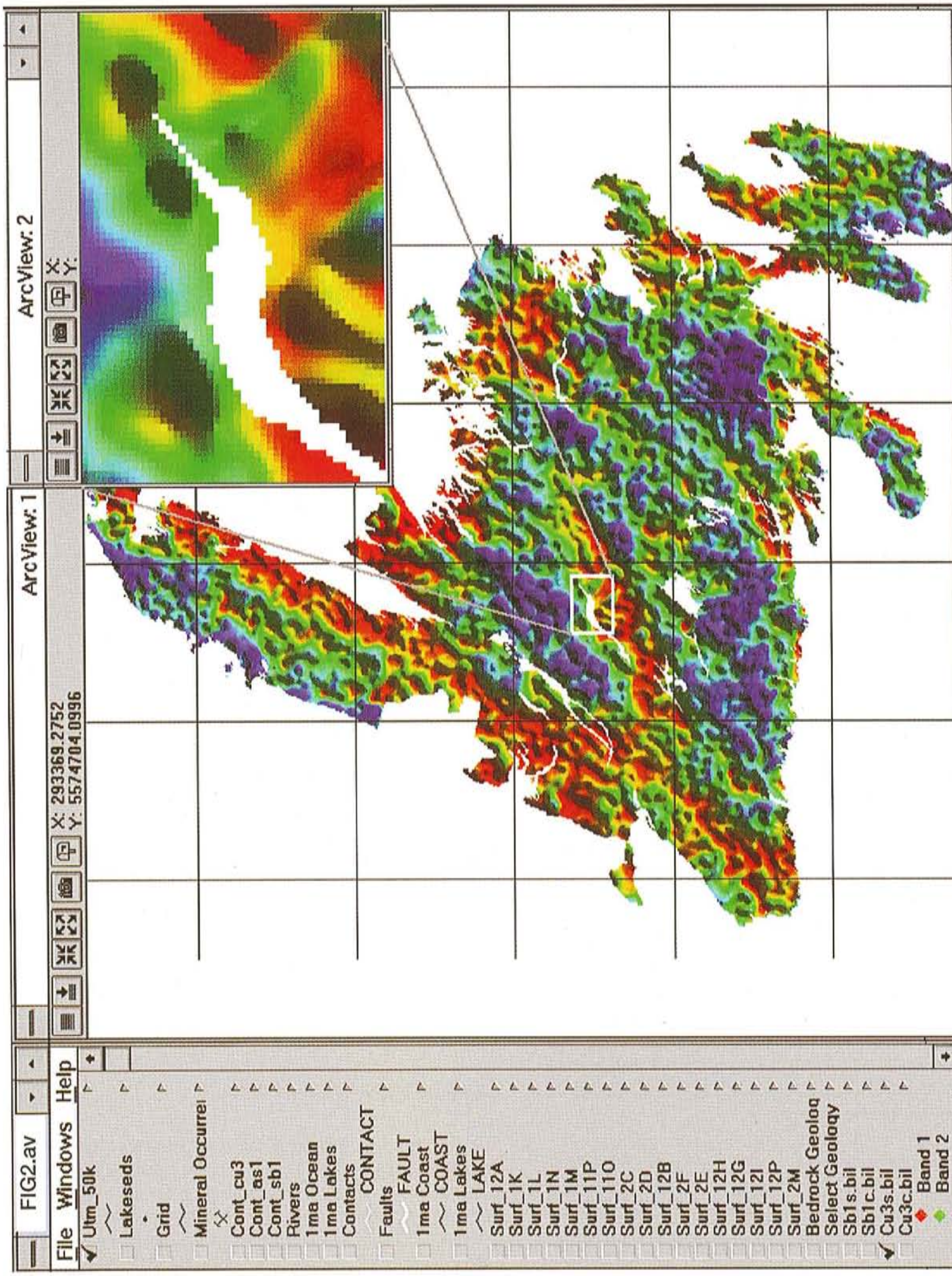

Figure 2. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu³) in lake sediment as a colour shaded-relief raster image (layer Cu3s.bil); right window shows a zoom of the area outlined in the complete image.*

Table 5. Raster Images included in the digital geochemical atlas of Newfoundland, version 1.0

1. Ag[6], Silver, colour contour image	2. Ag[6], Silver, colour shaded-relief image
3. As[1], Arsenic, colour contour image	4. As[1], Arsenic, colour shaded-relief image
5. Au[1], Gold, colour contour image	6. Au[1], Gold, colour shaded-relief image
7. Ba[1], Barium, colour contour image	8. Ba[1], Barium, colour shaded-relief image
9. Br[1], Bromine, colour contour image	10. Br[1], Bromine, colour shaded-relief image
11. Ce[1], Cerium, colour contour image	12. Ce[1], Cerium, colour shaded-relief image
13. Co[3], Cobalt, colour contour image	14. Co[3], Cobalt, colour shaded-relief image
15. Cr[1], Chromium, colour contour image	16. Cr[1], Chromium, colour shaded-relief image
17. Cs[1], Cesium, colour contour image	18. Cs[1], Cesium, colour shaded-relief image
19. Cu[3], Copper, colour contour image	20. Cu[3], Copper, colour shaded-relief image
21. Eu[1], Europium, colour contour image	22. Eu[1], Europium, colour shaded-relief image
23. F[9], Fluorine, colour contour image	24. F[9], Fluorine, colour shaded-relief image
25. Fe[3], Iron, colour contour image	26. Fe[3], Iron, colour shaded-relief image
27. Hf[1], Hafnium, colour contour image	28. Hf[1], Hafnium, colour shaded-relief image
29. La[1], Lanthanum, colour contour image	30. La[1], Lanthanum, colour shaded-relief image
31. Mn[3], Manganese, colour contour image	32. Mn[3], Manganese, colour shaded-relief image
33. Mo[5], Molybdenum, colour contour image	34. Mo[5], Molybdenum, colour shaded-relief image
35. Na[1], Sodium, colour contour image	36. Na[1], Sodium, colour shaded-relief image
37. Ni[3], Nickel, colour contour image	38. Ni[3], Nickel, colour shaded-relief image
39. Pb[3], Lead, colour contour image	40. Pb[3], Lead, colour shaded-relief image
41. Rb[1], Rubidium, colour contour image	42. Rb[1], Rubidium, colour shaded-relief image
43. Sb[1], Antimony, colour contour image	44. Sb[1], Antimony, colour shaded-relief image
45. Sc[1], Scandium, colour contour image	46. Sc[1], Scandium, colour shaded-relief image
47. Sm[1], Samarium, colour contour image	48. Sm[1], Samarium, colour shaded-relief image
49. Ta[1], Tantalum, colour contour image	50. Ta[1], Tantalum, colour shaded-relief image
51. Tb[1], Terbium, colour contour image	52. Tb[1], Terbium, colour shaded-relief image
53. Th[1], Thorium, colour contour image	54. Th[1], Thorium, colour shaded-relief image
55. U[8], Uranium, colour contour image	56. U[8], Uranium, colour shaded-relief image
57. W[1], Tungsten, colour contour image	58. W[1], Tungsten, colour shaded-relief image
59. Yb[1], Ytterbium, colour contour image	60. Yb[1], Ytterbium, colour shaded-relief image
61. Zn[3], Zinc, colour contour image	62. Zn[3], Zinc, colour shaded-relief image
63. LOI, loss-on-ignition, colour contour image	64. LOI, loss-on-ignition, colour shaded-relief image
65. Terrain Model, grey-tone shaded-relief image	66. Terrain Model, colour shaded relief image

with the mouse to bring the database information to a new window on the screen. By applying ArcView™ functions to the database files, sites for which the data meet user-specified criteria can be selected for display as symbols, and the user can also control the symbol shapes, sizes and colours.

Line Datasets. There are several layers of line data, each with its associated database file (Table 6). The database information can be displayed on the screen by pointing to a line with the mouse (Figure 4) and, as for the point data, can be used to control what line work is displayed and how (line type, thickness and colour).

Polygon Datasets. These are the lakes from the topographic data, the solid geology units from the 1:1 000 000-scale geological map (Colman-Sadd *et al.*, 1990), and surficial geology units from Liverman and Taylor (1990). Each set of information, e.g., surficial geology, comprises a layer of polygons, in which each polygon has an associated record in a database file containing attribute information such as its classification and area (Figure 5). This information can be used in ArcView™ as selection criteria so that, for example, only specific surficial geological units are displayed based on their class or area or both. These attributes can also be used to control colouring of the polygons, and for the geological layers, the unit classifications provide an abbreviated legend. Having the geological information as both a polygon layer and as a line or vector layer allows surficial and solid geology to be displayed together (Figure 5), in addition to geochemical data layers.

DISCUSSION

DESIGN CONSIDERATIONS

The atlas is designed for both extensive overviews at small scales as well as more intensive evaluations of smaller areas at larger scales. Portraying geochemical data at scales varying by two or more orders of magnitude from about 1:5 000 000 to 1:50 000 precludes the use of a single display format. When displaying the whole island on screen, neither proportional symbols at sample sites nor line contours produce legible displays. However, the colour images of the geochemical data (Figures 1 and 2) show the overall element distributions well, especially the shaded-relief images, which employ the greatest degree of generalization. At intermediate

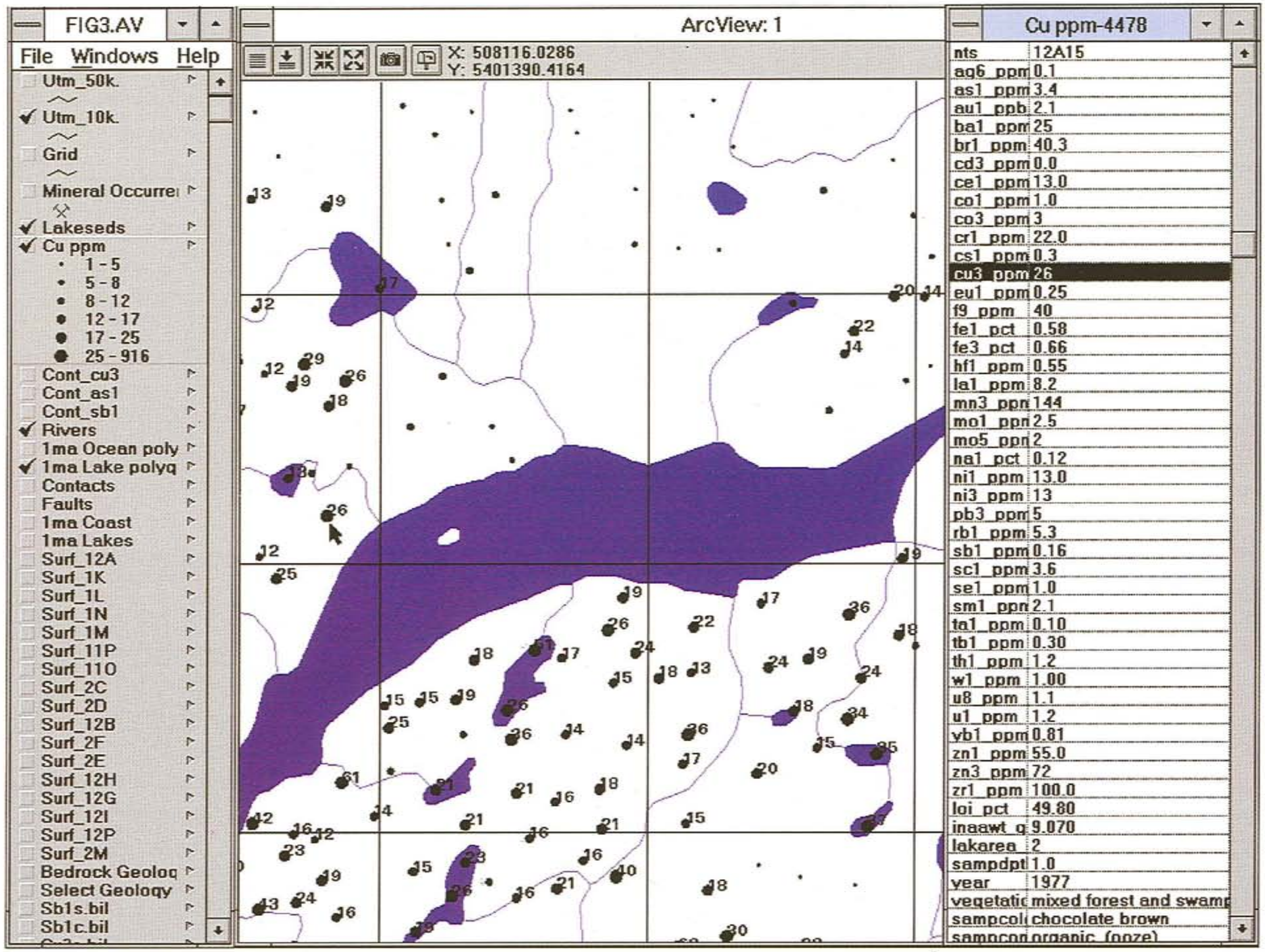

Figure 3. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu^3) in lake sediment as proportional symbols with site values in ppm and the drainage network of major lakes and rivers (in blue) for the area displayed in the right window of Figures 1 and 2 (32 km from north to south). Window on the right lists the geochemical data from the database file for the site marked by the arrow. The layer-control menu at left includes a key that relates the symbol sizes to Cu concentrations. Six classes of concentration level based on equal percentiles of values were selected in ArcView™ and the symbols automatically sized from small to large with increasing concentration.*

Table 6. Line datasets and associated database file in the digital geochemical atlas of Newfoundland

LAYER NAME	VARIABLES IN DATABASE FILE
Geochemical line contours for	
As[1], Ba[1], Br[1], Ce[1], Co[3], Cr[1], Cs[1], Cu[3], F[9], Fe[3], Hf[1], La[1], Mn[3], Mo[5], Na[1], Ni[3], Pb[3], Rb[1], Sb[1], Sc[1], Sm[1], Ta[1], Tb[3], Th[1], U[8], W[1], Yb[1], Zn[3], LOI.	Contour labels in ppm & as percentiles, length
Geological boundaries	Type (i.e., fault or unspecified), length
Streams and rivers	Length
Coastline	Length

scales, line contours become readable, particularly if the user selectively reduces the number of contours displayed through ArcView™ database commands. The colour images remain useful at these intermediate scales also, especially when combined with selected line contours (Figure 6). For detailed evaluation, the shaded-relief images are usually too generalized to be useful. In this situation, the contoured data combined with proportional symbol plots of the individual site values provide a clear portrayal of local geochemical variation. Individual element values can be posted at each site, either for all sites or for those where the values exceed some threshold (Figure 7). At this scale too it is often useful to bring up the complete information on a particular site from the database file.

The inclusion of the geochemical data in four formats also allows the user to take full advantage of the data query, selection and display capabilities of ArcView™ to gain a real understanding of the data and to fully interact with it. Although the raster images and some 'scenes' such as the coloured geology map are ready to display when called, the user can exercise a wide degree of control over how the different data layers are combined. Geochemical variation might be emphasised over geology by displaying a colour-contoured element distribution over geological line work in white (Figure 6). Alternatively the geology might be emphasized by displaying it in colour with the geochemical variation shown as line contours (Figure 8), or the surficial geology might be displayed in colour, with solid geology line work in black and geochemical variation as proportional symbols in red (Figure 9).

A full-featured GIS would permit the computation of the different styles of geochemical data display for the atlas from a single file of the basic data. In practice, this calls for a set of fairly complex data-transformation routines, all of which require the careful selection of parameters to produce, for example, satisfactory contour plots. Moreover, with large datafiles such as the regional geochemical database for Newfoundland, considerable computational resources are required. It would be impractical to create the interpolated geochemical layers in real time on a personal computer or even a workstation, and the knowledge and experience required to create satisfactory coverages would also be a major impediment to many would-be users of the data. The atlas is intended for general use, not exclusively for geochemists. The preparation of the geochemical layers by geochemists for query and display in ArcView™ has resulted in an easy to use but powerful and flexible tool for the general user and specialist alike that works well on a personal computer. The atlas will be released on CD-ROM, from which the parts of interest can be copied to the user's hard disc for faster retrieval.

LIMITATIONS OF VERSION 1

The initial version of this atlas has been prepared using release 1.0 of ArcView™ which imposes some limitations. The most serious limitation is the difficulty of plotting screen displays. In many cases, when a user has built a display of the information required to meet a particular objective, a hard copy at a standard scale is the most useful product. At present this can be accomplished only by exporting an ESRI graphics file to ARC/INFO® if a raster layer is part of the image.

A second limitation is its inability to link the separate database files to select on combinations of criteria from two or more of them. For example, to select for display all lake-sediment sites over granitic rocks, the user cannot link the database containing legend information for the polygons from the solid geology map with the database containing the geochemical site data. Rather, the geological information must be included within the geochemical database file (Table 3), so databases must be created with this type of selection in mind from the outset. This complicates design and also results in data redundancy. It is expected that these problems will be addressed in future releases of ArcView™.

Another set of limitations results from the geological and topographic reference information included. Just as several formats for the geochemical data are needed to allow effective display over a wide range of scales, so too for other types of data. For this initial version, only the solid and surficial geology and topographic data that were readily available in digital form are included. At larger scales, the inadequacy in the degree of detail in the solid geology and topographic data in particular become evident. As they become available in digital form, additional layers of more detailed information may be added. Despite these limitations, the atlas is regarded as a major step forward in the release of the geochemical information in a revolutionary format.

UPDATES

The comments of users will be important in improving the content and design of this atlas. For the geochemical database, coverages for additional elements will be added as the data become available. Mercury data will be added in 1994, and data for Li, Be, Mg, Al, P, K, Ca, Ti, V, Ga, Sr,

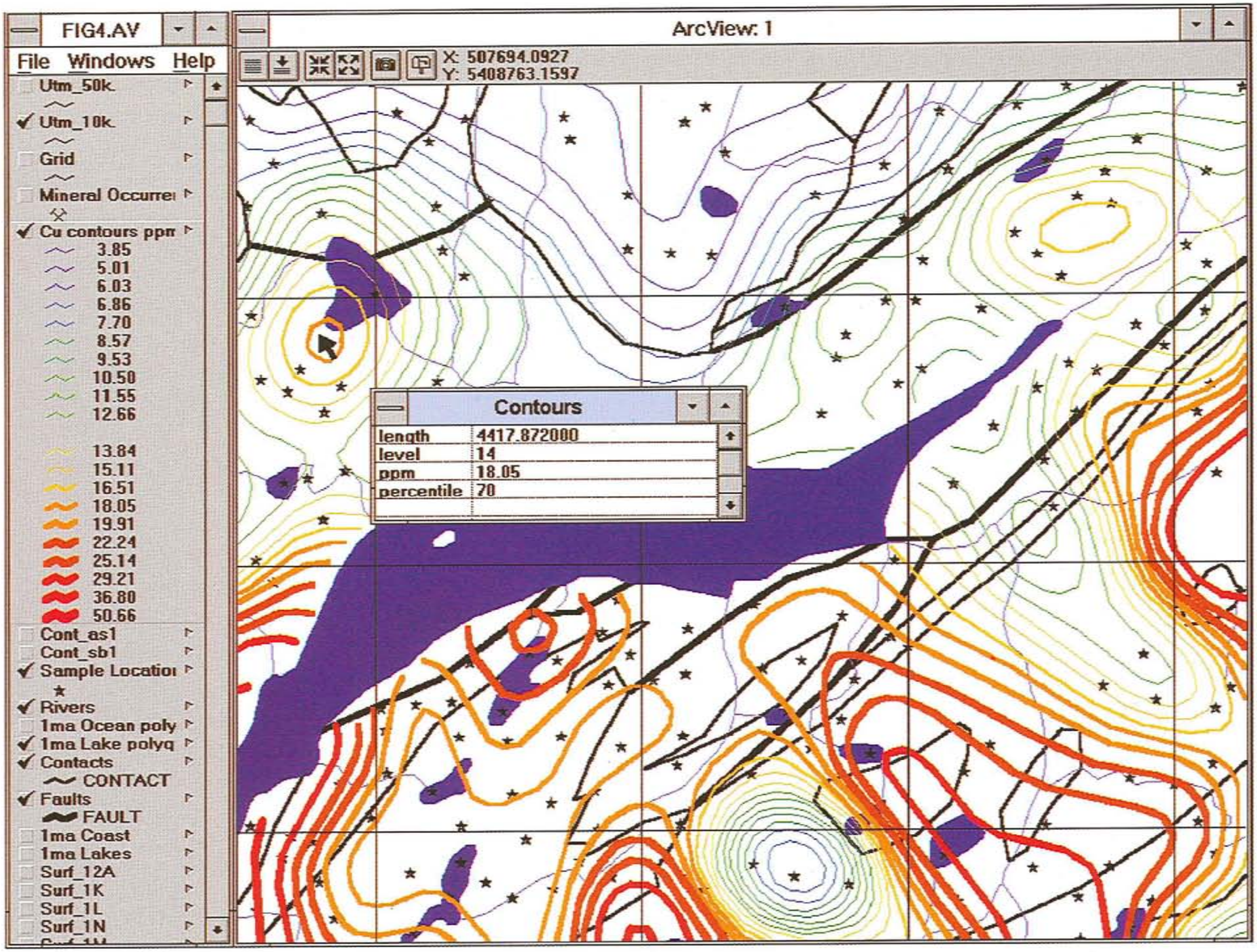

Figure 4. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu³) in lake sediment as line contours plotted on solid geology (in black, faults and contacts) and drainage (in blue) for the area displayed in Figure 3 (32 km from north to south). The Cu contours or isopleths were created in GEOSOFT at 5 percentile increments from the 5th to the 95th percentile and at the 98th percentile, and ArcView™ used to portray them with continuous variations in thickness and colour between blue (low) and red (high). The window on the right lists the attributes for the contour marked by the arrow from the associated database file that indicates that it is the 90th percentile or at 29.2 ppm Cu. The layer-control menu at left includes a key that relates the contour appearance to Cu concentration.*

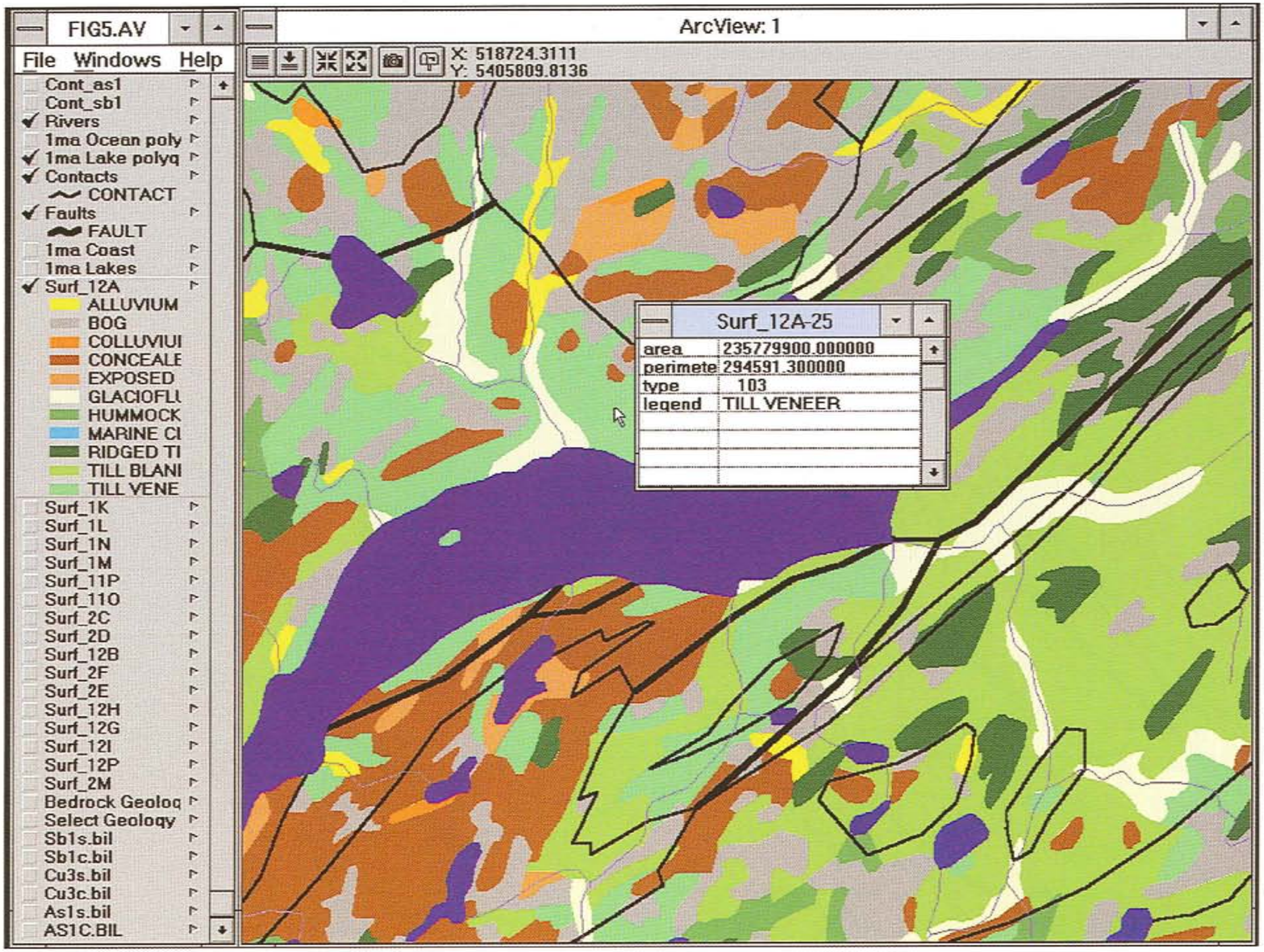

Figure 5. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing surficial geology in colour, with solid geology as black lines (faults and contacts) and drainage in blue, for the area displayed in Figure 3 (32 km from north to south). The window on the right lists the surficial geology legend from the database file for polygon marked by the arrow (till veneer). The layer-control menu at left includes an abbreviated legend for the surficial geology units.*

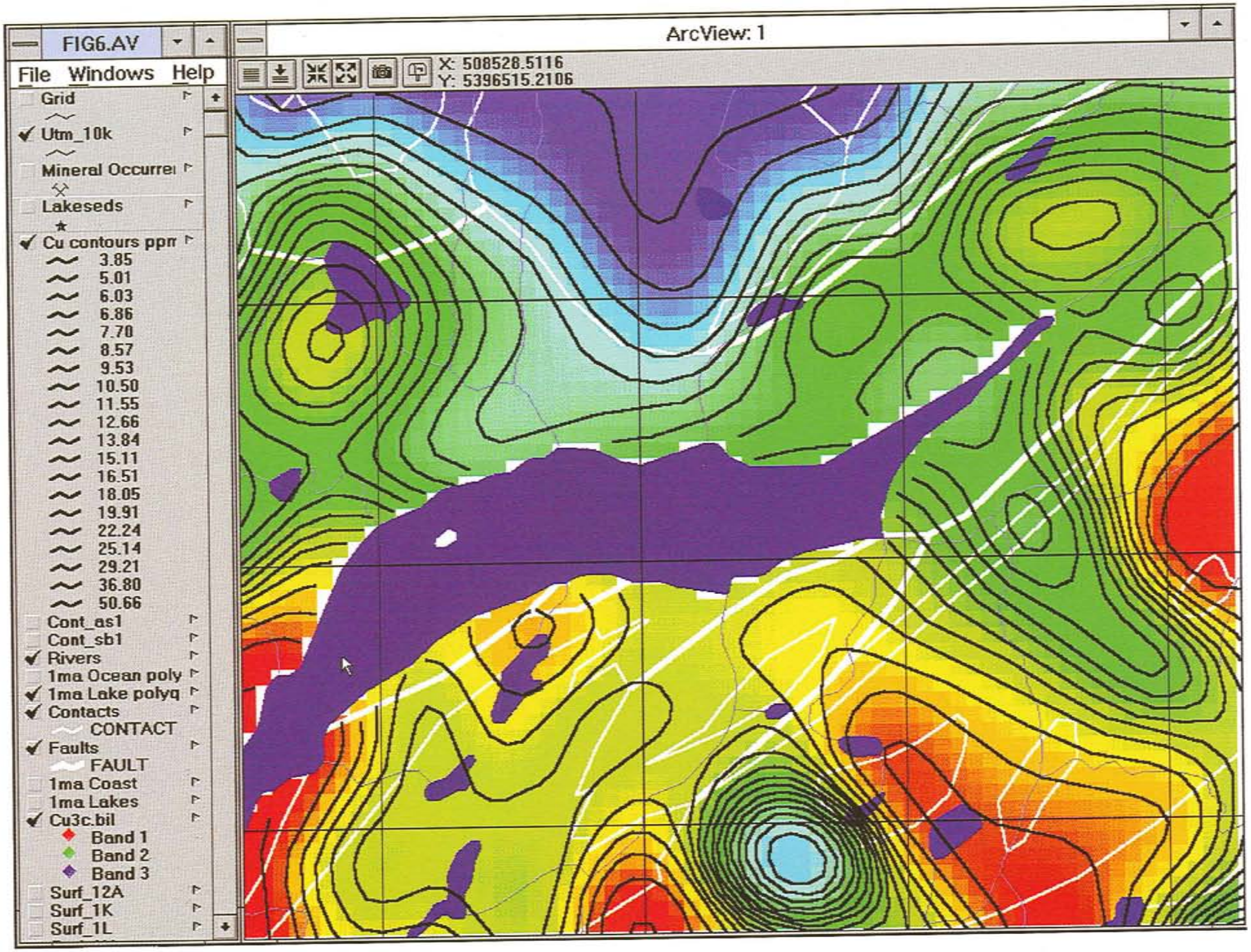

Figure 6. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu^3) in lake sediment as line contours (in black) and as a colour contour image with solid geology (faults and contacts) in white and drainage in blue, for the area displayed in Figure 3 (32 km from north to south). The layer-control menu at left includes a key for Cu contour levels.*

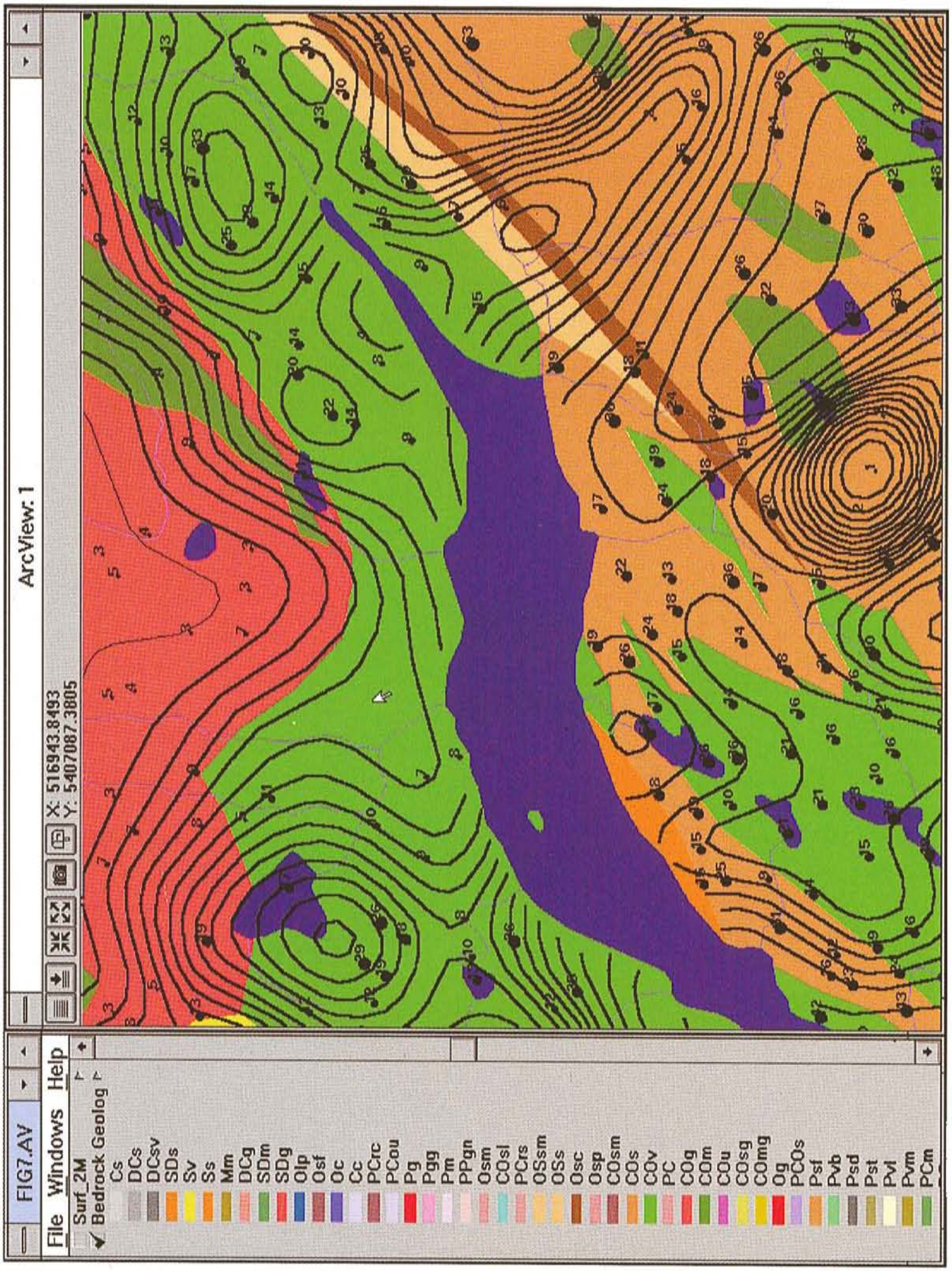

Figure 7. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu^3) in lake sediment as line contours (in black) and as proportional symbol plots (with values posted) displayed on the solid geology in colour and drainage in blue, for the area displayed in Figure 3 (32 km from north to south). The layer-control menu at left includes an abbreviated legend for the solid geology units.*

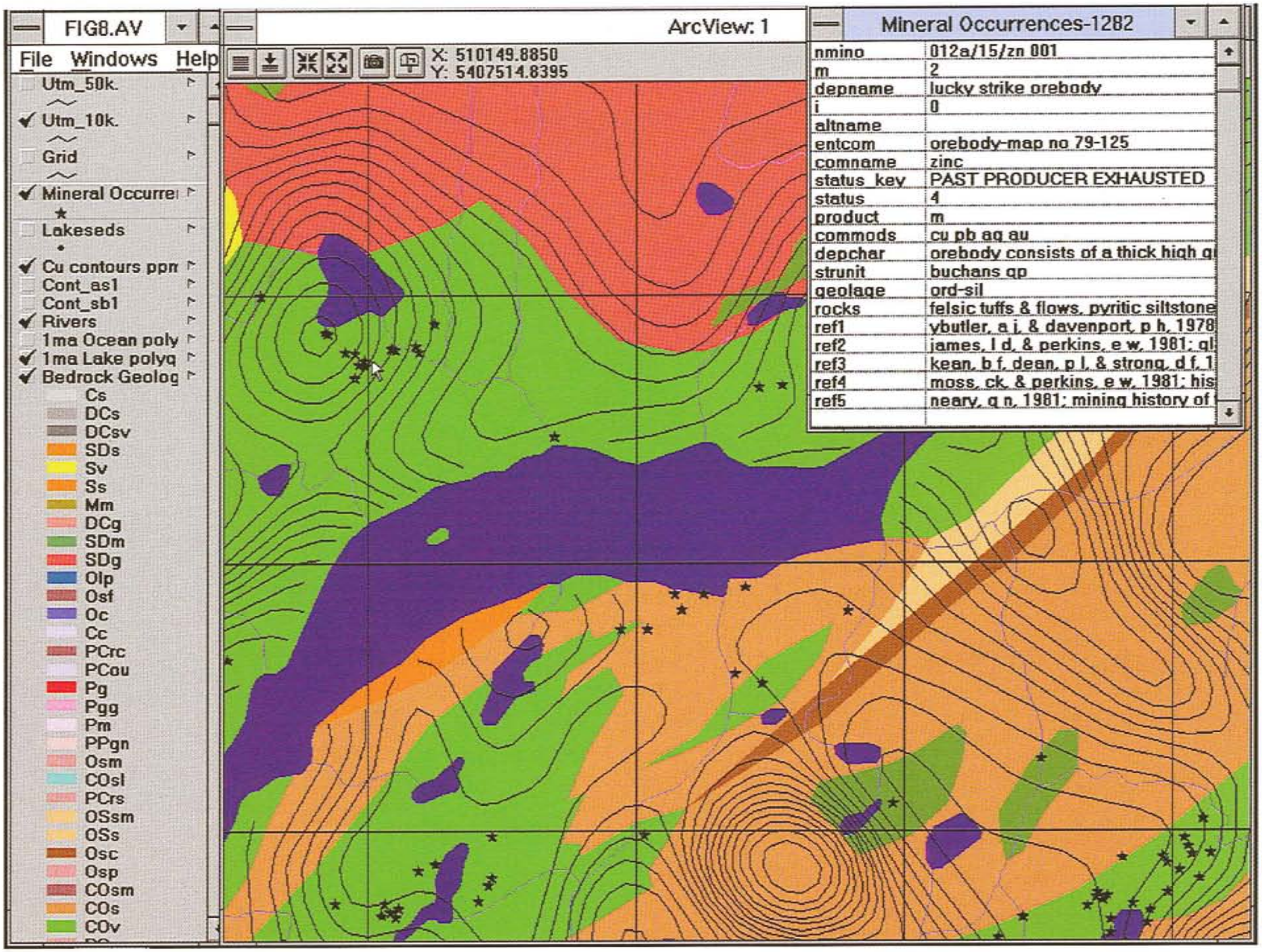

Figure 8. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu³) in lake sediment as line contours (in black) displayed on the solid geology in colour with Cu occurrences from the MODS/PC database and drainage in blue, for the area displayed in Figure 3 (32 km from north to south). The window on the right lists the MODS/PC information from the database file for the occurrence marked by the arrow (Lucky Strike Mine). The layer-control menu at left indicates the layers turned on for display; mineral occurrences (in this cases only those with Cu were selected through ArcView™), rivers, lma lakes (together making up the drainage network displayed), and solid geology (with part of the abbreviated legend shown).*

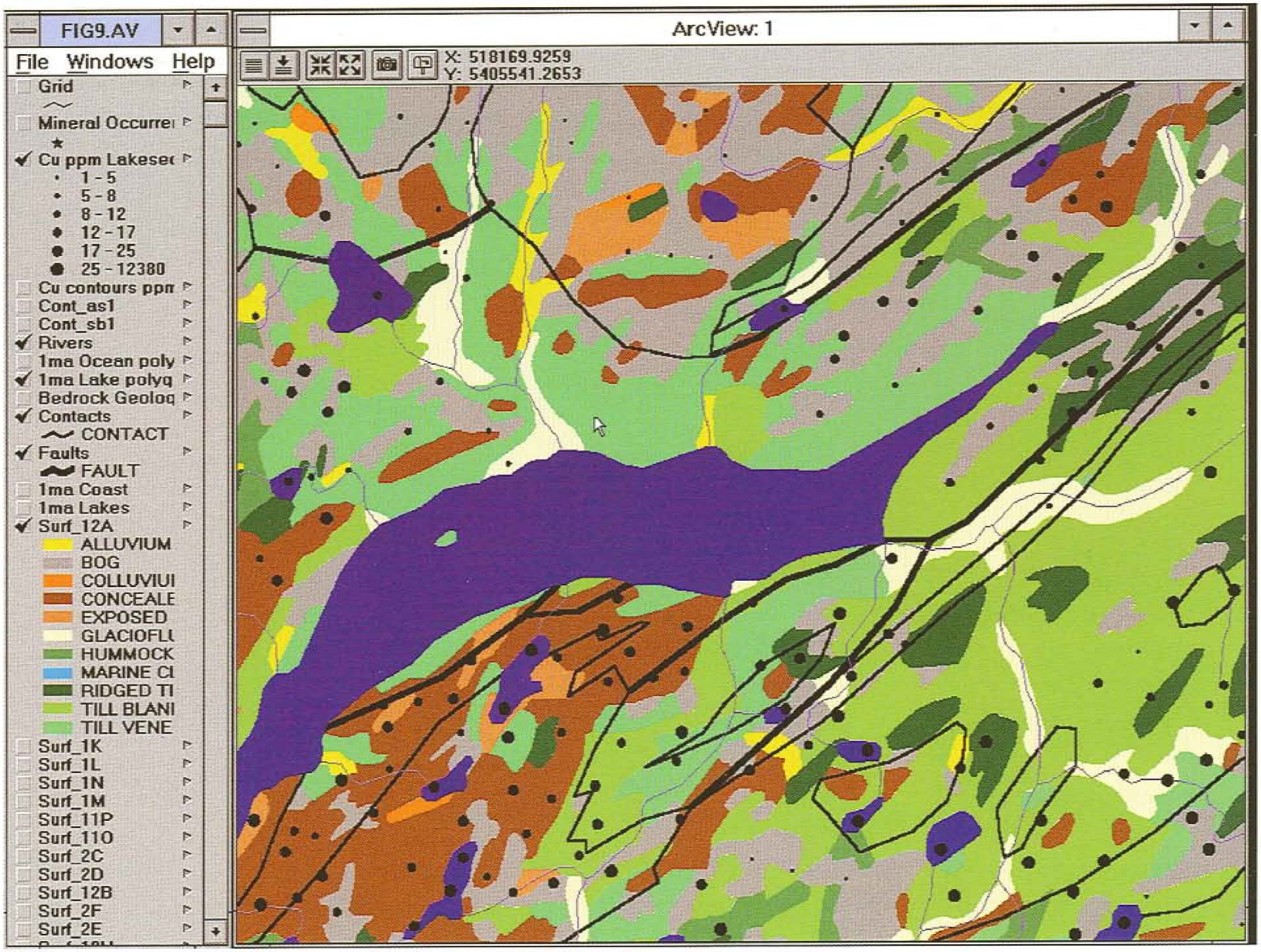

Figure 9. *Print of the screen display from the Digital Geochemical Atlas of Newfoundland showing copper (Cu³) in lake sediment as a proportional symbol plot (in red) displayed on the surficial geology in colour with the solid geology as black lines and drainage in blue, for the same area as Figure 3 (32 km from north to south). The layer-control menu at left indicates the layers turned on for display; Cu values as proportional symbols (with legend), contacts and faults (solid geology), rivers and 1 ma lakes (the drainage network), and surficial geology (with an abbreviated legend).*

Y, Zr, Nb, Cd and Dy probably in 1995. In addition to the regional data, several more detailed geochemical surveys have been conducted by the Geological Survey Branch throughout the island, employing till, soil, stream sediment and water, and lake sediment and water. These will be compiled into a second digital geochemical atlas module that can be added to the regional atlas.

Comparable regional and detailed geochemical atlases are planned for Labrador where there is similar coverage although at lower sample densities. Work on these will start in 1994. Companion atlases in compatible formats are in progress for airborne geophysical data (Kilfoil and Bruce, *this volume*) and are being planned for surficial geology and mineral aggegrate resources. More detailed, multiscale digital compilations of solid geology and topographic databases are also envisaged. The ultimate goal is the capture in digital atlas format of all map-referenced geoscientific data resident at the Geological Survey Branch, including eventually data from mineral-assessment files and other external sources. This would greatly increase the application and effectiveness of the geoscientific database for the province as a tool for environmentally sound mineral and industrial development.

CONCLUSIONS

The authors believe the digital atlas format to be the way of the future for data organization and dissemination. It allows both the presentation of well-designed thematic maps (interpreted information) with the flexibility of digital databases (hard data). Users of different backgrounds and interests can explore the data at many different levels and different scales, and bring together readily all the various types of data available for any area of interest. The digital atlas format will largely eliminate the need for costly colour-map production as printed maps will be replaced by on demand colour maps. These will not only be more up-to-date but can also be tailored to the user's special interests.

The digital geochemical atlas (version 1.0) is quite large (almost 300 Mb), and with planned additions it will grow larger. It will be released initially on CD-ROM. It is envisaged that typically only subsets of the data will be queried at any one time, and these will be copied to hard disc to improve file access times. Ever decreasing costs for hard-disc storage capacity and CD-ROM access times will probably diminish problems encountered with the size of the atlas. In the future, consideration will be given to making the data available in other formats; DAT tape and through INTERNET for example.

MacKenzie *et al.* (1989) concluded that developing the geoscientific database of the province has the greatest economic impact of all government mineral-development programs. Radically improving the way this database can be used will substantially increase its value as an economic development tool.

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