LITHCHEM — GEOLOGICAL DATABASE SYSTEM: RECENT DEVELOPMENTS*

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INTRODUCTION

LITHCHEM is a database system for storage, retrieval and graphic representation of whole-rock geochemical data. The first version of the LITHCHEM system was described by Harrop and Sinclair (1986). Since then, the system has been developed further. This paper briefly describes the structure and operational routines of the latest version, with emphasis on the recent achievements and developments. A detailed reference manual is available from the Department of Geological Sciences, The University of British Columbia. The system presently contains analyses of more than 2000 volcanic rock specimens from the Cordillera of British Columbia (Radlowski, 1988).

SYSTEM OBJECTIVE

LITHCHEM is designed for the following tasks: input and editing of lithogeochemical data, searching for individual records by various key data fields, plotting sets of records on a variety of petrogenetic, two-coordinate diagrams, and generating data subsets by selection based on graphical domains. These detailed procedures permit sequential selection of lithogeochemical data specifically to distinguish altered and unaltered samples in the existing compilation of chemical analyses of volcanic rocks in British Columbia.

HARDWARE/SOFTWARE REQUIREMENTS

The LITHCHEM system is written in Turbo Pascal and configured for the IBM PC(XT) with 576k RAM, 10 megabytes (or more) hard disk storage, IBM CGA, running under MS/DOS 3.0 or later versions. In addition, an 8087 numerical coprocessor is highly recommended. Any dot matrix printer which can perform a graphics screen dump can be used for hardcopy output.

RECORD FORMAT

A primary element of the database is a record that represents information for a single sample. A new record is always entered at the end of the data file, hence a record number becomes an unique sample identifier.

A sample record consists of 24 fields that are either numerical or string type. The string fields contain geological names (assemblage, formation, rock name/occurrence, age) or they describe a sample location (NTS map sheet, details of stratigraphic unit). The numerical fields represent geochemical analyses (12 major oxides and volatiles) and specify a bibliographic reference (reference number and sample number).

The record format can be modified or expanded with minor changes to the program.

SYSTEM STRUCTURE

The LITHCHEM system consists of two main programs, LITHED (Editor) and LITHP (Plotter), supported by a number of external subprograms and routines. The Editor and the Plotter comprise about 6000 lines each of source code, and the system requires approximately 120 kilobytes, plus 100 to 500 kilobytes for lithogeochemical data.

LITHCHEM is a menu-driven system with several options available from the Editor and/or the Plotter. The main menu commands relate to the following procedures:

- Editing and updating records
- Database file maintenance
- Compound search for records
- Graphic display
- Conversion of a LITHCHEM datafile to ASCII datafile and vice versa.

The LITHCHEM edit procedures have remained unchanged from those discussed by Harrop and Sinclair (1986). The file maintenance procedures are of marginal importance and are not discussed here. The most important achievement of the latest versions of the system is an extended development of the search and graphic procedures, and implementation of ASCII conversion routines.

SEARCH ROUTINES

LITHCHEM provides search routines to create, modify and maintain sets of data records. This procedure introduces two important concepts: source and target. The routines work with a general algorithm that searches in the source and processes in target. It is mandatory to specify explicitly which source is to be searched, and which target is to be processed; therefore, the system employs a flag concept. Each record has a 16-bit integer associated with it and 15 of these bits are used to signify a set membership. If the nth bit is ON, the corresponding record is a member of the set flagged with n-flag. The search source can be a whole database or an active flag, hence the source cannot be empty. The target might be an inactive flag unless the target and source are the same.

The search routines operate with the following sub-menu:

   (1) Create set
   (2) Remove set
   (3) Join set
   (4) Display set
   (5) Rename set
   (6) Clear set.

When a search command is executed, the submenu is activated and the flag lists are displayed on the screen. The flags are labelled from 1 to 15 and these labels function as flag identifiers. All active flags are associated with names entered by the user or generated by the system. In other words, the flag labels without names are currently empty. Although the flag name is not a set identifier it is still a valid indicator of the set presence. The algorithm assumes that a set contains at least one record, and a zero-size set means a set absence.

GRAPHIC ROUTINES

LITHCHEM provides several graphic routines to plot the flagged set(s) and to generate subsets by plot domains. The plot routine involves a submenu with functions keyed from 0 to 8. The function "0" (zero) sets graphic characters for plotting and it should be executed first. The program allows the user to set up to eight graphic symbols that will identify sets (flags) on all diagrams unless "zero" option is rerun.

The selected sets are displayed on plot diagrams while executing the menu functions 1 to 8. The diagram appears with specific curves contouring domains of rock compositions. The program mostly deals with two boundary curves that divide a plot plan into three domains. Each sample of the set can then be identified by its location on the plot diagram and a domain membership. The system introduces a new search procedure that enables the user to split (subset) the set into domains. This routine is called from the selected diagram, and can be applied only to one set at a time.

The "subset" routine works with the following algorithm:

- Identify all samples above the upper curve (or right to the rightmost curve) and move them from the parent set to the first available flag; generate a name for the new set by adding a prefix predefined for the upper/right domain to the parent name.
- Search for all samples below the lower curve (or left to the leftmost curve), proceed as above, adding a prefix predefined for the lower/left domain to the parent name.
- Rename the remainder of the parent set by adding a prefix predefined for the central domain.

As a result, the "subset" procedure creates three smaller sets of which an arithmetic sum is equal to the parent set. These sets are recognized by all LITHCHEM procedures as independent sets, can be further processed with search or plot routines and can be subset again.

At present, the possible plots for graphic representation are: MgO vs. CaO, MgO vs. SiO_2, CaO vs. SiO_2, Na_2O vs. SiO_2, K_2O vs. SiO_2, alkaline vs. SiO_2, TiO_2 vs. FeO total, and MgO vs. FeO total. Others can be added easily, as required.

CONVERSION ROUTINES

LITHCHEM provides conversion routines to translate its database into ASCII, and vice versa. Any set of the LITHCHEM data, or a whole database, may be converted into a text file with records of a fixed format. An ASCII file can be converted to the LITHCHEM database if its records have the required structure and format. This means that the

file should be checked as to record organization, and modified if necessary, prior to conversion to the LITHCHEM system.

The conversion routines are an important linkage between LITHCHEM and other systems, and allow an easy exchange of data.

CONCLUSIONS

LITHCHEM is a powerful tool for sorting, extracting, and grouping rock-chemistry records. Its search and plot routines can be applied repeatedly in different combinations, allowing one to select and display a very specific set of records.

The system is fully operational with a database of the whole-rock analyses of volcanic rocks of British Columbia compiled by A.F. de Rosen-Spence. The database has been used principally to define magmatic trends in various magmatic suites (de Rosen-Spence, 1985; de Rosen-Spence and Sinclair, 1987, 1988; Ray and de Rosen-Spence, 1986). It is presently being used to assist in the recognition of alteration in samples of volcanic rocks, and is being developed to further quantify alteration associated with mineralization in volcanic rocks, in cooperation with X. Cheng.

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