GEOQUIM: A COMPREHENSIVE GEOCHEMICAL TOOLBOX FOR THE BDGEO SOFTWARE PACKAGE

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SUMMARY- BDGEO 4.0, is our current version of a user-friendly, modular, integrated Windows95/NT application for storage, visualization and analysis of geothermal data. Its main goal is to standardize and simplify the assessment and management of geothermal fields at departmental level. BDGEO 4.0 is set up as a distributed application over a local area network. Its main modules are a control module, a database and a visualization package, collectively denominated KERNEL. The KERNEL is common to all users. In addition to the KERNEL there are toolboxes, which are a family of applications for geothermal analysis and interpretation (e.g., for geochemistry, well testing, production, etc.) running in the BDGEO computational environment. Toolboxes are meant to be installed mostly in specialists PCs. GEOQUIM is the geochemical toolbox. It allows computation of (1) chemical equilibrium in the reservoir (speciation); (2) gas geothermometers; (3) liquid phase geothemometers; and (4) chemical concentrations at reservoir conditions. Results are presented in tabular form, and whenever appropriate, in graphical form. They may be either printed or saved to files. GEOQUIM has been carefully tested with field data. This application greatly simplifies geochemical analysis of geothermal reservoirs.

1. INTRODUCTION

Last year (Iglesias et *al.,* 1997) we introduced BDGEO v4.0, our current version of a user-friendly, modular, integrated Windows95/NT application for storage, visualization and analysis of geothermal data. The main goal of this package is to standardize and simplify the assessment and management of geothermal fields at departmental level. BDGEO 4.0 is set up as a distributed, client-server application over a local area network.

The architecture of BDGEO 4.0 is modular (Fig. 1). A *Control Module* interacts with a number of structurally identical databases (*DB1, ...Dbn),* each belonging to a distinct geothermal field, and with several *Application* Modules. The main modules, collectively denominated KERNEL, are the Control *Module,* the *Database Access Module* and the *Visualization Module.* The KERNEL is installed in the server and in all the networked PCs and implements the BDGEO v4.0 computing environment. The environment's user interface is written in Spanish.

Other, independent *Application Modules* , called toolboxes, are designed for standard computations in some disciplines (e.g. geochemistry, reservoir engineering) and for specialized analysis (e.g., production, well tests). Toolboxes are meant to be installed mostly in specialists PCs, to save system resources. Thus, some users will work only with the KERNEL, while other users may work with the KERNEL plus one or more toolboxes, according to necessity. Data transfer between the modules is seamless and transparent to users.

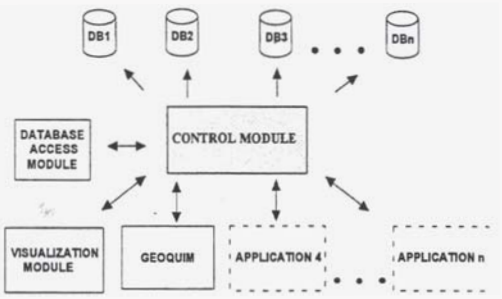

Fig. 1. Architecture of BDGEO v4.0

This paper introduces GEOQUIM, a toolbox that performs standard geochemical computations. Other toolboxes, including a geothermal wellbore flow numerical simulator and an expert system for well test analysis are currently under development.

2. GEOQUIM

GEOQUIM is programmed in Visual Basic (user interface, communications with *Control Module* and databases) and MATLAB (computations, visualization). This module, like all toolboxes, requires the BDGEO computational environment for its installation.

Users select GEOQUIM from BDGEO's main screen (Fig.2). This opens the screen shown in Fig. 3., which, among other things, allows users to select a database, corresponding to a particular g e o t h d field (button at upper right). The path to the selected database is then shown in the

upper left window. Clicking on the BDGEO logo retrieves a list of the available wells in the window that lies below that showing the path to the database. Users select the well of interest in this window, clicking on its name. They also select the time interval in which to perform the calculations in the twin small lower windows.

Fig.2. Starting GEOQUIM from BDGEO's main screen.

As shown in Fig. 3, GEOQUIM is capable of performing four types of standard geochemical computations. Going down fiom the top these are:

- Equilibrium distribution of species in the reservoir.
- Cl^- concentration in total discharge and in reservoir liquid.
- Gas geothermometers.
- Liquid phase geothemometers.

Fig. 3. GEOQUIM's main screen allows selection

The screen in Fig. 4 displays the name of the well and the date of the sample in the upper left and right windows respectively. Below the name of the well there is an area presenting the sampling conditions (starting from the top: wellhead pressure, separation pressure, specific enthalpy, separation temperature of the liquid sample, separation temperature of the steam sample, pH of the liquid sample and temperature of pH measurement). The adjacent area to the right displays the computed reservoir conditions (starting from the top: fraction of liquid phase, temperature, pH, steam fraction and steam deficit). Below these areas there are four scrollable windows. The first one starting from of database, well, time interval and computation to be performed.

2.1 Equilibrium distribution of species in the reservoir.

Clicking on the "Equilibrium ..." option and then on the lowermost button (Continue) (Fig. 3) starts these calculations.

This capability is based on EQQYAC, a program developed in IIE's Geothermal Unit (Barragán and Nieva, 1989). This program calculates the equilibrium distribution of inorganic aqueous ion species in geothermal reservoirs from the chemical composition of discharged fluids and *in situ* physical measurements. GEOQUIM retrieves the input data automatically and transparently from the selected database.

The original EQQYAC requires the reservoir temperature as input. Unlike it, GEOQUIM, more consistently, computes the required reservoir temperature fiom the composition of the discharge, by means of a liquid phase geothermometer. For greater flexibility, we plan to add an option to assign a reservoir temperature, bypassing the geothermometer calculation.

The results, together with the corresponding input data, can be displayed in the screen (Fig. 4), saved to a file or printed as a report.

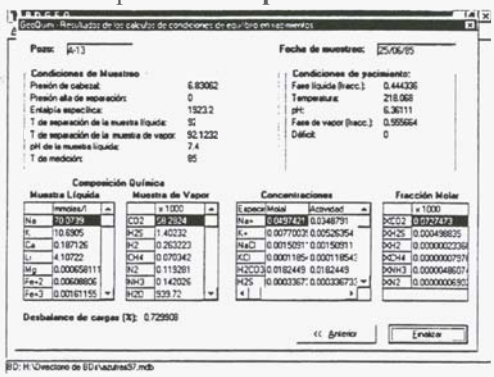

Fig. 4. Screen with results of *"Equilibrium distribution of species in the reservoir".*

the left (Muestra Liquida=Liquid Sample) shows the chemical composition of the liquid phase sample, in mmol/l. The second (Muestra de Vapor=Steam Sample) presents the chemical composition of the steam sample in mole fraction x1000. The third window depicts the inferred reservoir molal concentrations in the liquid phase and the corresponding activities. In the fourth window one finds the computed reservoir mole fractions of the volatile components in the steam phase. Finally, the bottom line presents the the charge imbalance (%) of the sample data.

2.2 Chloride concentration in total discharge and in reservoir liquid.

This is the second option fkom the top in GEOQUIM's main screen (Fig. **3).** Clicking in the bottom buton "Continuar" (="Continue") displays the screen of Fig. 5. As in the previous option, users must select a database, a well and a time interval. Then they may select to compute the Cl concentarion in total discharge andor the Cl concentration in the reservoir, by ticking the upper box/lower box or both, respectively, in the lowest area of the screen.

Fig. 5. This screen starts computation of Cl concentrations in total discharge and /or in the reservoir.

Clicking in the "Continuar" buton presents the screen of Fig. 6. Here users are asked in the upper area, whether the well is fed by: (top to bottom) ***liquid, liquid and steam*** or ***superheated steam.*** The lower area of this screen presents choices of relevant geothermometers to compute deep temperatures, depending on how the well is fed. Selecting ***"liquid"*** elicits three options (top to bottom): Cationic Composition Geothermometer (Nieva and Nieva, 1987), Na-K-Ca (Fournier and Truesdell, 1973) or silica (Foumier and Potter, 1982). If fed by ***"liquid and steam"*** users are offered only the first two options just mentioned. Finally, when selecting fed by ***"superheated steam",*** users are presented five choices: (top to bottom) TD (D'Amore and Panichi, 1980), TC02 (Amorsson, 1985), TH2S (Amorsson, 1985), TH2 (Amorsson, 1985) and TFT (Fischer-Tropsch; Arnorsson,1985).

When the results are ready, users **may** choose (Fig. ***6,*** top to bottom) to: display them in the screen (e.g., Fig. **7),** save them to a file, print a report, plot them (e.g., Fig. 7). Selections are chosen by ticking the corresponding boxes.

Fig. 6. Users must select which way the well is fed and a geothermometer to **compute deep** temperatures.

Fig. 7. Choice of how to display/save the results.

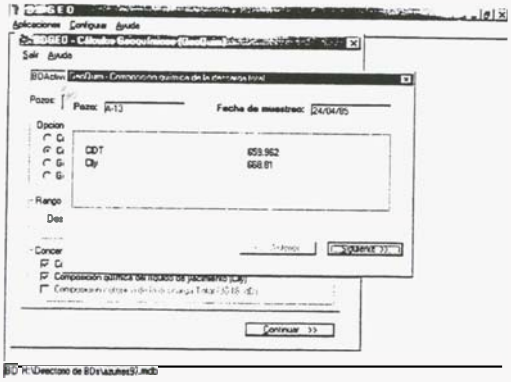

Fig. 8. Example of screen results.

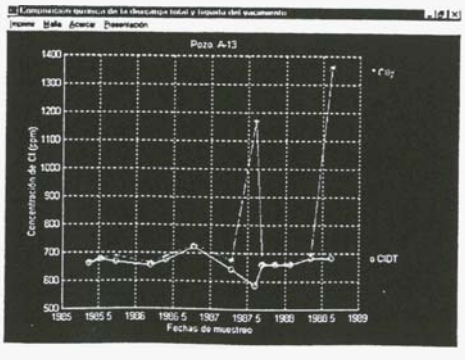

Fig. 9. Example of graphical results.

2.3 Gas geothermometers

The third option from the top in GEOQUIM's main screen (Fig. 3), allows computation of a comprehensive set of gas geothermometers. These are accessible through three tick boxes (Fig. 10).

Fig. 10. Selection of gas geothermometers.

Ticking the top box results in computation of the D'Amore and Panichi (1980) gas geothermometer.

Ticking the next box down brings about computation of five gas geothermometers from Arnorsson and Gunlaugsson (1985): TCO2, TH2S, TH2, TCO2/H2 and TH2S/H2. When selecting this choice users are required to indicate whether the Cl concentration is greater or less than 500 ppm (Fig. 11).

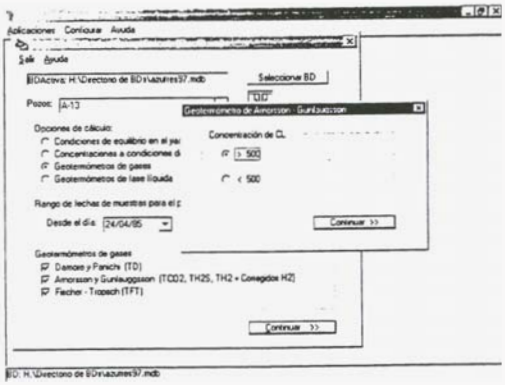

Fig. 11. To calculate Amorsson and Gunlaugsson geothetmometers users must provide idormation about Cl concentration.

Results may be diplayed in the screen, saved to a file or printed (Fig. 12). They are presented by sample date and geothermorneter (Fig. 13).

2.4 Liquid phase geothemometers

This is the last option of GEOQUIM's main screen (Fig.3). It is designed to compute a comprehensive set of liquid phase geothermometers (Fig. 14).

Fig. 12. Results of gas geothermometers may be shown in the screen (top box), saved to a file (middle box) or printed (lower box).

Fig. 13. Screen presentation of results for gas geothermometers.

Fig. 14. Selection of liquid phase geothermometers.

Ticking the upper box computes the silica geothermometer (Fournier and Potter, 1982). Ticking the next box down calculates the Cationic Composition Geothermometer (Nieva and Nieva, 1987). And ticking the last box brings about computation of four Na-K geothermometers: Na/K (Truesdell, 1975), Na/K (Foumier, 1979), Na-K-Ca (Foumier and Truesdell, 1973) and Na-K-Ca corrected by Mg (Fournier and Potter, 1979).

Results may be presented in the screen (Fig. 15), saved to a file, printed or ploted (Fig. 16).

Fig. 15. Results of liquid phase geothermometers.

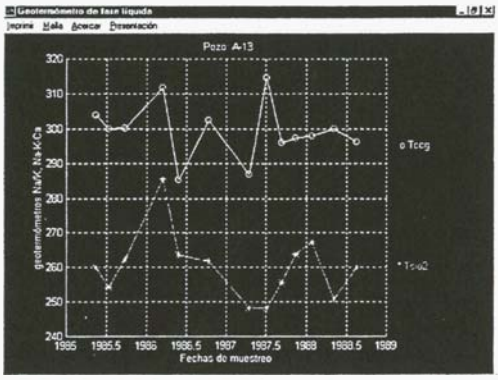

Fig. 16. Graphical results from gliquid phase. geothemometers.

3. CONCLUSIONS

We have developed GEOQUIM, a Windows95/NT toolbox that runs under the BDGEO v4.0 computing environment. This toolbox performs four types of standard geochemical computations:

- Equilibrium distriiution of species in the reservoir.
- Cl^- concentration in total discharge and in reservoir liquid.
- Gas geothermometers.
- Liquid phase geothemometers.

All the computations are based on well-known published algorithms.

The necessary data are automatically and transparently retrieved from databases each corresponding to a different geothermal field. Within each geothermal field the geochemical data are organized by well and by date.

The results can always be displayed in the screen, saved to a file and printed. Furthermore, results from Cl concentrations and liquid phase geothemometers may be ploted in the screen or in paper.

GEOQUIM is a user-friendly and efficient tool to perform standard geochemical computations. It saves untold man-hours by automatically routing data between different applications such as databases, computing algorithms and visualization tools.

4. ACKNOWLEDGEMENTS.

This work was performed under contract to México's Secretary of Energy .

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