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Application of hydrogeochemical modelling to the characterization and water quality control of coastal karst aquifers

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Abstract A set of computer systems (HIDROGEOQUIM, SAMA, GEOQUIM, BATOMET, SACAN, SIMUCIN, MODELAGUA and TEMADAT) for hydrochemical data processing with the aim of characterizing and controlling water quality, and simulating the water–rock interaction process, are detailed. Examples of their application to karst costal aquifers are discussed.

Key words hydrogeochemical models; water quality; karst costal aquifers

INTRODUCTION

To enable determination of the quality of the water resources, as well as the changes to them as a result of human activity, there are, in many countries, large networks of systematic sampling stations at which the local hydrometeorological conditions and some water quality indicators are continually monitored. The mathematical processing of these data by means of statistical and hydrogeochemical models can offer rich information about the regularities among the different variables and the environmental characteristics of the aquifers. These models apply the physical-chemical principles (thermodynamics and kinetics) to the interpretation of these hydrogeochemical systems. With this purpose, two approaches are used: (a) the inverse model (mass-balance), that uses the chemical composition data of the water and the rock with the objective of quantitatively identifying the geochemical reactions that give rise to the composition of waters; and (b) the direct model that, on the basis of some well-known initial conditions of the water–rock system, predicts the characteristics of the resulting solution through hypothetical chemical reactions (Gimeno & Peña, 1994; Plummer *et al*., 1991).

Since the 1990s, at the Cuban National Center for Scientific Research and at the National Center of Thermalism (now in the National Center of Natural and Traditional Medicine), a set of software based on statistical and hydrogeochemical (thermodynamic, kinetic, pattern recognition, mass balance and mixing water) models was developed with the aim to characterize and monitor the water quality of the karst aquifers and mineral water springs (Fagundo *et al*., 2004). The more recent version of the computer programs were designed in DELPHI3 language for WINDOWS. In this paper some of these informatics systems are described and examples of their applications for characterizing and controlling the water quality of the coastal karst aquifer in western Cuba, are discussed.

METHOD

The hydrogeochemical data were processed using the following computer programs: HIDROGEOQUIM (System for Hydrogeochemical Data Processing), SAMA (System for water quality monitoring), GEOQUIM (System for statistical data processing), BATOMET (System for monitoring the water quality of coastal aquifers), SACAN (System for water chemical composition characterization, based on a pattern recognition model), SIMUciN (System to process hydrochemical data from the water–rock interaction in a kinetics experiment), MODELAGUA (System for modelling the natural water chemical composition), and TEMADAT (database system).

RESULTS

The SAPHIQ system (Alvarez & Fagundo, 1991), and more recently, HIDROGEOQUIM (Fagundo *et al*., 2005), allow the hidrochemical characterization of the aquifers, to study the temporal variation of water quality and to determine the state of the water in its equilibrium with respect to the aquifer constituent minerals. These systems have been applied for the characterization of underground waters of the karst coastal aquifer in the Matanzas (Ferrera *et al*., 1999), Havana (Fagundo *et al*., 2002) and Pinar del Río (Fagundo & Arellano, 1991) provinces; gypsum aquifers of Punta Alegre (Fagundo *et al*., 1994) and saline waters at Cauto basin (Fagundo *et al*., 1995), some of them with high salinity. Also, these software systems were used to study the human effects (overexploitation of the aquifers for public and agricultural supply) on the karst coastal aquifers (Fagundo & González, 1999). Figure 1 shows a chronological series of electric conductivity (EC) and some parameters calculated by HIDROGEOQUIM.

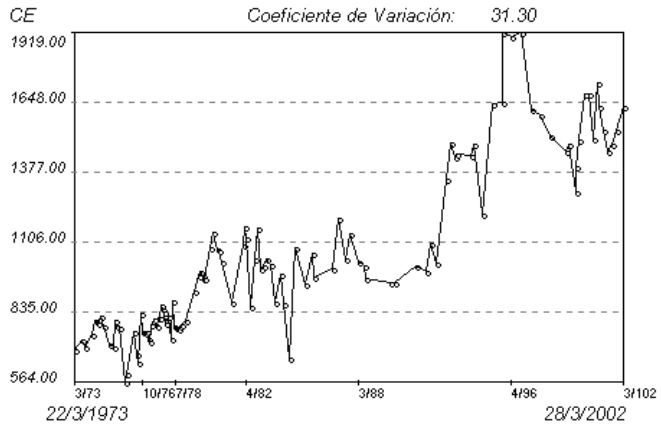

Fig. 1 Variation at time of the electric conductivity (HYDROGEOQUIM).

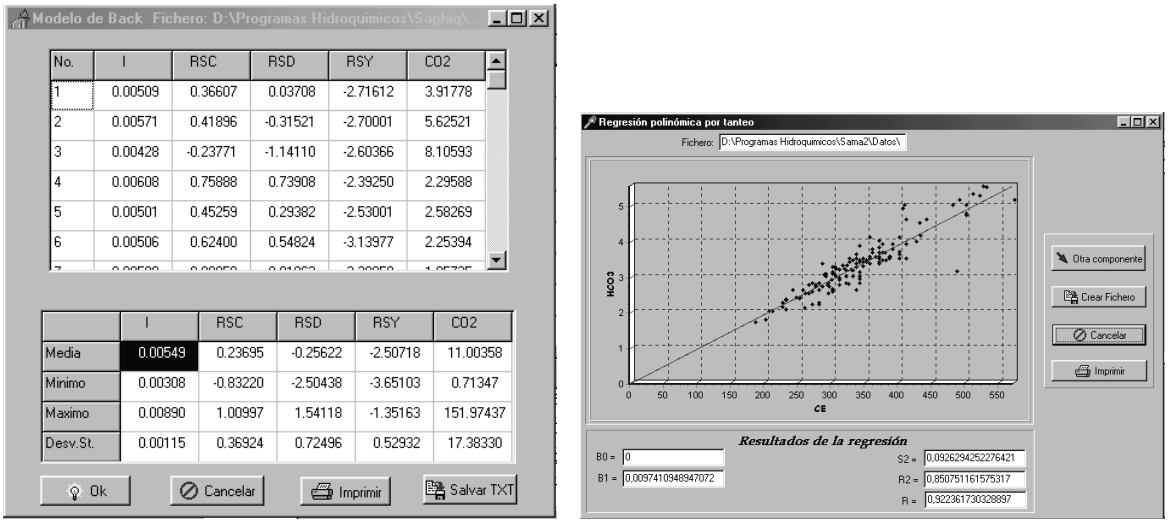

Fig. 2 (a) HYDROGEOQUIM output: ionic strength (I), calcite saturation ratio (RSC), dolomite saturation ratio (RSD), gypsum saturation ratio (RSY) and CO_2 content. (b) Plot by SAMA of the relationship between HCO_3^{2-} content and electric conductivity.

The SAMA system (Alvarez *et al*., 1990), designed to determine mathematical correlations among ionic concentration and EC, and later, to estimate the chemical composition using the above equations and measures of the EC, has been largely used for water quality monitoring for the basins and control network of the Cuban National Institute of Water Research (INRH). Some examples of the application of this software are discussed in Fagundo & Rodríguez (1992) and Fagundo *et al*. (1993, 1994, 1995). Figure 2(a) and (b) show two output windows with results of this system.

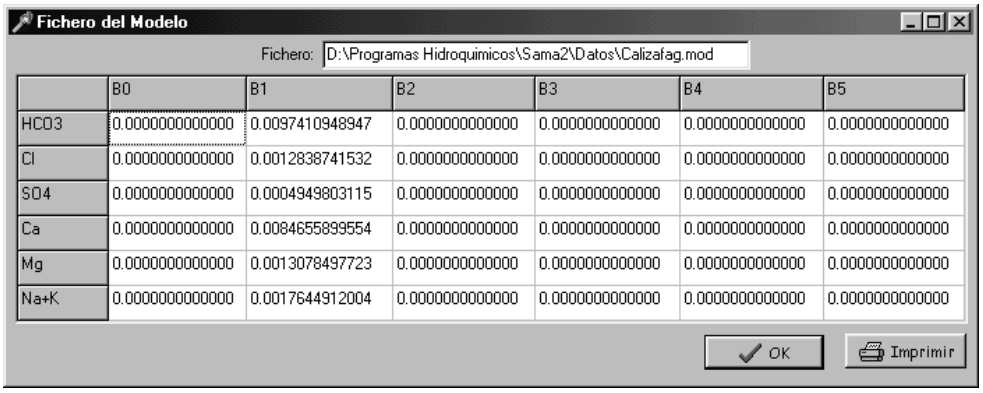

Fig. 3 Relationships between ionic contents and electric conductivity (SAMA).

The GEOQUIM system (Alvarez *et al*., 1993), was designed for the statistical processing of hydrochemical data, and was applied along with SAMA to determine the mathematical correlation equations established among chemical composition and electric conductivity of the water quality control net of INRH in the Pinar del Río region. BATOMET (Vinardell *et al*., 1995), based on a pattern recognition model, sorts the data according to its Cl^-/HCO_3^- ion ratio and later determines the mathematical correlations among chemical composition and EC of each sorted group, estimating the chemical composition of the water using mathematical equations (Fig. 3) and the measured EC (Fig. 3). This system has been applied for monitoring the water quality of the systematic observation well network of INRH in South Pinar del Río basin (Fagundo & Rodríguez, 1991); South Havana basin (Fagundo *et al*., 2002); as well as Zapata swamp, in Matanzas province (Fagundo *et al*., 1993). The karst waters of these coastal aquifers are stratified as a consequence of the mixing of the freshwaters with the seawaters. BATOMET, which joins SAPHIQ and SAMA, was also applied to evaluate the salinity and to control the water quality in the Cauto river basin (Fagundo *et al*., 1995), where the water composition changes drastically in short time intervals.

SACAN, has been used more in the context of mineral waters than in coastal aquifer waters (Tillán *el al*., 1996) due the minor component data available.

SIMUCIN was applied to study the laboratory chemical simulation processes established between the waters and aquifer materials of the karst aquifers (Alvarez *et al*., 1996), including experiments in mixing conditions with seawaters.

MODELAGUA (Fagundo-Sierra *et al*., 2001) was created to determine the geochemical processes that originate the chemical composition of natural waters, by means of mass-balance models and mixture analysis, also allowing the plot of Stiff graphics and the determination of

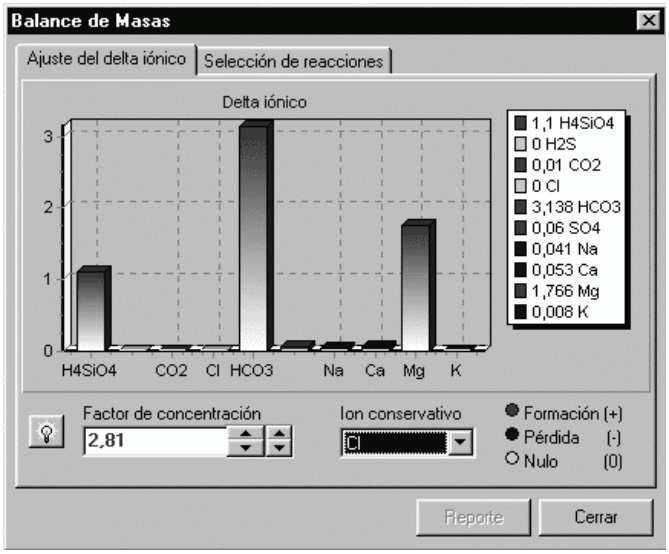

Fig. 4 Computation of ionic delta (Δi) by MODELAGUA.

hydrogeochemical patterns for the classification of different water types. By means of the algorithm of this computer program, the percent of freshwater–seawater mixing and the ionic delta (ΔSO_4^{2-}, ΔNa^+, ΔCa^{2+} and ΔMg^{2+} where Δ represents the mass transferred in the geochemical process) at the karst coastal aquifer of Zapata Swamp (Ferrera *el al*., 1999) and Güira-Quivicán Hydrogeologic Sector (Fagundo *et al*., 2002) were determined. The main hydrogeochemical processes, which explain the chemical composition of these waters, are: calcite and dolomite dissolution, calcite precipitation, dolomitization, sulfate anaerobic reduction and direct and inverse ionic interchange. At the karst coastal aquifer adjacent to a swamp, the variation of the Δ ion magnitude is more intense and also, is in these sites where there are disposed biodegradable organic wastes.

TEMADAT (Fagundo-Sierra *et al.*, 2002) is a database system used to store and manage the hydrochemical data.

CONCLUSION

The informatic systems, implemented by the authors, have been applied to study different underground basins of western Cuba, allowing hydrochemical characterization of the aquifer, analysis of the temporal variation of water quality, to determination of the state of the water and its equilibrium with respect to the aquifer constituent minerals, calculation of the degree of freshwater–seawater mixing as a consequence of marine intrusion, determination of the origin of the water's chemical composition and the geochemical processes which explain this composition, evaluation of water quality and design of water monitoring and automatic control systems. The results of these investigations have been published in different papers, and presented at scientific congresses as part of some Master and Doctoral theses.

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