SAPHIQ AND SIMUCIN: COMPUTER SYSTEMS FOR THE HYDROCHEMICAL CHARACTERIZATION AND WATER QUALITY MONITORING

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ABSTRACT

The computer systems SAPHIQ and SIMUCIN, for the hydrochemical data process with the aim to characterize and control the water quality, as well as to simulate the water-rock interaction process are presented.

INTRODUCTION

With the purpose to know the quality of the hydric resources, as well as the changes carried out in the waters as the result of man activity, there are, in many countries, large networks of systematic sampling stations, where continually the local hydrometeorological conditions and some water quality indicators as temperature, pH, electric conductivity (EC) and redox potential are recorded, while some samples are sent to the laboratory for chemical analysis. Also in many dependences devoted to control the water quality for the agriculture and population supply, or to elaborate beer and soft drinks, a vast quantity of historical hydrochemical data is available. The mathematical process of these data can offer rich information about the regularities among the different variables. For example, it is possible to find linear mathematical relations, at least in a discrete interval, which are near the real function, and allow the estimation of the water macrocomponent in function of other magnitudes easier of measurements.

The aim of this paper is to show the possibility to use a set of specific software in order to characterize aquifers and systematic sampling stations; to study the changes of the water chemical composition along the time; to simulate the natural process of chemical composition acquisition at the aquifer, and the changes in its properties by the action of the hydrogeologic and environmental conditions; to find mathematical regularities among the hydrochemical variables, and to establish an automatic monitoring system of the water quality, expressed as chemical composition and mineralization, taking into account the measurements of temperature, pH and EC.

THEORETICAL BASIS

The chemical composition acquisition of natural waters is a complex process determined by different factors: physico-chemical, geological, hydrogeological, geomorphological, climatic, microbiological and environmental. Elsewhere, in a determined place or area with certain homogeneity, some of the above factors can be made constant, and in these conditions, it is possible to find empirical relations between EC and water ionic macrocomponents (Fagundo, 1990; Fagundo and Rodríguez, 1991).

Theoretical considerations about EC and its applications to analytical control was discussed by Miller et al (1988). This parameter correlates with the sum of dissolved major-ion concentrations in waters and often with a single dissolved-ion concentration (Hem, 1970). Thus, electric conductivity is useful as a supplement of analytical determinations of major ions and can also be used for the analytical quality control in laboratory of major constituents (Dudley, 1972; Miles and Yost, 1982). Also, a significant correlation coefficient between EC and other groups of physico-chemical parameters as mineralization (Keith Todd, 1975; Bakalowicz, 1974), salinity (Accerboni and Mosseti, 1967), hardness (Bray, 1977) and the square root of the ionic strength (Shuster and White, 1965) has been reported.

On the basis of the mathematical relationships between EC and ionic concentration of the main macroconstituents of waters, and measurement field electric conductivity a method for quality monitoring was developed (Fagundo et al 1992).

In order to use this method it is necessary previously to perform and hydrological and hydrochemical characterization of the waters from the basin where the sampling points are located. The hydrogeochemical data needs to reflect the effect of the hydrologic cycle above the chemical composition and EC fluctuations along the time. The historical data from a systematical sampling at dry and wet periods in the network developed for quality control is good for this purpose.

With the aim to facilitate the calculus, some computer systems: ***SAPHIQ*** (Alvarez et al 1992, Alvarez et al 1993) and ***SIMUCIN*** (Alvarez and Fagundo 1995), have been designed. The data can be introduced directly by means of the systems or from other data files created by other systems. All data files have a similar structure or are transformed into others.

BRIEF DESCRIPTION OF THE SYSTEMS

SAPHIQ: From the values of the main physico-chemical parameters (temperature, pH, EC, CO_2 and ionic concentration in meq/l) the system expresses the ionic contents in mg/l, % meq/l and mmol/l, and calculates the hardness, mineralization, ionic strength, several ionic ratios of geochemical interest; the theoretical EC (by means of the Dudley and Miller models); the water aggressiveness degree (by means of the Back et al and

Tillmans-Trombe models); the theoretical CO_2 contents and other parameters. The results are displayed in tables and graphics. Comparing the real and theoretical electric conductivity it is possible to determine the precision of the analysis excluding those with analytical mistakes in order to select the representative data for the mathematical process. The results can be expressed in function of time, which constitutes a good tool for evaluating the seasonal fluctuation and the tendency of physico-chemical parameters.

A graphic output of the EC variation along the time from one stream at the San Marcos experimental basin, Pinar del Rio, Cuba (Fagundo and Rodríguez, 1991), at the interval 26/01/1984-14/06/1989 is observed in figure 1.

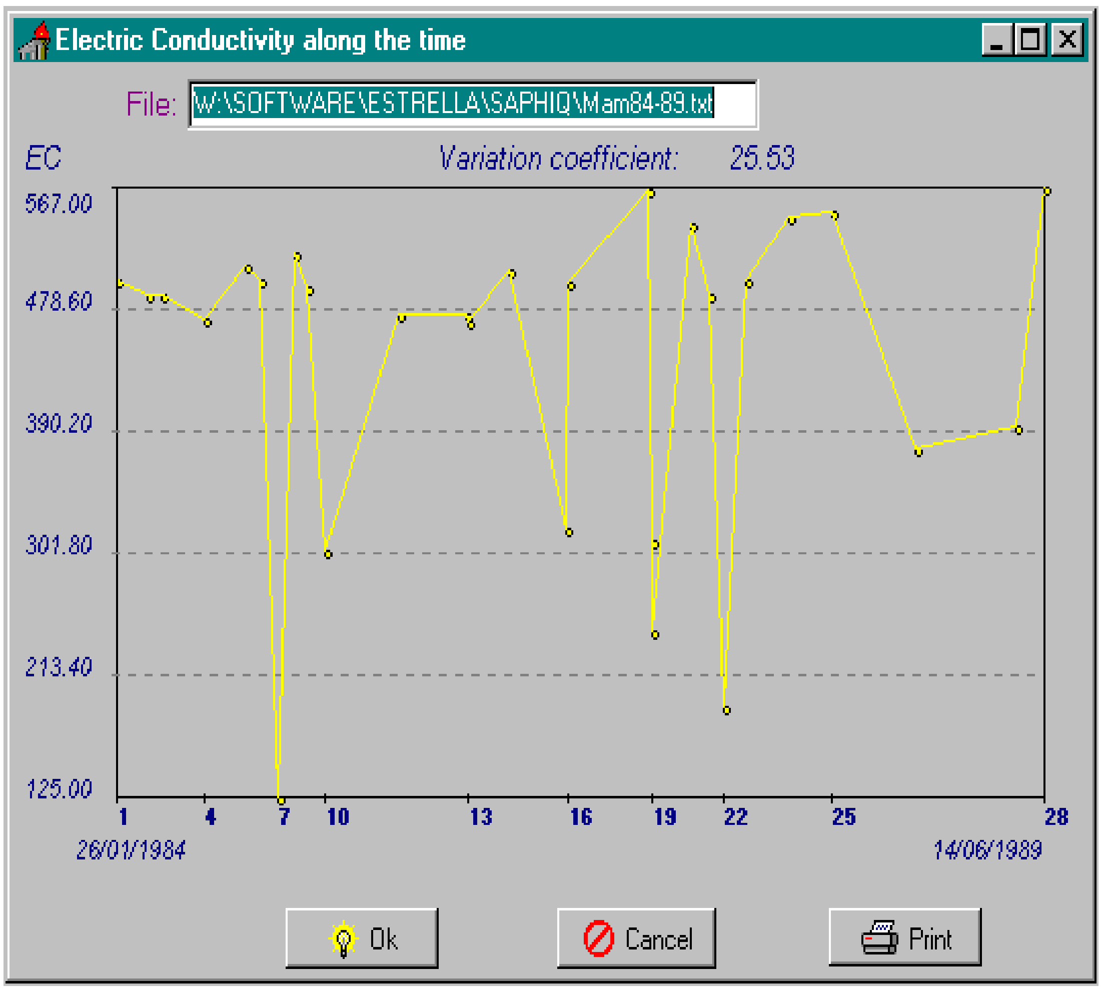

***Figure 1**: EC variation along the time*

SIMUCIN: The purpose of this system is to calculate the kinetic constants for the process of rock dissolution experiments in the laboratory. (Fagundo et al 1992 a) The system calculates the CO^2 contents on the basis of the pH, calcium concentration and alkalinity of the water, and represents graphically the variation in time of HCO_3^-, Ca^{2+}, Mg^{2+}, CO_2 as well as pH and EC by means of kinetic models:

$$C = C_{eq}(1-e^{-kt}) \text{ or } C = C_{eq}\, e^{-kt}$$

The former for the ionic concentration and EC, and the latter for the CO_2 contents. The similarity between the real and theoretical results are estimated by means of kinetic graphics and the mathematical simulation method. (Figure 2)

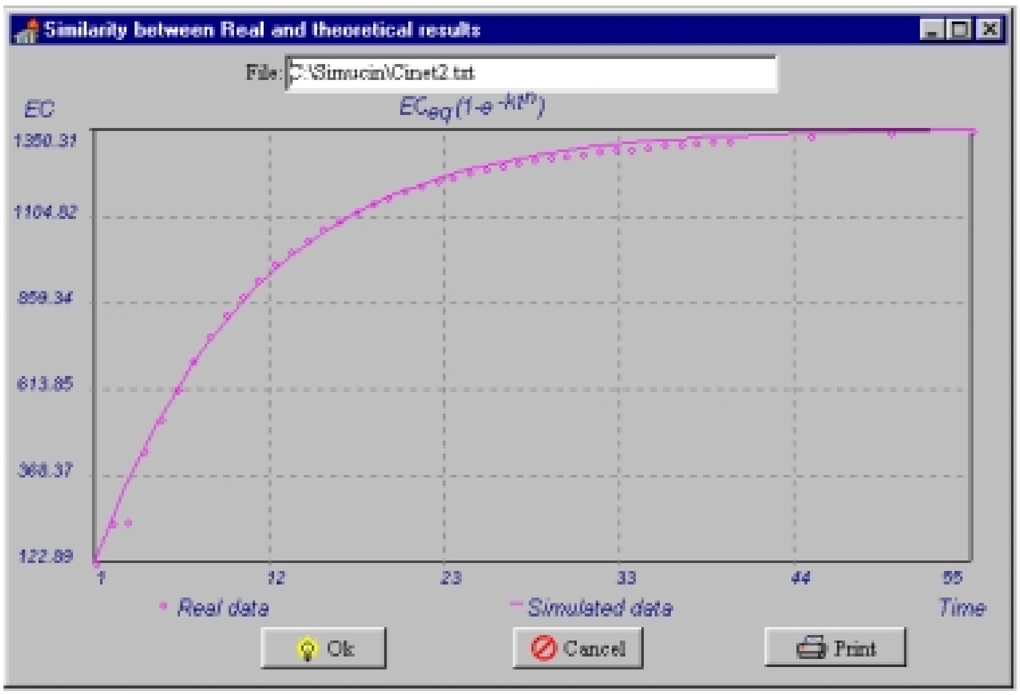

Figure 2: *The similarity between the real and theoretical results are estimated by means of kinetic graphics and the mathematical simulation method*

All these systems have been widely applied in the network established by the National Institute for Hydraulic Research of Cuba for monitoring the quality of the water used for supplying the main city population, the industry and the agriculture.

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