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SolGeo: A new computer program for solute geothermometers and its application to Mexican geothermal fields

Surendra P. Verma*, Kailasa Pandarinath, Edgar Santoyo

Departamento de Sistemas Energéticos, Centro de Investigación en Energía, Universidad Nacional Autónoma de México, Priv. Xochicalco s/no., Col Centro, A.P. 34, Temixco, Mor. 62580, Mexico

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Abstract

The freely available computer program Solute Geothermometers (SolGeo) was written and tested using geochemical data and reported geothermometric temperatures from several geothermal wells from around the world. Subsurface temperatures for the Mexican geothermal fields of Cerro Prieto, Las Tres Vírgenes, Los Azufres, and Los Humeros were estimated based on different solute geothermometers and found to be generally in close agreement with measured well temperatures when considering errors in the calculations and measurements. For Los Humeros wells it was concluded that a better agreement of chemical geothermometric temperatures is observed with static formation than with bottom-hole temperatures (BHTs). It was also found that the widely used Na–K geothermometric equations generally give more consistent and more reliable temperature estimates than the other geothermometers, which should therefore be applied with caution.

Keywords: Geothermal; Geochemistry; Mexico; Computer software; Geothermal exploration; Geothermometry

1. Introduction

A plethora of geothermometric equations put forth for estimating subsurface temperatures from solute concentrations in geothermal waters are difficult to use without suitable computer software. In the 1970s, Truesdell (1976) reported computer program GEOTHERM, which was

* Corresponding author. Tel.: +52 55 5622 9745; fax: +52 55 5622 9766.
E-mail address: spv@cie.unam.mx (S.P. Verma).

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capable of calculating temperatures from seven geothermometric equations (see also Henley et al., 1984). Since then, numerous new equations have been proposed and used in geothermometric temperature calculations (see D'Amore and Arnórsson, 2000, or Verma, 2002, for relatively recent compilations of such equations).

Commercial program AquaChem (Version 5.1.33; http://www.swstechnology.com/software_product.php?tab=3&ID=1#index) contains 18 geothermometric equations (four for Na–K; one for K–Mg; one for Mg–Li; three for Na–Li; two for Na–K–Ca; four for quartz; three for sulfate-waters) and provides for modifying regression coefficients corresponding to most of the programmed equations, but does not allow changes to the sign (+ or −) of the coefficients. More recent equations such as those proposed by Nieva and Nieva (1987), Fournier (1991), Verma and Santoyo (1997), and Can (2002) are absent from AquaChem. El-Naqa and Zeid (1993) presented a computer program (GEOTHERM) for applying Na–K, Na–K–Ca, and silica (or quartz) geothermometers, but so far temperatures computed using this program have not been reported in the published literature.

Most geochemists use some kind of spreadsheets or hand calculators that probably lead to frequent errors, as discussed below. Therefore, there is a special need for developing freely available software that could facilitate these computations in an easy, friendly, efficient, and reliable way. With this need in mind, we developed computer program Solute Geothermometers (i.e., SolGeo) that includes 35 geothermometric equations for solute geothermometers (Table 1). A salient feature of the program is that the concentration of each chemical variable is converted to the measurement units required by each geothermometric equation (see Table 1 for these requirements) using updated values of atomic weights (e.g. Vocke, Jr., 1999; Verma et al., 2003; Wieser, 2006) and proper geothermal water density calculations and corrections (McCutcheon et al., 1993; Nicholson, 1993). Here, we present validation of SolGeo from a worldwide geothermal database and results from application to four Mexican geothermal fields.

2. SolGeo: a new computer program

Computer program SolGeo (for Solute Geothermometers) was written in Visual Basic 6.0; the main functions of the code are summarized in Fig. 1. It accepts input data as an Excel (*.xls) or a Statistica (*.sta; Version 5) file (example files are available from any of the authors on request). Thirty-five geothermometric equations and their respective applicability constraints used in SolGeo are listed in Table 1.

For each sample, the chemical variables Cl, HCO_3, SO_4, Na, K, Li, Ca, Mg, and SiO_2 (indicated without the respective charge) are compiled in an input file, and the units (mg/kg, mg/l, or the sometimes ambiguously used ppm) in a single column as reported in the literature reference. The input file also has a provision to include relative standard deviation (R.S.D.) data (analytical errors expressed as R.S.D.%) for Na, K, Li and SiO_2, if the information is available. Otherwise, typical values of 2% R.S.D. are used as default values in the error propagation module as inferred by some workers (e.g. Arnórsson, 2000; Santoyo et al., 2005).

An important feature of SolGeo is the data validation option that checks the input file for probable typographical errors such as characters in place of numbers and negative concentration values. The program also computes "% ionic balance" in several different ways according to the availability of ionic species data; either all of them (i.e. anions Cl, HCO_3, and SO_4; cations Na, K, Li, Ca, and Mg) or without Li and/or Mg if not reported. However, because of the presence of other charged species in solution that generally are not routinely determined, the use of the ionic balance as the sole indicator of data quality should be done with caution.