

Integrated multicomponent solute geothermometry



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ABSTRACT

The previously developed and well-demonstrated mineral saturation geothermometry method is revisited with the objective to ease its application, and to improve the prediction of geothermal reservoir temperatures using full and integrated chemical analyses of geothermal fluids. Reservoir temperatures are estimated by assessing numerically the clustering of mineral saturation indices computed as a function of temperature. The reconstruction of the deep geothermal fluid compositions, and geothermometry computations, are implemented into one stand-alone program, allowing unknown or poorly constrained input parameters to be estimated by numerical optimization using existing parameter estimation software. The geothermometry system is tested with geothermal waters from previous studies, and with fluids at various degrees of fluid–rock chemical equilibrium obtained from laboratory experiments and reactive transport simulations. Such an integrated geothermometry approach presents advantages over classical geothermometers for fluids that have not fully equilibrated with reservoir minerals and/or that have been subject to processes such as dilution and gas loss.

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1. Introduction

Solute geothermometers have been used for decades to infer the temperature of deep geothermal reservoirs from analyses of fluid samples collected at ground surface from springs and exploration wells. The most commonly applied such geothermometers include those based on the concentration of silica (Fournier and Rowe, 1966; Fournier and Potter, 1982; Fournier, 1977) and of sodium, potassium and calcium (Fournier and Truesdell, 1973; Fournier, 1979; Giggenbach, 1988). Other similar geothermometers also take into account the concentration of magnesium (Giggenbach, 1988) and lithium (Fouillac and Michard, 1981). These “classical” geothermometers and several of their modifications have been successfully applied to many geothermal waters and can be easily implemented through simple equations either directly or through various available software packages (e.g., Verma et al., 2008; Powell and Cumming, 2010). As a result, classical geothermometers have become important and essential geothermal exploration tools. However, these geothermometers can fail because of the assumptions on which they are based on. The Na–K geothermometers assume chemical equilibrium between the fluid and the minerals albite and K-feldspar, while the K–Mg

geothermometers consider equilibrium of the fluid with muscovite, clinocllore and K-felspar (Giggenbach, 1988). These minerals are usually common in geothermal systems, however their composition may vary. Also, especially in lower temperature systems, the Na–K and K–Mg ratios might be controlled by other minerals such as smectites, causing these geothermometers to fail. In addition, geothermal fluids ascending to ground surface are typically affected by gas loss, mixing and/or dilution with shallower waters, masking their deep geochemical signatures (Fournier, 1977).

In the late 1970s and early 1980s, with the availability of increasingly powerful computers, numerical multicomponent geochemical models were developed specifically for the study of hydrothermal systems, with direct application to chemical geothermometry (e.g., Michard et al., 1981; Michard and Roekens, 1983; Arnorsson et al., 1982, 1983a,b; Reed, 1982; Reed and Spycher, 1984). These studies showed that given a fluid composition, numerical models could be used to compute the (theoretical) equilibration temperature of a suite of reservoir minerals and thus infer reservoir temperature. Such multicomponent approaches present advantages over classical geothermometers because they rely on complete fluid analyses and a solid thermodynamic basis, rather than the solubility of a few minerals or (semi-)empirical correlations, and thus in principle apply to any geochemical system. However, because multicomponent geothermometry methods require a numerical model and a priori assumptions regarding reservoir minerals, these methods are much less practical than classical geothermometers. For this reason, multicomponent

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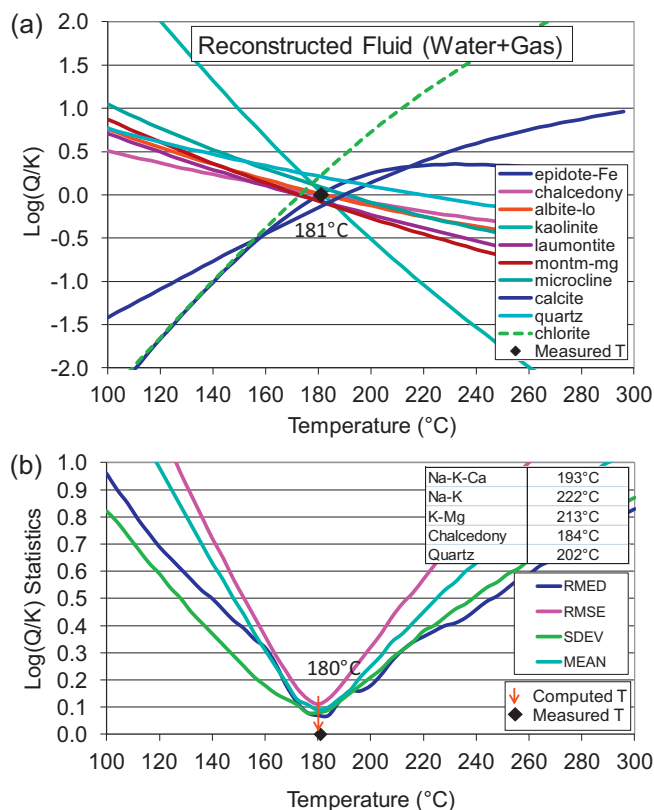


Fig. 1. Multicomponent geothermometry using an Icelandic geothermal water (Hveragerdi Well 4, Arnorsson et al., 1983a) previously used as an example by Reed and Spycher (1984): (a) Computed saturation indices, $\log(Q/K)$, as a function of temperature, showing clustering near zero close to the measured temperature (181°C). The amount of $\text{H}_2\text{O}_{(\text{g})}$ in steam was adjusted by numerical optimization (see text). (b) Statistical analyses of saturation indices: median (RMED), mean root square error (RMSE), standard deviation (SDEV) and average (MEAN) of absolute $\log(Q/K)$ values. The reservoir temperature is inferred from the temperature at which RMED is minimum (see text). Results of classical geothermometers are also shown for comparison, calculated using the reconstituted deep fluid composition (Na–K–Ca, Fournier and Truesdell, 1973; Na–K, Giggenbach, 1988; chalcedony, Fournier, 1977; quartz, Fournier and Potter, 1982).

geothermometry methods have been applied much less frequently than classical geothermometers.

Here, we revisit the multicomponent chemical geothermometry method presented by Reed and Spycher (1984) and further developed by Pang and Reed (1998) and Palandri and Reed (2001).

The method consists of using full chemical analyses of water samples to compute the saturation indices ($\log(Q/K)$) of reservoir minerals over a range of temperatures (e.g., 25–300 $^{\circ}\text{C}$). The saturation indices are graphed as a function of temperature, and the clustering of $\log(Q/K)$ curves near zero at any specific temperature (for a group of certain reservoir alteration minerals) is inferred to yield the reservoir temperature (e.g., Fig. 1a). Prior to computing saturation indices, the composition of the deep fluid is reconstructed by applying corrections for any dilution and/or mixing effects and by numerically adding back (to the analyzed fluid composition) any gases that may have exsolved from the deep fluid on its way to the ground surface. As shown by these earlier studies, the scatter of $\log(Q/K)$ curves can also be used to decipher, and correct for, dilution and/or other processes affecting the evolution of deep geothermal fluids.

The method of Reed and Spycher (1984) was developed for single-point fluid analyses and, although quite powerful, requires somewhat tedious data processing followed by temperature estimations relying on fairly subjective “eyeballing” of the clustering of computed $\log(Q/K)$ curves. For these reasons, the first goal of this

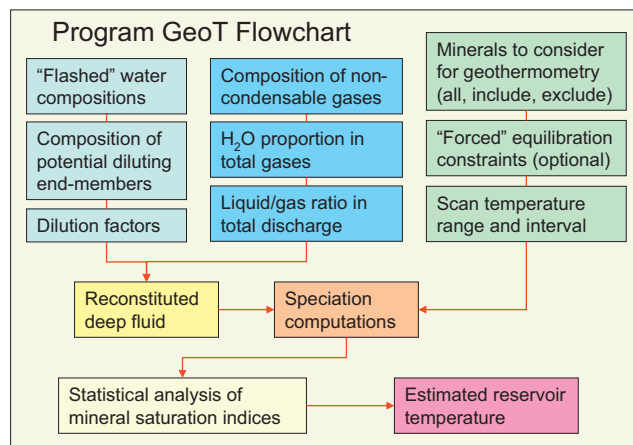


Fig. 2. General structure of the multicomponent geothermometry computer program GeoT. See Fig. 3 for the temperature estimation methodology.

study was to implement the method into a practical software tool that uses a set of objective criteria to estimate reservoir temperatures from computed mineral saturation indices for any given water composition. The second goal was to integrate the method with numerical optimization to allow simultaneous processing of multiple water analyses to estimate reservoir temperatures as well as unknown input parameters affecting the temperature estimations (such as the amount of dilution, if any, the degassed steam fraction and/or composition, or the concentrations of aqueous species that may not have been measured or that do not reflect reservoir conditions).

The approach followed in this study is essentially the automation of the method presented by Reed and Spycher (1984) into a stand-alone computer program (GeoT²), to ease and standardize temperature estimations, and to allow numerical optimization of model input parameters using existing parameter-estimation software. This paper presents the methodology implemented into the GeoT computer program, and its application to two previously published examples of geothermal waters. The program is then applied to experimental and simulated fluid compositions to examine the impact of fluid–rock disequilibrium on estimated temperatures by both multicomponent and classical geothermometry. This work extends preliminary materials presented earlier in a conference paper (Spycher et al., 2011). In a complementary paper (Peiffer et al., 2014), the integrated geothermometry approach presented below is applied to the Dixie Valley geothermal system, Nevada, including the simultaneous processing of multiple datasets with numerical optimization to provide insights on this complex geothermal field. The pros and cons of multicomponent and classical geothermometry is also further investigated by Peiffer et al. (2014) and Wanner et al. (2013, 2014), with application of both methods to Dixie Valley.

2. Technical approach

A computer program (GeoT, Fig. 2) was developed drawing on existing routines and methods implemented into programs TOUGHREACT (Xu et al., 2006, 2011), SOLVEQ/CHILLER (Reed, 1982, 1998) and GEOCAL (Spycher and Reed, unpublished, U. Oregon, 1985). The core of the software is essentially a homogeneous geochemical speciation algorithm solving mass-balance/mass-action equations by Newton–Raphson iterations (e.g., Reed, 1982). Using complete fluid analyses, the saturation indices of minerals ($\log(Q/K)$) are obtained from the computed ion activity product

² This computer program is available at <http://esd.lbl.gov/research/projects/geot/>.

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