QrtzGeotherm: A revised algorithm for quartz solubility geothermometry to estimate geothermal reservoir temperature and vapor fraction with multivariate analytical uncertainty propagation

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Abstract

The quartz solubility geothermometry to calculate geothermal reservoir temperature and vapor fraction with multivariate analytical uncertainty propagation is programmed as two classes, $\text{SiO}_2\text{TD}$ and $\text{QrtzGeotherm}$ in Visual Basic in Visual Studio 2010 (VB.NET). The class, $\text{SiO}_2\text{TD}$ calculates the total discharge concentration, $\text{SiO}_2\text{TD}$ and its uncertainty, $\text{SiO}_2\text{TD}\text{Err}$ from the analytical concentration of silica, $\text{SiO}_2\text{msd}$ and uncertainty, $\text{SiO}_2\text{msd}\text{Err}$ of separated water, sampled after N-separations of vapor and liquid. The class, QrtzGeotherm uses the following properties as input parameters: (i) $H\text{Res}$—reservoir enthalpy (kJ/kg), (ii) $H\text{Res}\text{Err}$—uncertainty in the reservoir enthalpy (kJ/kg), (iii) $\text{SiO}_2\text{TD}$—total discharge silica concentration (ppm), (iv) $\text{SiO}_2\text{TD}\text{Err}$—uncertainty in the total discharge silica concentration (ppm), (v) $\text{GeoEq}$—number of quartz solubility regression equation, (vi) $\text{TempGuess}$—a guess value of the reservoir temperature (°C). The properties corresponding to the output parameters are (i) $\text{TempRes}$—reservoir temperature (K), (ii) $\text{TempRes}\text{Err}$—uncertainty in the reservoir temperature (K), (iii) $\text{VaporRes}$—reservoir vapor fraction and (iv) $\text{VaporRes}\text{Err}$—uncertainty in the reservoir vapor fraction. Similarly, it has a method, $\text{SiO}_2\text{Eqn}(\text{EqNo}, \text{Temp})$ to provide the silica solubility as function of temperature corresponding to the regression equation. Four quartz solubility equations along the liquid–vapor saturation curve: (i) a quadratic equation of $1/T$ and pressure, (ii) a linear equation relating log $\text{SiO}_2$ to the inverse of absolute temperature ($T$), (iii) a polynomial of $T$ including logarithmic terms and (iv) temperature as a polynomial of $\text{SiO}_2$ including logarithmic terms are programmed. A demonstration program, QGeotherm is written in VB.NET. Similarly, the applicability of classes $\text{SiO}_2\text{TD}$ and QrtzGeotherm in MS-Excel is illustrated considering Los Azufres geothermal field as an example.

1. Introduction

The development of silica solubility geothermometers to estimate geothermal reservoir temperature from the fluid composition of surface manifestations was commenced with the pioneer work of White et al. (1956). The thermodynamic properties (or state functions) like solubility, equilibrium constant of a chemical reaction, etc. are functions of two independent thermodynamic variables (e.g. temperature and pressure). Therefore, the experimental data of quartz solubility have been fitted in various types of regression equations: (i) a quadratic equation of $1/T(K)$ and $P(MPa)$ (Verma, 2003), (ii) a linear equation relating log $\text{SiO}_2$ to the inverse of absolute temperature (Verma, 2002), (iii) a polynomial of absolute temperature including logarithmic terms (Gunnarsson and Arnórsson, 2000) and (iv) temperature as a polynomial of $\text{SiO}_2$ including logarithmic terms (Fournier and Potter, 1982). Using these equations, Verma (2008) presented an algorithm to calculate the deep geothermal reservoir temperature and vapor fraction with the quartz solubility geothermometry. The algorithm contemplates the conservation of mass and energy (enthalpy) and quartz solubility equilibrium in the geothermal reservoir and preservation of its signature in the fluid of surface manifestations (Henley et al., 1984).

The earlier version of QrtzGeotherm was written in Visual Basic 6.0 as an ActiveX component (Verma, 2008). ActiveX components had various problems which were described as DLL hell.1 These problems have been resolved in Visual Studio 2010. So, the new version of QrtzGeotherm is written as two classes, $\text{SiO}_2\text{TD}$ and QrtzGeotherm in Visual Basic in Visual Studio 2010 (VB.NET). The vital improvement in this new version is the incorporation of the multivariate analytical uncertainty propagation. Similarly, its use in MS-Excel is illustrated considering Los Azufres geothermal field as an example.

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2. Theory and algorithm

Fig. 1 shows the conceptual diagram of geothermal system for sample collection and chemical analysis of geothermal fluids. The numbering order of separators is inverted in the present computer code from that was presented by Verma (2008) since the programming of error propagation is easy to manage in the present order of separators. The algorithm is divided in two parts: (a) calculation of total discharge concentration and (b) geothermal reservoir temperature and vapor fraction. The measured uncertainties in the silica concentration and total discharged enthalpy are propagated first in the calculation of total discharge silica concentration and then in the calculation of geothermal reservoir temperature and vapor fraction.

2.1. Total discharge concentration with uncertainty propagation

The vapor fraction at the \(i\)th separator is expressed as:

\[
y(i) = \frac{H_l(i+1) - H_l(i)}{H_r(i) - H_l(i)}, \quad i = 1, 2, \ldots, NSep-1
\]

where \(NSep\) is the total number of separators. \(H\) is enthalpy and subscripts \(l\) and \(v\) represent the liquid and vapor phase.

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### Table 1

Quartz solubility regression equations, programmed in the class \(\text{QrtzGeotherm}\) (modified after Verma, 2008).

<table>
<thead>
<tr>
<th>Equation</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. [\log_{10}(\text{SiO}_2) = (5.8983 - 1894.6)T^{-0.27348}/C_0 + 0.23734 \times 10^{-6}P + (1.3577 \times 10^{10})/T^2 - 153.23 \times 10^{-6}3.3112 \times 10^{-15}/C_0^6 + 12.245\log T]</td>
<td>Quadratic of 1/T and P (Verma, 2003)</td>
</tr>
<tr>
<td>2. [\log_{10}(\text{SiO}_2) = -1117.34(\pm 13.05)/T + 4.78(\pm 0.03)]</td>
<td>Linear of 1/T (Verma, 2002)</td>
</tr>
<tr>
<td>3. [\log_{10}(\text{SiO}_2) = -38.955 + 197.47/T - 5.851 \times 10^{-6}T^2 + 12.245\log T]</td>
<td>Polynomial of T (Gunnarsson and Arnórsson, 2000)</td>
</tr>
<tr>
<td>4. [T = 230.952 + 0.28315\text{SiO}_2 - 3.6686 \times 10^{-6}\text{SiO}_2^2 + 3.1665 \times 10^{-7}\text{SiO}_2^3 + 77.03\log\text{SiO}_2]</td>
<td>Polynomial of SiO2 (Fournier and Potter, 1982)</td>
</tr>
</tbody>
</table>

* Temperature \((T)\) in K, pressure \((P)\) in Pa and SiO2 in ppm.

### Table 2

Properties of class, \(\text{SiO2TD}\).

<table>
<thead>
<tr>
<th>Property</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N\text{Sep})</td>
<td>Read–write</td>
<td>Number of separators.</td>
</tr>
<tr>
<td>(H\text{Res})</td>
<td>Read–write</td>
<td>Measured reservoir enthalpy ((\text{J/kg})).</td>
</tr>
<tr>
<td>(H\text{ResErr})</td>
<td>Read–write</td>
<td>Uncertainty in the measured reservoir enthalpy ((\text{J/kg})).</td>
</tr>
<tr>
<td>(P\text{Sep}(i))</td>
<td>Read–write</td>
<td>Measured pressure ((\text{Pa})) at the separator (i), where (i = 1) to (N\text{Sep}). The order of separators is defined in Fig. 1.</td>
</tr>
<tr>
<td>(T\text{Sep}(i))</td>
<td>Read only</td>
<td>Temperature ((\text{K})) along the separation boundary (i.e. liquid–vapor saturation curve) at the separator (i).</td>
</tr>
<tr>
<td>(\text{SiO2msd})</td>
<td>Read–write</td>
<td>Measured silica concentration ((\text{ppm})) in the liquid water sample in the first separator.</td>
</tr>
<tr>
<td>(\text{SiO2msdErr})</td>
<td>Read–write</td>
<td>Uncertainty in the measured silica concentration ((\text{ppm})) in the liquid water sample.</td>
</tr>
<tr>
<td>(\text{SiO2Sep}(i))</td>
<td>Read only</td>
<td>SiO2 concentration ((\text{ppm})) in the liquid phase at the separator (i). The concentration in the first separator ((\text{SiO2Sep}(1))) is internally assigned equal to (\text{SiO2msd}).</td>
</tr>
<tr>
<td>(\text{SiO2SepErr}(i))</td>
<td>Read only</td>
<td>Uncertainty ((\text{ppm})) in the SiO2 concentration in the liquid phase at the separator (i). The value in the first separator ((\text{SiO2SepErr}(1))) is internally assigned equal to (\text{SiO2msdErr}).</td>
</tr>
<tr>
<td>(y\text{Sep}(i))</td>
<td>Read only</td>
<td>Vapor fraction at the separator (i).</td>
</tr>
<tr>
<td>(\text{SiO2TD})</td>
<td>Read only</td>
<td>Calculated total discharge concentration ((\text{ppm})).</td>
</tr>
<tr>
<td>(\text{SiO2TDErr})</td>
<td>Read only</td>
<td>Uncertainty ((\text{ppm})) in the calculated total discharge concentration.</td>
</tr>
</tbody>
</table>
respectively. The vapor fraction at the NSep-separator is calculated as

\[ y_{\text{NSep}}(i) = \frac{H_{\text{Res}} - H_{l}(\text{NSep})}{H_{l}(\text{NSep}) - H_{l}(\text{NSep})} \]  

(2)

where \( H_{\text{Res}} \) is the reservoir enthalpy. The concentration of silica at the first separator is the measured concentration of water sample. The concentration at other separators is calculated as

\[ \text{SiO}_2(i + 1) = (1 - y(i)) \cdot \text{SiO}_2(i), \quad i = 1, 2, \ldots \text{to} \ldots \text{NSep} - 1 \]  

(3)

The total discharged concentration is

\[ \text{SiO}_2 TD = (1 - y(\text{NSep})) \cdot \text{SiO}_2(\text{NSep}) \]  

(4)

Similarly, the measured uncertainty of silica in the water sample is the uncertainty of silica at the first separator. The uncertainty of measured silica concentration is propagated according to the following equation:

\[ \text{SiO}_2 Err(i + 1) = (1 - y(i)) \cdot \text{SiO}_2 Err(i), \quad i = 1, 2, \ldots \text{to} \ldots \text{NSep} - 1 \]  

(5)

Table 3: Properties of class, QrztGeotherm.

<table>
<thead>
<tr>
<th>Property</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>HRes</td>
<td>Read–write</td>
<td>Measured reservoir enthalpy (J/kg)</td>
</tr>
<tr>
<td>HResErr</td>
<td>Read–write</td>
<td>Uncertainty in the measured reservoir enthalpy (J/kg)</td>
</tr>
<tr>
<td>SiO2TD</td>
<td>Read–write</td>
<td>Total discharge concentration (ppm)</td>
</tr>
<tr>
<td>SiO2TDErr</td>
<td>Read–write</td>
<td>Uncertainty (ppm) in the total discharge concentration</td>
</tr>
<tr>
<td>GeoEq</td>
<td>Read–write</td>
<td>Number of quartz solubility regression equation as given in Table 1</td>
</tr>
<tr>
<td>TempGuess</td>
<td>Read–write</td>
<td>The guess value of geothermal reservoir temperature (K)</td>
</tr>
<tr>
<td>TempRes</td>
<td>Read only</td>
<td>Calculated geothermal reservoir temperature (K)</td>
</tr>
<tr>
<td>TempResErr</td>
<td>Read only</td>
<td>Uncertainty (K) in the geothermal reservoir temperature</td>
</tr>
<tr>
<td>VaporRes</td>
<td>Read only</td>
<td>Vapor fraction in the geothermal reservoir</td>
</tr>
<tr>
<td>VaporResErr</td>
<td>Read only</td>
<td>Uncertainty in vapor fraction in the geothermal reservoir</td>
</tr>
</tbody>
</table>

Thus the uncertainty of total discharged concentration is

\[ \text{SiO}_2 TD Err = (1 - y(\text{NSep})) \cdot \text{SiO}_2 Err(\text{NSep}) \]  

(6)

2.2. Geothermal reservoir temperature and vapor fraction with uncertainty propagation

The distribution of fluid enthalpy between the liquid and vapor phases in the geothermal reservoir is written as

\[ H_{\text{Res}} = y_{\text{Res}} H_{\text{l},\text{Res}} + (1 - y_{\text{Res}}) H_{\text{v},\text{Res}} \]  

(7)

where \( H_{\text{l},\text{Res}} \) and \( H_{\text{v},\text{Res}} \) are the enthalpies of vapor and liquid phases in the geothermal reservoir, respectively. According to the conservation of enthalpy, the reservoir enthalpy (\( H_{\text{Res}} \)) is equal to the total discharge enthalpy (\( H_d \)).

Similarly, the equation for the conservation of silica is written as

\[ \text{SiO}_2 TD = (1 - y_{\text{Res}}) \cdot \text{SiO}_2(l,\text{Res}) \]  

(8)

where \( \text{SiO}_2(l,\text{Res}) \) is the silica concentration in the liquid phase in the geothermal reservoir. From Eq. (8), the fraction of vapor in the geothermal reservoir is

\[ y_{\text{Res}} = 1 - \frac{\text{SiO}_2 TD}{\text{SiO}_2(l,\text{Res})} \]  

(9)

The procedure to solve Eqs. (7)–(9) for geothermal reservoir temperature and vapor fraction is described by Verma (2008). It uses any of the four quartz solubility equations given in Table 1.

The independent variables are the measured enthalpy (\( H_d \)) and silica concentration (\( \text{SiO}_2 TD \)) in the total discharge, whereas the dependent variables are reservoir temperature (\( T_{\text{Res}} \)) and vapor fraction (\( y_{\text{Res}} \)). The uncertainty of independent variables is propagated to the dependent variables through the uncertainty propagation law (Arras, 1998). The equations for the uncertainty propagation are expressed in matrix notation as

\[ C_Y = F_X C_X F_X^T \]  

(10)

where \( C_Y \) is the \( p \times p \) output covariance matrix, \( F_X \) is a \( p \times n \) Jacobian matrix of a \( p \)-dimensional vector-valued function \( f(X) = [f_1(X), f_2(X), \ldots, f_p(X)]^T \), and \( C_X \) is \( n \times n \) input covariance matrix, which contains all variances and covariances of the input random...
Table 4
Listing of functions for calculating geothermal reservoir temperature and vapor fraction with multivariate uncertainty propagation in a Workbook in MS-Excel.

Public Function SIO2TD(NSep As Integer, PSep As Range, Hr As Double, SIO2md As Double, SIO2mdErr As Double) As Variant
Dim ObjSIO2TD As New Geotherms.SIO2TD
Dim MyMat() As Variant
Dim i As Integer
ObjSIO2TD.NSep = NSep
For i = 1 To NSep
  ObjSIO2TD.PSep(i) = PSep.Cells(i).Value
Next
ObjSIO2TD.HRes = Hr * 1000
ObjSIO2TD.SIO2md = SIO2md
ObjSIO2TD.SIO2mdErr = SIO2mdErr
ReDim MyMat(1 To 4)
MyMat(1) = ObjSIO2TD.SIO2TD
MyMat(2) = ObjSIO2TD.SIO2TDErr
SIO2TD = MyMat
End Function

Public Function GeoRes(Hr As Double, HrErr As Double, GeoEq As Integer, TGuess As Double) As Variant
Const TCK As Double
GeoEq = GeoEq
MyMat(1) = ObjGeoRes.TempRes-TCK
MyMat(2) = ObjGeoRes.TempResErr
MyMat(3) = ObjGeoRes.VaporRes
MyMat(4) = ObjGeoRes.VaporResErr
GeoRes = MyMat
End Function

Public Function GeoRes(Hr As Double, HrErr As Double, GeoEq As Integer, TGuess As Double) As Variant
Const TCK As Double
GeoEq = GeoEq
MyMat(1) = ObjGeoRes.TempRes-TCK
MyMat(2) = ObjGeoRes.TempResErr
MyMat(3) = ObjGeoRes.VaporRes
MyMat(4) = ObjGeoRes.VaporResErr
GeoRes = MyMat
End Function

Public Function GeoRes(Hr As Double, HrErr As Double, GeoEq As Integer, TGuess As Double) As Variant
Const TCK As Double
GeoEq = GeoEq
MyMat(1) = ObjGeoRes.TempRes-TCK
MyMat(2) = ObjGeoRes.TempResErr
MyMat(3) = ObjGeoRes.VaporRes
MyMat(4) = ObjGeoRes.VaporResErr
GeoRes = MyMat
End Function

Public Function TSiO2(SiO2TD As Double) As Double
End Function

Variables, $X_1, X_2, \ldots, X_n$. If the $X_i$'s are independent, all $\sigma_y$ with $i \neq j$ disappear and $C_X$ is diagonal.

In the case of quartz solubility geothermometry the input covariance matrix is

$$
C_X = \begin{bmatrix}
\sigma_{H_2}^2 & 0 \\
0 & \sigma_{SO_2TD}^2
\end{bmatrix}
$$

(11)

where $\sigma_{H_2}$ and $\sigma_{SO_2TD}$ are the uncertainties in the measured reservoir enthalpy and calculated total discharge silica concentration, respectively. From Eqs. (7)–(9), we can write the partial derivatives of $f_1$ and $f_2$ as

$$
\frac{\partial f_1}{\partial H_R} = \frac{1}{H_R-H_1}
$$

(12)

$$
\frac{\partial f_2}{\partial SO_2TD} = 0
$$

On substituting the Eqs. (11) and (12) in (10), we calculate the uncertainty in the geothermal reservoir temperature and vapor fraction.

3. Description of QtzGeotherm

A library, Geotherms.DLL was created in VB.NET. It contains two classes, SIO2TD and QtzGeotherm whose properties are given in Tables 2 and 3, respectively. The class QtzGeotherm has a method, SIO2Eqn(EqNo, Temp) to provide the silica solubility as function of temperature for the regression equations, where EqNo is the silica solubility equation number and Temp is the temperature in K. The method will be used in Excel to write a function to illustrate the difference between algorithms, presented here and used earlier for the silica geothermometry. The thermodynamic properties of water for internal calculation are calculated with SteamTables (Verma, 2003). Now, the SteamTables is rewritten in VB.NET and it is located in the library, ThermoData.DLL. The classes encapsulate the data and methods, and serve as blueprints for creating objects. The use of the classes in Excel will be presented later.

3.1. QGeotherm: a demo

A demonstration program was written in VB.NET. The program can be downloaded from the journal webpage or requested from the author. It can be installed with running the setup program which is contained in the default folder, C:\ProgramFiles\QGeotherm.

Fig. 2 shows the user interface of QGeotherm. User has to provide the following parameters: number of separators, pressures, reservoir enthalpy, error (uncertainty) in enthalpy, measured silica concentration, error in the measured silica concentration and guess value of reservoir temperature, and select at least one silica solubility regression equation. Then press the button “Calculate”. It calculates the reservoir temperature and vapor fraction with their corresponding uncertainties. The XY plot serves for the visualization of calculations. The white horizontal line intersects the corresponding quartz solubility curves as a function of enthalpy and temperature at the reservoir temperature (Fig. 2). The calculated results with respective uncertainties are shown in the group boxes: total discharge and results.
3.2. Using QrtzGeotherm in MS-excel

The library (Geotherms.DLL) can be used in any computer programming language in the Windows environment. However, its use in Excel for geochemical calculations will be explained here; since most geochemists use Excel for geochemical data management and calculations. During the installation of the demonstration program QGeotherm the installation of Microsoft Framework and registration of the libraries QrtzGeotherm and ThermoData are carried out automatically. The libraries were compiled on the framework version “v4.0.030319”. Otherwise one has to download and install a higher version of Framework from Microsoft Webpage and register the libraries. The first step is to extract the libraries, Geotherms and ThermoData from the file “QrtzGeotherm.MSI” in a folder. To extract files from a.msi file at the command line, type:2

```
msiexec/a PathToMSIFile/qb TARGETDIR=D:\ToExtractTo
```

Then change the folder, which contains the libraries in the command window and issue the following command to register the library, Geotherms

```
C:\Windows\Microsoft.NET\Framework\v4.0.30319\regasm.exe Geotherms.DLL
```

Similarly, the command to unregister the library, Geotherms is

```
C:\Windows\Microsoft.NET\Framework\v4.0.30319\regasm.exe/u Geotherms.DLL
```

The path of “regasm.exe” may be different in your computer. So, search for “regasm.exe” to find its path in your computer. Similarly, the library ThermoData.DLL for the thermodynamic properties of water must be registered.

Verma (2003) explained the procedure for writing a function in the personal workbook of Excel. A macro stored in this location will be available for all the workbooks. For using the classes in the libraries, QrtzGeochem and Thermodata it is needed to perform the following steps:


2. Creating functions: write the code given in Table 4 in a module in the personal workbook (PERSONAL.XLSB). There are three functions, SI02TD, GeoRes and TSIO2 in Table 4. Save the personal workbook. Now, the function can be used in any workbook.

The functions, SI02TD(NSep, PSep, Hr, SI02msd, SI02msdErr) and GeoRes(Hr, HrErr, SI02TD, SI02TDErr, GeoEq, TGuess) are written as array formulas. An Array Formula in Excel is a formula that uses arrays (many cells) instead of single cell value as input–output and may be considered as many formulas packed into a single super formula.3 The input parameters of SI02TD are the number of separators, separation pressures as a variable of range type, total discharge enthalpy, measured silica concentration and its uncertainty, respectively. It calculates the total discharge silica concentration and its uncertainty as an array formula. Similarly, the input parameters of function GeoRes are total discharge enthalpy and its uncertainty, and the total discharge silica concentration and its uncertainty, respectively. It calculates the geothermal reservoir temperature and vapor fraction and their respective uncertainties as an array formula.

3.3. Los Azufres geothermal system

The analytical data of wells from Los Azufres geothermal field are taken from Arellano et al. (2005). The data are well ID (Well), total discharge enthalpy (Hr), separation temperature (TSep) and

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measured silica concentration \( (\text{SiO}_2\text{msd}) \) of water samples, collected at the weir box (Fig. 3). The atmospheric pressure is considered as \( 1 \times 10^5 \text{ Pa} \). Firstly, the separation pressure \( (P_{\text{sep}}) \) is calculated using the SteamTables (Verma, 2003). For example, the separation temperature of well 5 is 180 °C. Using the SteamTables, the separation pressure is calculated as 1,002,635 Pa. The analytical uncertainty (error) is not reported in the analytical data of geothermal system. Verma et al. (submitted for publication) conducted an interlaboratory comparison of silica analysis in water samples. They found that the analytical uncertainty in the silica analysis is more than 10%. Similarly, the uncertainty in the measurement of enthalpy is considered as 2%. Using the Excel function \( \text{SiO}_2\text{TD} \), the total discharge silica concentration \( (\text{SiO}_2\text{TD}) \) and its uncertainty \( (\text{SiO}_2\text{TDErr}) \) are calculated. In the case of well 5, the input parameters are the number of separators \( (N_{\text{sep}}=2) \), separation pressures \( (P_{\text{sep}} \text{ as range type} = 100,000, 1,002,635 \text{ Pa}) \), total discharge enthalpy \( (H_r = 2224 \text{ kJ/kg}) \), silica concentration in the water sample \( (\text{SiO}_2\text{msd} = 991 \text{ ppm}) \) and its uncertainty \( (\text{SiO}_2\text{msdErr} = 99.1 \text{ ppm}) \). Thus the total discharge concentration is 230.5 ppm with its uncertainty as 23.1 ppm. The propagation of uncertainty for the total discharge concentration is linear; therefore, the uncertainty in \( \text{SiO}_2\text{TD} \) is also 10%.

Now, the geothermal reservoir temperature and vapor fraction and their uncertainties are calculated using the Excel function GeoRes. In the case of well 5, the input parameters are \( H_r = 2224 \text{ kJ/kg}) \), \( H_{\text{Err}} = 2\% = 444.8 \text{ kJ/kg} \), \( \text{SiO}_2\text{TD} = 230.5 \text{ ppm} \), \( \text{SiO}_2\text{TDErr} = 23.1 \text{ ppm} \), GeoEQ = 1 to 4 and \( T_{\text{Guess}} = 150 \text{ °C} \). Thus the calculated reservoir temperature and vapor fraction are \( T_{\text{Res}} = 293.3 ± 20.7 \text{ °C} \) and \( y_{\text{Res}} = 0.631 ± 0.03 \). The present algorithm is based on the conservation of enthalpy; therefore, the enthalpy of the liquid and vapor at the reservoir temperature is the same as the total discharge enthalpy, i.e. we assume there has been no vapor loss or vapor gain between the deep fluid and the fluid reaching the surface.

The quartz geothermometry is mostly applied considering only the liquid phase in the reservoir (e.g. Henley et al., 1984). To illustrate it, a function, \( \text{TSio2}/\text{SiO}_2\text{TD} \) is written with using Eq. (2) of quartz solubility in Excel (Table 4). The function \( \text{TSio2} \) is written considering the second quartz solubility equation, but it can be modified for any equation. The algorithm for Eq. (1) will be slightly different. The input parameter is the total discharge concentration \( (\text{SiO}_2\text{TD} = 230.5 \text{ ppm}) \). Thus the calculated reservoir temperature for well 5 is \( \text{TSio2} = 189.08 \text{ °C} \). This value of temperature is lower than that calculated with the present algorithm based on the conservation of enthalpy. However, if we calculate the geothermal reservoir enthalpy, \( H_{\text{LiqSiO2}} \) at the reservoir temperature \( \text{TSio2} \), the enthalpy 808.3 kJ/kg is much lower than the measured total discharge enthalpy 2224 kJ/kg (see Fig. 3). This means that the conservation of enthalpy in silica geothermometry is a prerequisite.

The uncertainty in the geothermal reservoir temperature obtained from quartz geothermometry is relatively large. The range of uncertainty is \( ± 10 \text{ to } ± 25 \text{ °C} \) with an average of \( ± 18 \text{ °C} \). Therefore, the analytical quality of silica analysis in geothermal water is very important (Verma et al., submitted for publication).

Fig. 4 shows the comparison of temperature and reservoir enthalpy, calculated from quartz geothermometry using the present algorithm (i.e. conservation of enthalpy) and the algorithm used in literature (i.e. liquid only in the reservoir). It can be observed in Fig. 4(a) that the geothermal reservoir temperature of all the wells is significantly higher for the present algorithm than that used in the literature except for wells 22 and 26.

Fig. 4(b) shows a relation between the measured and calculated enthalpies using the both the algorithms. The calculated enthalpies for well 26 are close since the vapor fraction \( (y_{\text{Res}} = 0.131) \) is low. As the vapor fraction increases the difference between the calculated enthalpies increases. The present algorithm is based on the conservation of enthalpy; therefore the measured and calculated enthalpies are same. If we consider the liquid only in the reservoir, there will be substantially low enthalpy in the reservoir. The energy loss is not feasible; therefore the present algorithm is an improved in the quartz geothermometry.

4. Conclusions

The quartz solubility geothermometry programmed as two classes, \( \text{SiO}_2\text{TD} \) and \( \text{QrtzGeotherm} \) in the library, \text{Geotherm} in VB.NET is an accurate and efficient approach to estimate the deep geothermal reservoir temperature and vapor fraction with multivariate analytical uncertainty propagation. The library \text{Geotherm} can be implemented in any programming environment including Excel.

The calculation of temperature and vapor fraction in the geothermal reservoir of Los Azufres geothermal system is...
illustrated with considering the analytical uncertainty of enthalpy (2%) and SiO₂ concentration (10%). The average uncertainty in the calculated reservoir temperature is ±18 °C, which is relatively high to understand reservoir processes during the exploitation of the geothermal reservoir. Thus the geochemical analysis of geothermal water is first improvement that must be made to obtain a better understanding of the characteristics of geothermal systems with fluid geochemistry. The algorithm of quartz geothermometry with considering only liquid phase in the geothermal reservoir is conceptually incorrect due to lacking of energy (enthalpy) balance. However, both the algorithms provide same results for the wells, which are fed from a single phase liquid reservoirs.

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Appendix A. Supplementary materials

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.cageo.2012.01.008.

References


