United States Department of the Interior
Geological Survey

FORTRAN Program to Compute
Chemical Geothermometers for Geothermal Fluids

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Preface

The GEOTHERM Information System is a comprehensive system of databases and software to maintain data on the geology, geochemistry and hydrology of geothermal systems, both nationally and internationally. The information system is made up of four databases and software to assist in data entry, quality assurance, operations, and to generate useful outputs for system users. The system is housed on the U.S. Geological Survey Amdahl computer and inquiries for retrievals from system databases may be made of the GEOTHERM staff at the address given below. The database on geochemistry is also available to subscribers of the General Electric Mark III System, an internationally available timeshare network. General Electric customer support is available at 800-638-8730.

This report addresses a GEOTHERM user-support software package used to generate geothermometer values from data in the Sample File which contains geochemical information on fluids from geothermal springs and wells. Both the FORTRAN code and associated documentation have been included. The program has been carefully checked and used for some time but users are advised to spot check the results from it as computer software can be less fool proof than one might hope. Readers of this report are encouraged to inform the Data Base Manager, GEOTHERM Information System, U.S. Geological Survey, 345 Middlefield Rd. MS 84, Menlo Park, CA 94024, of any omissions or errors. Comments or requests for further information are invited.

James D. Bliss
Data Base Manager
GEOTHERM Information System
INTRODUCTION

Chemical geothermometers represent one method of estimating temperature conditions at depth in geothermal systems. However, geothermometer results are not valid unless reaction rates are sufficient to bring fluid and minerals in the confining rock to equilibrium at the temperature of the geothermal reservoir. At the same time, the water-mineral reactions must be sluggish enough so as not to re-equilibrate as the fluids move to the surface or to the point at which the sample was collected. Concentrations of elements used for geothermometers should be high enough for equilibrium processes to be valid (Ellis and Mahon, 1977).

Geothermometer results should always be evaluated with respect to geology, hydrology and chemical properties of the fluids. Variation between the geothermometers for the same sample may reflect different chemical species equilibrating at different points in the geothermal system (Fournier, 1981). Mixing of geothermal fluids with other subsurface water can radically modify the chemistry. Geothermometer results should therefore be used with care, and the limitations and strengths of each should be fully understood.

The FORTRAN program given here calculates geothermometer values using silica, sodium, potassium and calcium from the results of chemical analyses of geothermal waters. In the case of the Na-K-Ca geothermometer, a correction is available using magnesium. This operation is described in Fournier and Potter (1978).

This program was specifically designed to be used with data from the GEOTHERM Sample file. The portions of the program that deal with the peculiarities of the GEOTHERM format are explained and a modified version of the program, suitable for use with more generalized data, is given. This paper documents the program so that it can be used by those with a rudimentary understanding of FORTRAN.
BACKGROUND OF PROGRAM

The geothermometer program was developed in order to facilitate the U. S. Geological Survey's assessment of low-temperature geothermal resources of the United States. The source of input data for the program is the Sample File. This program requires input data and generates some output which may or may not be necessary for general applications. In addition to the chemical constituents used to calculate the geothermometers, the input and output include the GEOTHERM record number; the temperature of the sample; the name of the sample source; the state, county, township, and range in which the source is located; the depth if the source is a well; pH; total dissolved solids; and the flow rate. The program calculates the total dissolved solids, the silica and the cation geothermometers and calculates and applies a magnesium correction when appropriate.

The equations used in the program are taken from Fournier (1977) and are given below:

GEOTHERMOMETERS

Silica

Quartz (conductive) \[ TQC = \frac{1309}{5.19 - \log SiO_2} - 273.15 \]

Quartz (adiabatic) \[ TQA = \frac{1522}{5.75 - \log SiO_2} - 273.15 \]

Chalcedony \[ TCH = \frac{1032}{4.69 - \log SiO_2} - 273.15 \]

Alpha-cristobalite \[ TCR = \frac{1000}{4.78 - \log SiO_2} - 273.15 \]

Amorphous silica \[ TAM = \frac{731}{4.52 - \log SiO_2} - 273.15 \]

All concentrations are in mg/l or ppm and results are given in degrees C.
Cations

\[
\text{NA-K (TNAK)} = \frac{1217}{\log(\text{Na/K}) + 1.483} - 273.15
\]

\[
\text{NA-K-Ca (T13 or T43)} = \frac{1647}{\log(\text{Na/K}) + B \log(\sqrt{\text{Ca}}/\text{Na}) + 2.24} - 273.15
\]

Where \(B = \frac{1}{3}\) and \(\frac{4}{3}\) for T13 and T43 respectively.

All concentrations are in molality and results are given in degrees C.

A correction is made to the NA-K-Ca geothermometers for the Mg content of the solution if the ratio of Mg/(Mg+Ca+K) (in equivalent percent) is greater than 0.5 and less than 50. The criteria, procedure and equations for application of this correction are given in Fournier and Potter (1978). The equations used for the Mg correction are as follows:

For \(5.0 < R < 50\).

\[
\text{DMG13 or} \quad = 10.66 - 4.7415xR + 325.9(\log R)^2 - \frac{103210(\log R)^2}{TKb} - \\
\text{DMG43} \quad \frac{1.97 \times 10^7(\log R)^2 + 1.61 \times 10^7(\log R)^3}{(TKb)^2}
\]

For \(0.5 < R < 5\).

\[
\text{DMG13 or} \quad = -1.03 + 59.97(\log R) + 145.05(\log R)^2 - \frac{36711.(\log R)^2 - 1.67 \times 10^7(\log R)}{TKb} \frac{1}{(TKb)^2}
\]

Where \(R = 100 \times \frac{\text{MGE}}{(\text{MGE+CAE+KE})}\)

\(\text{MGE} = \frac{\text{Mg/molecular weight Mg}}{}\)

\(\text{CAE} = \frac{\text{Ca/(molecular weight Ca/2)}}{}\)

\(\text{KE} = \frac{\text{K/molecular weight K}}{}\)

\(\text{TKb} = \frac{\text{Na-K-CA(1/3) or Na-K-Ca(4/3) temperature in Kelvin for b equal to 1/3 or 4/3 respectively}}{}\)
The equation used for calculation of total dissolved solids is given below:

\[ \text{CTDS} = \frac{\text{HC03}}{2.03} + \text{SI02} + \text{NA} + \text{CA} + \text{MG} + \text{CL} + \text{CO3} + \text{SO4} + \text{B} + \text{F} \]

All concentrations are in mg/l or ppm.

**EXPLANATION OF OUTPUT**

Three possible outputs of the geothermometer program are shown in figures la, lb, and lc. In all cases four sections are given for each output record: site identification and location, physical properties (temperature, flow, etc.), water chemistry, and geothermometers. Temperatures given under 'Mg corrected' in figure la are the results for the Na-K-Ca geothermometers, if adjusted for the Mg content. When this adjustment is made, a reduction in geothermometer temperature occurs. If the Mg correction is less than zero it is not used. If the Mg content is very low relative to the other constituents (i.e. \( \text{Mg}/(\text{Mg}+\text{Ca}+\text{K}) < 0.5 \), in equivalent percent) no correction is calculated. In either case, 'none' will appear under 'Mg corrected' (Figure lb). If the Mg content is relatively high, (i.e. \( \text{Mg}/(\text{Mg}+\text{Ca}+\text{K}) > 50 \), in equivalent percent), Fournier and Potter (1978) suggest that the measured temperature probably represents the point at which the solution equilibrated. Therefore higher values derived from Na-K-Ca geothermometers calculations are invalid. In this case the word 'cool' will appear under 'Mg corrected' (Figure lc) and the measured temperature is likely to be the maximum temperature.

The structure of the Sample File allows numeric fields, such as the results of chemical analyses, to be qualified and the presence of a qualifier will cancel calculation of a geothermometer. Possible qualifiers are G (greater than), L (less than), R (mid-point of a range), E (estimate), N (not detected), T (trace) or Q (qualified, further explanation included in record). Qualifiers precede numeric observations and are separated from them by at least one blank (Figure la).
**Figure 1a.** Output of geothermometer program. Adjusted cation geothermometers appear under 'MG CORRECTED'. CL is an example of a qualified field. The L preceeding the 2.00 indicates that there were less than 2.00 mg/l of Cl in the solution.
RECORD NO. ..........  1469
NAME OF SOURCE... UNNAMED WELL WEST OF HUECO AIRPORT (1)
STATE............. TEXAS
COUNTY............ EL PASO

TOWNSHIP RANGE SECTION

WELL DEPTH (M) ..  146.
FLOW RATE .......  38.
WATER TEMPERATURE ........ 38.

WATER CHEMISTRY (MG/L)
SiO2 .... 29.00  Cl .... 0.00  F .... 0.90
Na .... 97.80  HCO3 .... 158.00  PH .... 8.2
K ...... 1.30  CO3 .... 0.0  TOTAL DISSOLVED SOLIDS
Ca ...... 2.80  SO4 .... 32.80  RECORDED .... 285.
Mg ...... 0.20  B ...... 0.06  CALCULATED .... 276.

GEOTHERMOMETERS (DEGREES C)
SILICA - CONDUCTIVE ....  76.
ADIABATIC ....  82.
CHALCEDONY ....  47.
CRISTOBALITE ....  28.
AMORPHOUS .... -34.
 NA-K .............  66.
NA-2-Ca(1/3) ....  97.
NA-K-Ca(4/3) ....  74.
MG CORRECTED
NONE

Figure 1b. The word 'NONE' appearing below 'MG CORRECTED' indicates
that either the magnesium correction produced a negative value or the ratio
of Mg/Mg+Ca+K was less than 0.5.
RECORD NO........ 17623
NAME or SOURCE... HONEY POT
STATE............ UTAH
COUNTY........... GARFIELD

TOWNSHIP RANGE SECTION
36S 011E 06

WELL DEPTH(M)....
FLOW RATE......... E 7.6
WATER TEMPERATURE... 23.

WATER CHEMISTRY (MG/L)

<table>
<thead>
<tr>
<th>SIO2</th>
<th>CL</th>
<th>F</th>
<th>TEMP</th>
<th>TDS</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.00</td>
<td>15.00</td>
<td>0.40</td>
<td>23.00</td>
<td>2790.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Na</th>
<th>300.00</th>
<th>HC03</th>
<th>405.00</th>
<th>PH</th>
</tr>
</thead>
<tbody>
<tr>
<td>300.00</td>
<td>0.00</td>
<td>23.00</td>
<td>2790.00</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>K</th>
<th>13.00</th>
<th>CO3</th>
<th>0.00</th>
<th>2790.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.00</td>
<td>0.00</td>
<td>23.00</td>
<td>2790.00</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ca</th>
<th>190.00</th>
<th>S04</th>
<th>1800.00</th>
<th>2790.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>190.00</td>
<td>0.00</td>
<td>23.00</td>
<td>2790.00</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mg</th>
<th>260.00</th>
<th>B</th>
<th>0.12</th>
<th>2780.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>260.00</td>
<td>0.12</td>
<td>23.00</td>
<td>2780.00</td>
<td></td>
</tr>
</tbody>
</table>

GEOTHERMOMETERS (DEGREES C)

<table>
<thead>
<tr>
<th>SILICA - CONDUCTIVE</th>
<th>NA-K</th>
<th>NA-K-Ca(1/3)</th>
<th>NA-K-Ca(4/3)</th>
<th>MG CORRECTED</th>
</tr>
</thead>
<tbody>
<tr>
<td>42.0</td>
<td>122.0</td>
<td>131.0</td>
<td>70.0</td>
<td>COOL</td>
</tr>
</tbody>
</table>

Figure 1c. The work 'COOL' appearing below 'MG CORRECTED' indicates that the ratio of Mg/Mg+Ca+K was greater than 50.
Whenever a geothermometer can not be calculated, either because a critical solute was not present in the analysis or one of the solutes is qualified, zero (0.0) will be printed in the output for that geothermometer.

PROGRAM EXPLANATION

The program consists of three loops. The first reads the input and stores it in arrays. The second loop carries out the necessary computations on all input records and the third writes the output. The program can handle up to 1000 records, however, this amount can easily be increased or decreased by changing the dimension of the arrays. If the program is to be used on substantially fewer than 1000 input records it would be advisable to decrease the dimension so that large amounts of unused core space would not be allocated.

In order to calculate geothermometers, the minimum input requirements of the program are SiO₂, Na, K, and Ca. Mg concentration is needed if that correction is used. Other input variables are not necessary for the calculations and were included to fill the needs of the low-temperature assessment work. Some or all these input variables may be eliminated from the program or not entered as input without affecting the geothermometer calculations. However, some factors such as pH are very useful for evaluating the validity of the results. For example, the silica geothermometers are not valid for pH greater than 8.5.

DEFINITION OF VARIABLES

Input Variables

NUM - GEOTHERM record number. 'I' format, maximum length = 7

NAME1, NAME2, NAME3, NAME4, NAME5 - Name of sample source, that is the name of the spring or well from which the sample was taken. The NAME variables are read using an 'A' format, therefore any alphanumeric character is an acceptable value for the variables and, taken together, can handle a name up to 40 characters in length.
STATE1, STATE2 - The name of the state in which the sample site is located. 'A' format, maximum length = 8 (total of 16)

COUN1, COUN2 - The name of the county in which the sample site is located. 'A' format, maximum length = 8 (total of 16)

TWNS - Township. 'A' format, maximum length = 3

RANGE - Range. 'A' format, maximum length = 4

SECT - Section. 'A' format, maximum length = 3

WELLD - The depth of well if sample is from a well. 'A' format, maximum length = 7

FLOW, RATE - FLOW is the discharge of the sample and RATE is the units used in measuring it. FLOW, 'A' format, maximum length = 8

RATE, 'A' format, maximum length = 8

WTEMP - Measured temperature of the sample. All GEOTHERM temperatures are given in degrees C. 'A' format, maximum length = 6

UNITS - Units used for measuring solutes in sample. 'A' format, maximum length = 4

PH - pH of sample. 'A' format, maximum length = 6

SIO2, NA, K, CA, MG, F, CL, HCO3, CO3, SO4, B - Solutes measured in sample, each variable is the same as the chemical abbreviation (Except all letters are upper case). All are real variables and must include a decimal point. 'F' format, maximum length = 8.2 (Two places to the right of the decimal)

QSI02, QNA, QK, QCA, QMG, QF, QCL, QHCO3, QC03, QS04, QB - Qualifier for each solute. These variables are necessary because no qualified value is used in the geothermometer calculations, qualified fields are treated by the program as if they have a value of zero. 'A' format, maximum length = 1

RTDS - Recorded total dissolved solids (i.e. any value listed in the GEOTHERM record for dissolved solids). 'A' format, maximum length = 8

Calculated Variables

CTDS - Total dissolved solids as calculated by this program from concentrations of the chemical variables entered as input. The resultant value of the calculation is rounded to the nearest ten if it exceeds 1000. 'F' format, maximum length = 8.0

TQC - Silica geothermometer, quartz conductive. 'F' format, maximum
length = 6.0

TCH - Silica geothermometer, chalcedony. 'F' format, maximum length = 6.0

TQA - Silica geothermometer, quartz adiabatic. 'F' format, maximum length = 6.0

TCR - Silica geothermometer, alpha-cristobalite. 'F' format, maximum length = 6.0

TAM - Silica geothermometer, amorphous silica. 'F' format, maximum length = 6.0

TNAK - NA-K geothermometer. 'F' format, maximum length = 6.0

T13 - NA-K-CA (1/3) geothermometer, uncorrected. 'F' format, maximum length = 6.0

T43 - NA-K-CA (4/3) geothermometer, uncorrected. 'F' format, maximum length = 6.0

TMG13 - NA-K-CA (1/3) geothermometer, corrected for MG. 'F' format, maximum length = 6.0

TMG43 - NA-K-CA (4/3) geothermometer, corrected for MG. 'F' format, maximum length = 6.0

Miscellaneous Variable

LABEL - This variable is used as a flag which keeps track of status of the MG corrections for each record. The value of label determines the format to be used in the 'MG corrected' portion of the output. Integer variable, possible values = 0,1,2,3,4

INPUT FORMAT

Consists of two lines, each having a blank in column one.

Line one = NUM  cols 2-8
NAME1, NAME2, NAME3, NAME4, NAME5  cols 9-48
STATE1, STATE2  cols 49-64
COUN1,COUN2  cols 65-80
TWNS  cols 81-83
RANGE  cols 84-87
SECT  cols 88-90
WELLD  cols 91-97
FLOW  cols 98-115
RATE  cols 116-121
WTEMP  cols 122-127
UNITS  cols 128-131
PH  cols 132-137
A listing of the original program, which uses Sample File input is given in Appendix A. Appendix B lists a modified version of the program which can be used on more generalized input data. The portions of the original program that were altered or removed to create the revised version are outlined in Appendix A. The major effect of the revisions is to reduce the number of input and output variables and to eliminate all lines that deal with the Sample File qualifiers. In the new version of the program, the input and output consists of the concentration of the solutes which are required to calculate the geothermometers and some basic identifying information (e.g., Sample number, source name, state, county, temperature and pH). Appendix B also contains a sample of an input file for the revised version of the program and output produced by it.

The program listings follow. Any line with a 'C' in column one is a
comment and a '1' in column six indicates the line is a continuation of the preceding line.

Appendix C is an annotated listing of the Job Control Language (JCL) and Gipsy commands which must surround the program if it is run on the Amdahl computer system in Reston and GEOTHERM is used as the source of input data.

REFERENCES CITED


APPENDIX C

(job name) (acct. num) (user name) (class in descending priority may be H,A,B,C,D,E,F)

//MG9279MN JOB ($$$,B200,15,100), 'RAPPORT', CLASS=A
//A EXEC QUESTRAN, DNAME='RIF.W0020.THERM', RNAME='RIF.W0020.THERM', RVOL=CCD821,
// DUNIT='3330-1', RNAME='RIF.W0040.GEOD1', RVOL=CCD812,
// UNIT='3330-1', CLOCK=15, SPACE=800, RGN=110K, LINE=132
// QUESTRAN.SYSWRKO DD DSN=&&TEMP, UNIT=SYSDK, DISP=(NEW, PASS),
// DCB=(RECFM=FB, LRECL=132, BLKSIZE=132),
// SPACE=(CYL, (10, 1), RLSE)
// QUESTRAN.SYSRDR DD *
FORM
SAMPLE
SELECT
A. B60<UTAH> (Gipsy select variable and logic statement)
LOGIC A
SORT
B60 20
B65 20
B20 25
COPY
A10 7
B20 40
B60 16
B65 16
B95 3
B105 4
B115 3
M25 7
M220 8
M23 6
M210 6
M341 4
M20 6

NEW RECORD

M130 10
M40 10
M50 10
M60 10
M70 10
M80 10
M140 10
M580 10
M110 10
M120 10
M90 10
M23 8

/*
//B EXEC FTGICLGL, REGION.FORT=120K, REGION.GO=450K (FORTRAN compiler, load and go.)
//FORT.SYSIN DD *

// GO.FT02F001 DD DSN=&&TEMP, UNIT=SYSDK, DISP=(OLD, DELETE) (Input to program)
// GO.FT04F001 DD SYSOUT=A, DCB=(RECFM=FAB, LRECL=133, BLKSIZE=12901) (Output from program)
*/
APPENDIX A

Original Geothermometer program.

IMPLICIT REAL*8 (A-Z)
DIMENSION NAME1(1000),NAME2(1000),NAME3(1000),NAME4(1000)
DIMENSION STATE1(1000),STATE2(1000),COUN1(1000),COUN2(1000)
DIMENSION TWNS(1000),SECT(1000),WELLD(1000),RANGE(1000)
DIMENSION FLOW(1000),RATE(1000),WTEMP(1000),UNITS(1000),PH(1000)
DIMENSION SI02(1000),NA(1000),K(1000),CA(1000),MG(1000),F(1000)
DIMENSION CL(1000),HCO3(1000),CO3(1000),SO4(1000),B(1000)
DIMENSION RTDS(1000),CTDS(1000),TQC(1000),TCH(1000)
DIMENSION TA(1000),TCR(1000),NAME5(1000)
DIMENSION TAM(1000),TNAK(1000),T13(1000),T43(1000),TMG13(1000)
DIMENSION RTDS(1000),CTDS(1000),TQC(1000),TCH(1000)
DIMENSION TQA(1000),TSTR(1000)
DIMENSION TAM(1000),TNAK(1000),T13(1000),T43(1000),TMG13(1000)
DIMENSION RTDS(1000),CTDS(1000),TQC(1000),TCH(1000)
DIMENSION TQA(1000),TSTR(1000)
DIMENSION TAM(1000),TNAK(1000),T13(1000),T43(1000),TMG13(1000)

INTEGER*2 QSI02(1000),QNA(1000),QK(1000),QCA(1000),QMG(1000)
INTEGER*2 QCL(1000),QHCO3(1000),QCO3(1000),QSO4(1000),QB(1000)
INTEGER*2 QF(1000),BLANK

INTEGER I,LABEL(1000),NUM(1000),J,M,N,L
DATA BLANK/1HJ/

TK=273.15

C-- MWNA=MOLECULAR WEIGHT NA, MWK=MOLECULAR WEIGHT K, MWCA=MOLECULAR WEIGHT CA AND MWMG=MOLECULAR WEIGHT MG

MWNA=23.
MWK=39.1
MWCA=40.08
MWMG=12.16

C-- READ VALUES OF ALL VARIABLES

DO 5 J=1,1000
READ(2,10,END=30) NUM(J),NAME1(J),NAME2(J),NAME3(J),NAME4(J),
1 NAME5(J),
1 STATE1(J),STATE2(J),COUN1(J),COUN2(J),TWNS(J),RANGE(J),SECT(J),
1 WELLD(J),FLOW(J),RATE(J),WTEMP(J),UNITS(J),PH(J)
10 FORMAT(1X,I7,9A8,A3,A4,A3,A7,A8,A6,A6,A4,A6)
IF (NUM(J).EQ.O) GO TO 30

C-- INITIALIZE ALL QUALIFIERS TO BLANK WHICH CONSISTS OF A NONPRINTING PAD CHARACTER

QSI02(J)=BLANK
QNA(J)=BLANK
QK(J)=BLANK
QMG(J)=BLANK
QCL(J)=BLANK
QHCO3(J)=BLANK
QSO4(J)=BLANK
QB(J)=BLANK
QF(J)=BLANK
QCA(J)=BLANK
QCO3(J)=BLANK

C-- READ VALUES OF ALL SPECIES AND THEIR QUALIFIERS

READ(2,25) QSI02(J),SI02(J),QNA(J),NA(J),QK(J),K(J),QCA(J),CA(J),
1QMG(J),MG(J),QCL(J),CL(J),QHC03(J),HC03(J),QC03(J),C03(J),QS04(J),
1SO4(J),QB(J),B(J),QF(J),F(J),RTDS(J)
25 FORMAT(1X,11(A1,1X,F8.2),A8)___________________________
5 CONTINUE
30 DO 80 M=1,L
   LABEL(M)=0_______________________________________
   XCT£ 03=HC03(M)
   XSI02=SI02(M)
   XNA=NA(M)
   XK=K(M)
   XCA=CA(M)
   XMG=MG(M)
   XCL=CL(M)
   XC03=C03(M)
   XS04=S04(M)
   XB=B(M)
   XF=F(M)
C-- CHECK FOR QUALIFIERS AND SET INTERMEDIATE VALUES TO ZERO
C-- QUALIFIED VALUES ARE NOT USED IN ANY OF THE GEOTHERMOMETER
C-- CALCULATIONS
C--
   IF(QHC03(M).NE.BLANK) XHC03=0.
   IF(QSI02(M).NE.BLANK) XSI02=0.
   IF(QNA(M).NE.BLANK) XNA=0.
   IF(QK(M).NE.BLANK) XK=0.
   IF(QCA(M).NE.BLANK) XCA=0.
   IF(QMG(M).NE.BLANK) XMG=0.
   IF(QCL(M).NE.BLANK) XCL=0.
   IF(QC03(M).NE.BLANK) XC03=0.
   IF(QS04(M).NE.BLANK) XS04=0.
   IF(QB(M).NE.BLANK) XB=0.
   IF(QF(M).NE.BLANK) XF=0._______________________________
C-- CALCULATE TOTAL DISSOLVED SOLIDS
C-- VALUES OF TOTAL DISSOLVED SOLIDS GREATER THAN 1000 ARE ROUNDED
C-- TO THE NEAREST 10 PPM OR MG/L
C--
   CTDS(M) = (XHC03/2.03)+XSI02+XNA+XK+XCA+XMG+XCL+XC03+XS04+XB+XF
   IF(CTDS(M).LT.1000.) GO TO 50
   I = CTDS(M)/10
   CTDS(M) = 1*10.
50 IF(SI02(M).LE.0..OR.XSI02.LT.0.) GO TO 55
C-- CALCULATE SILICA GEOTHERMOMETERS
C--
   LS102=DLOG10(SI02(M))
   TQC(M)=-TK+1309./(5.19-LS102)
   TQA(M)=-TK+1522./(5.75-LS102)
   TCH(M)=-TK+1032./(4.69-LS102)
   TCR(M)=-TK+1000./(4.78-LS102)
   TAM(M)=-TK+731./(4.52-LS102)
GO TO 91
55 TQC(M)=0.
   TOA(M)=0.
   TCH(M)=0.
   TAM(M)=0.
   TCR(M)=0.
91 IF(NA(M).LE.0. OR K(M).LE.0.) GO TO 95
   IF(XNA.LE.0. OR XK.LE.0.) GO TO 95
C-----------------------------------------------C
C-- CALCULATE NA-K GEOTHERMOMETERS ---
C-----------------------------------------------C
NAE=NA(M)/MWNA
NAM=NAE/1000.
KE=K(M)/MWK
KM=KE/1000.
LNAK=DLOG10(NAM/KM)
TNAK(M)=-TK+1217./(LNAK+1.483)
94 IF(CA(M).LE.0. OR XCA.LE.0.) GO TO 82
C  CALCULATE NA-K-CA (1/3 & 4/3) GEOTHERMOMETERS
C
CAE=CA(M)/(MWCA/2.)
CAM=(CA(M)/MWCA)/1000.
SCAM=DSQRT(CAM)
LCANA=DLOG10(SCAM/NAM)
T13K=1647./(LNAK+.333*LCANA+2.24)
T43K=1647./(LNAK+1.333*LCANA+2.24)
T13(M)=T13K-TK
T43(M)=T43K-TK
T13KS=T13K**2
T43KS=T43K**2
C-----------------------------------------------C
C-- CALCULATE MG CORRECTIONS (1/3 & 4/3) ---
C-----------------------------------------------C
96 IF(MG(M).LE.0. OR XMG.LE.0.) GO TO 800
MGE=MG(M)/MWMG
R=100*MGE/(MGE+CAE+KE)
IF (R.GT.50.) GO TO 98
LR=DLOG10(R)
LRS=LR**2
LRC=LR**3
IF(R.LT.0.5) GO TO 800
IF(R.LT.5.) GO TO 92
DMG13=10.66-4.7415*R+325.9*LRS-103210.*LRS/T13K-1.97E7*LRS/T13KS
  +1.61E7*LRC/T13KS
DMG43=10.66-4.7415*R+325.9*LRS-103210.*LRS/T43K-1.97E7*LRS/T43KS
  +1.61E7*LRC/T43KS
GO TO 93
92 DMG13=-1.03+59.97*LR+145.05*LRS-36711.*LRS/T13K-1.675E7*LR/T13KS
  DMG43=-1.03+59.97*LR+145.05*LRS-36711.*LRS/T43K-1.675E7*LR/T43KS
93 IF(DMG13.LE.0.) LABEL(M)=3
   IF(DMG43.LE.0.) LABEL(M)=4
   IF(DMG13.LE.0. AND DMG43.LE.0.) LABEL(M)=1
C-- RECALCULATE NA-K-CA GEOTHERMOMETERS WITH MG CORRECTION
C--------------------
TMG13(M)=T13(M)-DMG13
TMG43(M)=T43(M)-DMG43
GO TO 80
C--------------------
C-- LABEL IS A FLAG FOR PRINTING MG CORRECTED VALUES
C--------------------
800 LABEL(M)=1
GO TO 80
98 LABEL(M)=2
GO TO 80
95 TNAK(M)=0.
82 T13(M)=0.
T43(M)=0.
LABEL(M)=1
80 CONTINUE
C--------------------
C-- PRINT RESULTS
C--------------------
DO 500 N=1,L
99 WRITE(4,100) NUM(N)
100 FORMAT('1',3X,'RECORD NO....... ',I7)
   WRITE(4,105) NAME1(N),NAME2(N),NAME3(N),NAME4(N),NAME5(N)
105 FORMAT(4X,'NAME OF SOURCE... ',5A8)
   WRITE(4,110) STATE1(N),STATE2(N)
110 FORMAT(4X,'STATE............ ',2A8)
   WRITE(4,120) COUN1(N),COUN2(N)
120 FORMAT(4X,'COUNTY.......... ',2A8)
   WRITE(4,130)
130 FORMAT('0',4X,'TOWNSHIP RANGE SECTION')
   WRITE(4,140) TWNS(N),RANGE(N),SECT(N)
140 FORMAT(6X,A3,6X,A4,4X,A3)
   WRITE(4,150) WELLD(N)
150 FORMAT('0',3X,'WELL DEPTH(M)... ',A7)
   WRITE(4,160) FLOW(N),RATE(N)
160 FORMAT(4X,'FLOW RATE....... ',A8,3X,A6)
   WRITE(4,170) WTEMP(N)
170 FORMAT(4X,'WATER TEMPERATURE... ',A6)
   WRITE(4,180) UNITS(N)
180 FORMAT('0',3X, 'WATER CHEMSITRY (',A4,')')
   WRITE(4,190) QSI02(N),SI02(N),QCL(N),CL(N),QF(N),F(N)
190 FORMAT(7X,'SI02... ',A1,1X,F8.2,4X,'CL...... ',A1,1X,F8.2,4X,
   1F........ ,A1,1X,F8.2)
   WRITE(4,200) QNA(N),NA(N),QHC03(N),HC03(N),PH(N)
200 FORMAT(7X,'NA...... ',A1,1X,F8.2,4X,'HC03... ',A1,1X,F8.2,
   14X,'PH...... ',2X,A8)
   WRITE(4,205) QK(N),K(N),QCO3(N),CO3(N)
205 FORMAT(7X,'K...... ',A1,1X,F8.2,4X,'CO3.... ',A1,1X,F8.2,
   14X,'TOTAL DISSOLVED SOLIDS')
   WRITE(4,210) QCA(N),CA(N),QSO4(N),SO4(N),RTDS(N)
210 FORMAT(7X,'CA..... ',A1,1X,F8.2,4X,'SO4.... ',A1,1X,F8.2,
   14X,'RECORDED.... ',A8)
WRITE(4,215) QMG(N),MG(N),QB(N),B(N),CTDS(N)
215 FORMAT(7X,'MG..... ',A1,1X,F8.2,4X,'B...... ',A1,1X,F8.2,
14X,'CALCULATED.. ',2X,F8.0)__________________
WRITE(4,220)
220 FORMAT('0',3X,'GEOTHERMOMETERS (DEGREES C)')
WRITE(4,230) TQC(N),TNAK(N)
230 FORMAT(7X,'SILICA - CONDUCTIVE.... ',F6.0,8X,'NA-K......... '1,F6.0)
WRITE(4,235) TQA(N),T13(N)
235 FORMAT(16X,'ADABATIC....... ',F6.0,8X,'NA-K-CA(1/3)... ',F6.0)
WRITE(4,240) TCH(N),T43(N)
240 FORMAT(16X,'CHALCEDONY.... ',F6.0,8X,'NA-K-CA(4/3)... ',F6.0)
WRITE(4,245) TCR(N)
245 FORMAT(16X,'CRISTOBALITE.. ',F6.0,8X,'MG CORRECTED')
   IF (LABEL(N).NE.0) GO TO 400
WRITE(4,250) TAM(N),TMG13(N)
250 FORMAT(16X,'AMORPHOUS...... ',F6.0,8X,'NA-K-CA(1/3)... ',F6.0)
WRITE(4,255) TMG43(N)
255 FORMAT(16X,'NA-K-CA(4/3)... ',F6.0)
goto 500
400 IF (LABEL(N).EQ.1.OR.LABEL(N).EQ.2) GO TO 411
   IF (LABEL(N).EQ.3) GO TO 413
   IF (LABEL(N).EQ.4) WRITE(4,250) TAM(N),TMG13(N)
goto 500
413 WRITE(4,267) TAM(N),TMG43(N)
267 FORMAT(16X,'AMORPHOUS...... ',F6.0,8X,'NA-K-CA(4/3)... ',F6.0)
goto 500
411 IF (LABEL(N).EQ.1) WRITE(4,260) TAM(N)
260 FORMAT(16X,'AMORPHOUS...... ',F6.0,8X,'NONE')
   IF (LABEL(N).EQ.2) WRITE(4,265) TAM(N)
265 FORMAT(16X,'AMORPHOUS...... ',F6.0,8X,'COOL')
500 CONTINUE
STOP
END
Revised geothermometer program

IMPLICIT REAL*8 (A-Z)
DIMENSION NAME1(1000),NAME2(1000),NAME3(1000),NAME4(1000)
DIMENSION STATE1(1000),STATE2(1000),COUN1(1000),COUN2(1000)
DIMENSION WTEMP(1000),PH(1000)
DIMENSION SI02(1000),NA(1000),K(1000),CA(1000),MG(1000)
DIMENSION TQC(1000),TCH(1000)
DIMENSION TQA(1000),TCR(1000),NAME5(1000)
DIMENSION TAM(1000),TNAK(1000),T13(1000),T43(1000),TMG13(1000)
1,TMG43(1000)
INTEGER I,LABEL(1000),NUM(1000),J,M,N,L
TK=273.15

C-- MWNA=MOLECULAR WEIGHT NA, MWK=MOLECULAR WEIGHT K, MWCA=MOLECULAR WEIGHT CA AND MWMG=MOLECULAR WEIGHT MG

MWNA=23.
MWK=39.1
MWCA=40.08
MWMG=12.16

C-- READ VALUES OF ALL VARIABLES

DO 5 J=1,1000
READ(2,10,END=30) NUM(J),NAME1(J),NAME2(J),NAME3(J),NAME4(J),
1NAME5(J),
1STATE1(J),STATE2(J),COUN1(J),COUN2(J)
1,WTEMP(J),PH(J)
10 FORMAT(1X,I7,9A8,A6,A6)
IF (NUM(J).EQ.O) GO TO 30

C-- READ VALUES OF ALL SPECIES

READ(2,25) SI02(J),NA(J),K(J),CA(J),MG(J)
25 FORMAT(1X,5(2X,F8.2))
L = J
5 CONTINUE

C-- CALCULATION LOOP

30 DO 80 M=1,L
LABEL(M)=0
50 IF(SI02(M).LE.O.) GO TO 55

C-- CALCULATE SILICA GEOTHERMETERS

LSI02=DLOG10(SI02(M))
TQC(M)=-TK+1309./(5.19-LSI02)
TQA(M)=-TK+1522./(5.75-LSI02)
TCH(M)=-TK+1032./(4.69-LSI02)
TCR(M)=-TK+1000./(4.78-LSI02)
TAM(M)=-TK+731./(4.52-LSI02)
GO TO 91
55  TQC(M)=0.
    TQA(M)=0.
    TCH(M)=0.
    TAM(M)=0.
    TCR(M)=0.
91  IF(NA(M).LE.0. OR. K(M).LE.0.) GO TO 95

C---------------------------------------------------------------
C--                CALCULATE NA-K GEOTHERMOMETERS               
C---------------------------------------------------------------

    NAE=NA(M)/MWNA
    NAM=NAE/1000.
    KE=K(M)/MWK
    KM=KE/1000.
    LNAK=DLOG10(NAM/KM)
    TNAK(M)=-TK+1217./(LNAK+1.483)
94  IF(CA(M).LE.0.) GO TO 82

C---------------------------------------------------------------
C--                CALCULATE NA-K-CA (1/3 & 4/3) GEOTHERMOMETERS 
C---------------------------------------------------------------

    CAE=CA(M)/(MWCA/2.)
    CAM=(CA(M)/MWCA)/1000.
    SCAM=DSQRT(CAM)
    LCANA=DLOG10(SCAM/NAM)
    T13K=1647./(LNAK+.333*LCANA+2.24)
    T43K=1647./(LNAK+1.333*LCANA+2.24)
    T13(M)=T13K-TK
    T43(M)=T43K-TK
    T13KS=T13K**2
    T43KS=T43K**2

C---------------------------------------------------------------
C--                CALCULATE MG CORRECTIONS (1/3 & 4/3)          
C---------------------------------------------------------------

96  IF(MG(M).LE.0.) GO TO 800
    MGE=MG(M)/MWMG
    R=100*MGE/(MGE+CAE+KE)
    IF (R.GT.50.) GO TO 98
    LR=DLOG10(R)
    LRS=LR**2
    LRC=LR**3
    IF(R.LT.0.5) GO TO 800
    IF(R.LT.5.) GO TO 92
    DMG13=10.66-4.7415*R+325.9*LRS-103210*LRS/T13K-1.97E7*LRS/T13KS
    1+1.61E7*LRC/T13KS
    DMG43=10.66-4.7415*R+325.9*LRS-103210*LRS/T43K-1.97E7*LRS/T43KS
    1+1.61E7*LRC/T43KS
    GO TO 93
92  DMG13=-1.03+59.97*LR+145.05*LRS-36711.*LRS/T13K-1.675E7*LR/T13KS
    DMG43=-1.03+59.97*LR+145.05*LRS-36711.*LRS/T43K-1.675E7*LR/T43KS
93  IF(DMG13.LE.0.) LABEL(M)=3
    IF(DMG43.LE.0.) LABEL(M)=4
    IF(DMG13.LE.0. AND. DMG43.LE.0.) LABEL(M)=1

C---------------------------------------------------------------
C--               RECALCULATE NA-K-CA GEOTHERMOMETERS WITH MG CORRECTION 
C---------------------------------------------------------------
TMG13(M) = T13(M) - DMG13
TMG43(M) = T43(M) - DMG43
GO TO 80

C---- LABEL IS A FLAG FOR PRINTING MG CORRECTED VALUES ----

800 LABEL(M) = 1
   GO TO 80
98 LABEL(M) = 2
   GO TO 80
95 TNAK(M) = 0.
82 T13(M) = 0.
   T43(M) = 0.
   LABEL(M) = 1
80 CONTINUE

C---- PRINT RESULTS ----

DO 500 N = 1, L
   WRITE(4, 501)
501 FORMAT('O', '---------')
99 WRITE(4, 100) NUM(N)
100 FORMAT('O', 3X, 'RECORD NO......... ', I7)
   WRITE(4, 105) NAME1(N), NAME2(N), NAME3(N), NAME4(N), NAME5(N)
105 FORMAT(4X, 'NAME OF SOURCE..... ', A5A8)
   WRITE(4, 110) STATE1(N), STATE2(N)
110 FORMAT(4X, 'STATE........... ', A2A8)
   WRITE(4, 120) COUN1(N), COUN2(N)
120 FORMAT(4X, 'COUNTRY........... ', A2A8)
   WRITE(4, 170) WTEMP(N), PH(N)
170 FORMAT(4X, 'WATER TEMPERATURE... ', A6, 4X, 'PH..... ', A8)
502 FORMAT('O', 3X, 'WATER CHEMISTRY')
   WRITE(4, 190) SI02(N)
190 FORMAT(7X, 'SI02... ', 2X, F8.2)
   WRITE(4, 200) NA(N)
200 FORMAT(7X, 'NA..... ', 2X, F8.2)
   WRITE(4, 205) K(N)
205 FORMAT(7X, 'K...... ', 2X, F8.2)
   WRITE(4, 210) CA(N)
210 FORMAT(7X, 'CA..... ', 2X, F8.2)
   WRITE(4, 215) MG(N)
215 FORMAT(7X, 'MG..... ', 2X, F8.2)
   WRITE(4, 220)
220 FORMAT('O', 3X, 'GEOTHERMOMETERS (DEGREES C)')
   WRITE(4, 230) TQC(N), TNAK(N)
230 FORMAT(7X, 'SILICA - CONDUCTIVE.... ', F6.0, 8X, 'NA-K......... ')
   WRITE(4, 235) TQA(N), T13(N)
235 FORMAT(16X, 'ADABATIC...... ', F6.0, 8X, 'NA-K-CA(1/3).... ', F6.0)
   WRITE(4, 240) TCH(N), T43(N)
240 FORMAT(16X, 'CHALCEDONY.... ', F6.0, 8X, 'NA-K-CA(4/3).... ', F6.0)
22

WRITE(4,245) IC(R(N)

245 FORMAT(16X,'Cristobalite.. ','F6.0,8X,'MG Corrected')
    IF (LABEL(N).NE.0) GO TO 400
    WRITE(4,250) TAM(N),TMG13(N)

250 FORMAT(16X,'Amorphous..... ',F6.0,8X,'Na-K-Ca(1/3)... ',F6.0)
    WRITE(4,255) TMG43(N)

255 FORMAT(16X,'Na-K-Ca(4/3)... ',F6.0)
    GO TO 500

400 IF(LABEL(N).EQ.1.OR.LABEL(N).EQ.2) GO TO 411
    IF(LABEL(N).EQ.3) GO TO 413
    IF(LABEL(N).EQ.4) WRITE(4,250) TAM(N),TMG13(N)
    GO TO 500

413 WRITE(4,267) TAM(N),TMG43(N)

267 FORMAT(16X,'Amorphous..... ',F6.0,8X,'Na-K-Ca(4/3)... ',F6.0)
    GO TO 500

411 IF (LABEL(N).EQ.1) WRITE(4,260) TAM(N)

260 FORMAT(16X,'Amorphous..... ',F6.0,8X,'None')
    IF (LABEL(N).EQ.2) WRITE(4,265) TAM(N)

265 FORMAT(16X,'Amorphous..... ',F6.0,8X,'Cool')

500 CONTINUE
STOP
END
Sample Input for Revised Version of Program

17623 HONEY POT UTAH GARFIELD 23.
11. 300. 13. 190. 260.

17311 ELBERTA UTAH UTAH 22. 6.8
70. 52. 15. 278. 101.

1469 UNAMED WELL WEST OF HUECO AIRPORT (1) TEXAS EL PASO 38. 8.2
29. 97.8 1.3 2.8 0.2
Sample of output of revised version on geothermometer program

---

**Record No.:** 17311  
**Name of Source:** ELBERTA  
**State:** UTAH  
**County:** UTAH  

**Water Temperature:** 22.0  
**pH:** 6.8  

**Water Chemistry**  
- SiO₂: 70.00  
- Na: 52.00  
- K: 15.00  
- Ca: 278.00  
- Mg: 101.00

**Geothermometers (Degrees C)**  
- Silica - Conductive: 118  
- Adiabatic: 117  
- Chalcedony: 93  
- Cristobalite: 61  
- Amorphous: 31

---

**Record No.:** 17623  
**Name of Source:** HONEY POT  
**State:** UTAH  
**County:** GARFIELD  

**Water Temperature:** 23.0  
**pH:** 6.8  

**Water Chemistry**  
- SiO₂: 11.00  
- Na: 300.00  
- K: 13.00  
- Ca: 190.00  
- Mg: 260.00

**Geothermometers (Degrees C)**  
- Silica - Conductive: 42  
- Adiabatic: 50  
- Chalcedony: 10  
- Cristobalite: -6  
- Amorphous: -63

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**Record No.:** 1469  
**Name of Source:** UNNAMED WELL WEST OF HUECO AIRPORT (1)  
**State:** TEXAS  
**County:** EL PASO  

**Water Temperature:** 38.0  
**pH:** 8.2  

**Water Chemistry**  
- SiO₂: 29.00  
- Na: 97.80  
- K: 1.30
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<tr>
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<th>Geothermometers (Degrees C)</th>
<th>Value</th>
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<tr>
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<td>Na-K-CA(4/3)</td>
<td>74</td>
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<tr>
<td>Mg Corrected</td>
<td>None</td>
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