User's Manual

GaS_GeoT: A computer program for an effective use of newly improved gas geothermometers in predicting reliable subsurface geothermal temperatures

1. Introduction

A quick user manual of the computer program GaS_GeoT is presented. This computer program was developed for an effective use of newly improved gas geothermometers in predicting reliable subsurface geothermal temperatures. GaS_GeoT is an object-oriented code in Java programming language developed to have minimum application dependencies.

Eight new improved gas geothermometers have been derived from an optimized evaluation based on artificial neural networks (ANN) and multi-criteria decision analysis (MCDA) for solving the multivariate analysis between the gas-phase composition of geothermal fluids and true bottom-hole temperature measurements (BHT_m). A detailed description of the overall optimized methodology has been reported in the following manuscript:

A. Acevedo-Anicasio, E. Santoyo, D. Pérez-Zárate, K. Pandarinath, M. Guevara, L. Díaz-González (2020). GaS_GeoT: A computer program for an effective use of newly improved gas geothermometers in predicting reliable subsurface geothermal temperatures. Manuscript submitted to: Computers & Geosciences (August, 2020).

The eight new gas geothermometers (referred as $GasG_1$ to $GasG_8$) use the gas-phase composition of geothermal fluids as main input data (CO_2, H_2S, CH_4, and H_2) for the calculation of the subsurface geothermal temperatures. The concentration units of the gas-phase composition are in mmol/mol (dry-basis).

Hardware and Software Requirements

For the execution of the GaS_GeoT, a hardware with the following minimum specifications is recommended:

- Operating system: Windows 7 Home Premium 64 bits or higher
- Processor: Intel Core i5-2300, 2.80GHz
- RAM memory: 4 GB
- Hard Drive: 500 GB

The installation of the Java virtual machine (version 7 or higher which is freely available on the following web site: https://www.java.com/es/download/ is required to decode the intrusions

of the Jar executable files, and the Excel spreadsheet (with a filename extension: xlsx). The Excel file is used by the program as a template for storing and processing the input and output data, respectively. The input data template.xlsx is available from the Help menu option for downloading and running the executable version of the GaS_GeoT program.

A flow chart showing the main computer execution steps used by the computer program GaS_GeoT is presented in Fig. 1 of this user's manual.

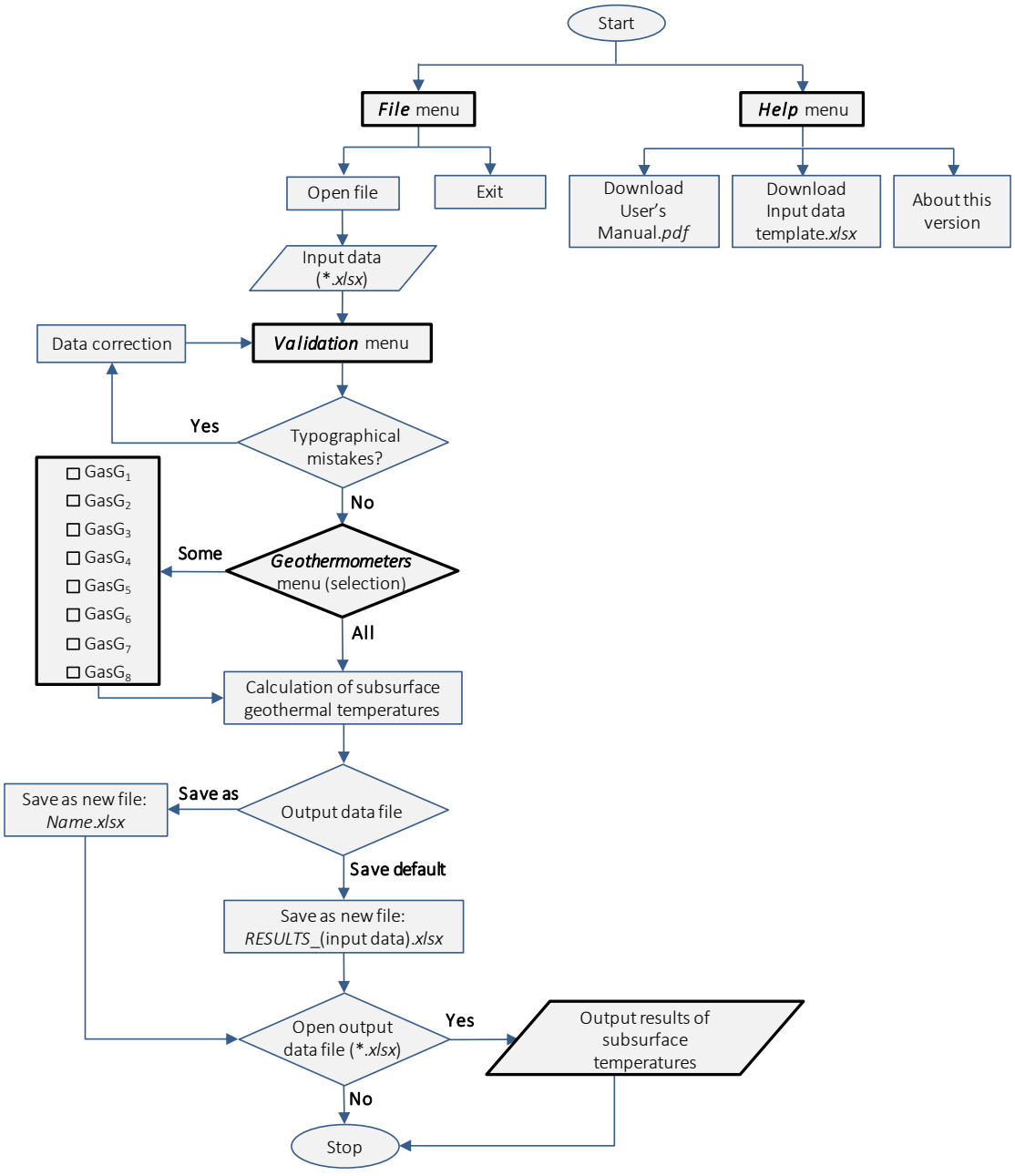


Fig. 1 Schematic flow diagram for showing the execution of the computer program GaS_GeoT.

2. Main menu options used by the computer program GaS_GeoT

A schematic view of the computing environment, and main menu options of the GaS_GeoT program is shown in Fig. 2.

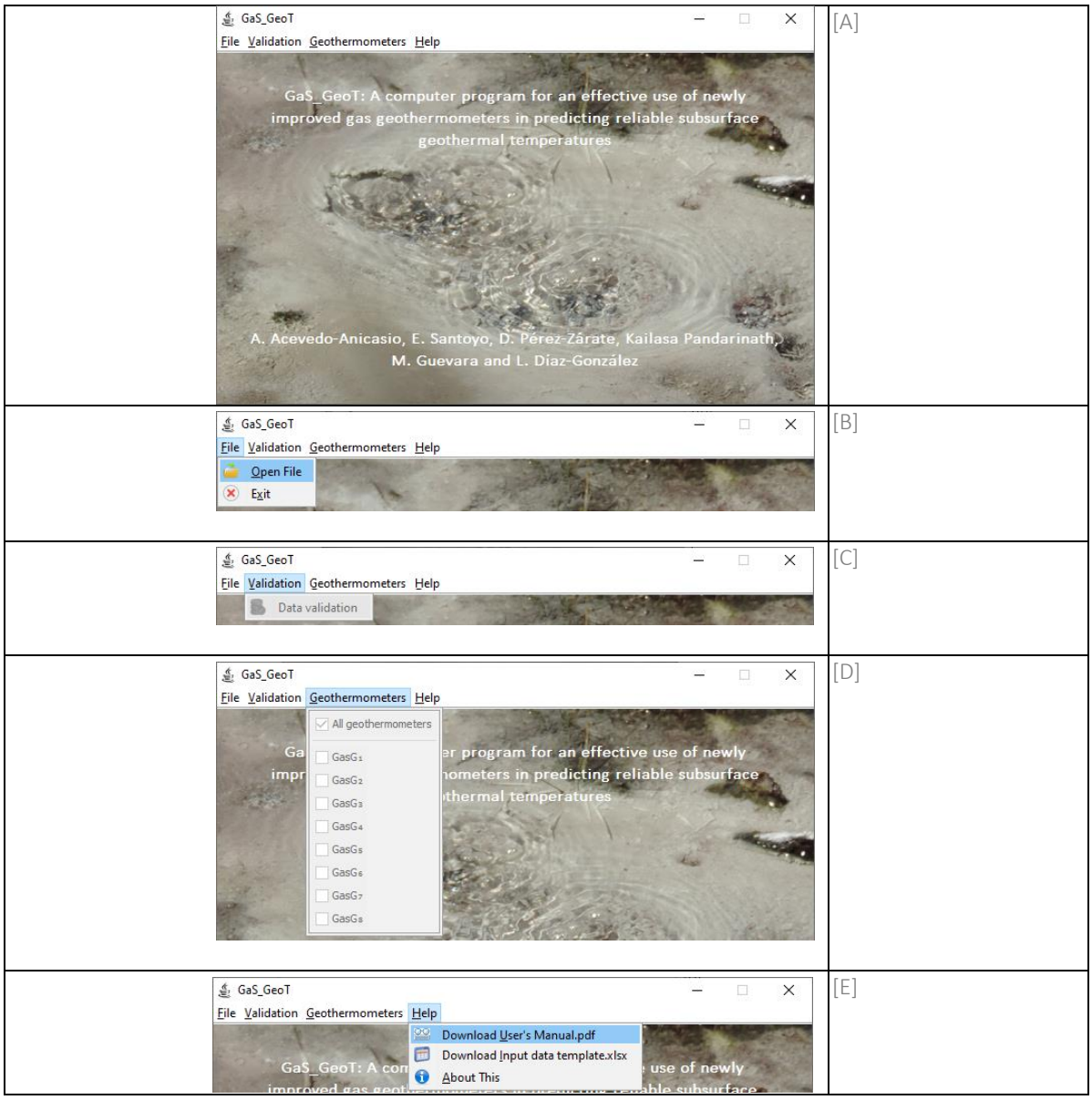


Fig. 2 Main screens and menu of options of the computer program GaS_GeoT.

2.1. File menu

It contains two possible options (Fig. 2B): (*i*) the option <Open File>, which allows the user to select the input data file (with the Excel filename extension: xlsx) to be processed with the following information in each column: Column 1: Sample ID (numerical data: integer); Columns

2-4 designed to enter the Geothermal Well, Geothermal Field, and Country information, respectively (in alphanumerical format); and the Columns 5-8 to compile the gas-phase composition of the CO_2, H_2S, CH_4, H_2 in mmol/mol (dry-basis), respectively (numerical data in floating format); and (*ii*) <Exit>, which closes the computer program GaS_GeoT.

The input data file to be entered in the computer program must have a similar format to the template available in the Help menu option (i.e., the same number of input columns, and the input data format or specification). As shown in Fig. 3, the input data file (with the Excel filename extension: xlsx) must contain data (numeric and alphanumeric) in eight columns. In case of entering data in more than eight columns, GaS_GeoT will display an error message with the location of the mistake (Fig. 4). GaS_GeoT does not have a limited number of samples to be processed (i.e., size of the input file). The CPU time elapsed by running the GaS-GeoT program will depend on the number of samples to be processed (e.g., an input data with 2,000 samples used 355 s of CPU time).

	A	B	C	D	E	F	G	H
1	Sample ID	Geothermal Well	Geothermal Field	Country	CO2	H2S	CH4	H2
2	1	well-01	Field-A	Mexico	900.099	49.951	6.429	26.212
3	2	well-02	Field-A	Mexico	912.5	135.349	0.997	1.937
4	3	well-03	Field-A	Mexico	856.950	52.632	17.544	12.146
5	4	well-04	Field-A	Mexico	789.474	137.336	9.046	38.651
6	5	well-05	Field-A	Mexico	939.2	19.7	15.2	17.7
7	6	well-06	Field-A	Mexico	972.7	9.2	3.65	13.8
8	7	well-07	Field-A	Mexico	931.117	10.08	0.187	3.038
9	8	well-08	Field-A	Mexico	976.994	11.853	1.332	1.926
10	9	well-09	Field-A	Mexico	817.2	7.81	0.176	22.589
11	10	well-10	Field-A	Mexico	902.099	52.951	10.429	31.212
12	11	well-11	Field-A	Mexico	914.500	138.349	4.997	6.937
13	12	well-12	Field-A	Mexico	858.950	55.632	21.544	17.146
14	13	well-13	Field-A	Mexico	791.474	140.336	13.046	43.651
15	14	well-14	Field-A	Mexico	941.200	22.700	19.200	22.700
16	15	well-15	Field-A	Mexico	974.700	12.200	7.650	18.800
17	16	well-16	Field-A	Mexico	933.117	13.080	4.187	8.038
18	17	well-17	Field-A	Mexico	978.994	14.853	5.332	6.926
19	18	well-18	Field-A	Mexico	819.200	10.810	4.176	27.589
20	19	well-19	Field-A	Mexico	904.099	55.951	14.429	36.212
21	20	well-20	Field-A	Mexico	916.500	141.349	8.997	11.937

Fig. 3 A typical input data file showing an example with the columns required for the validation of the input data, and the calculation processing of the subsurface temperatures.

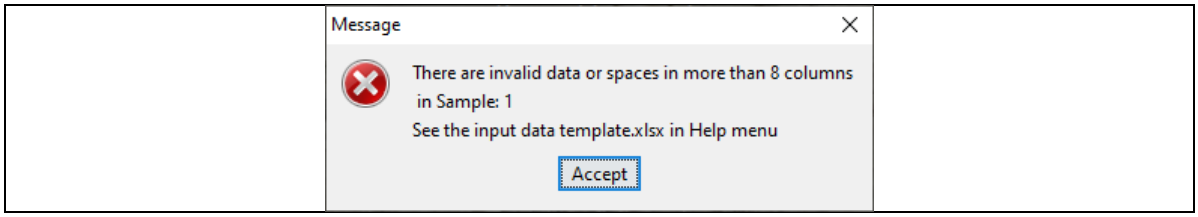
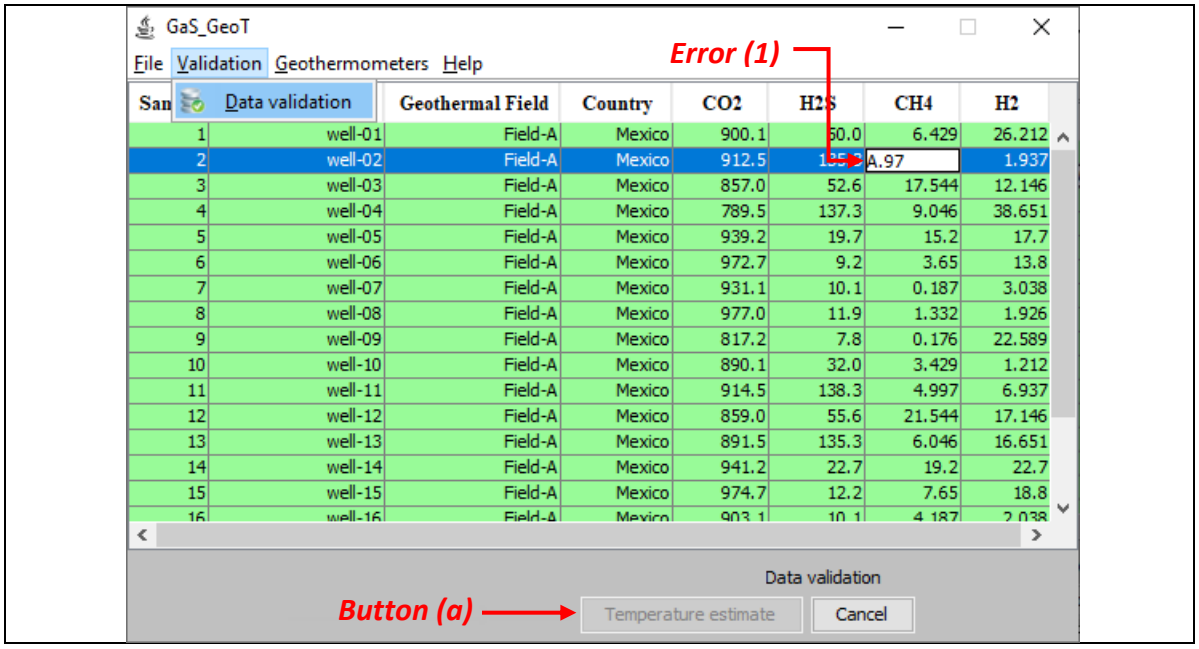


Fig. 4 A typical error message displayed by the computer program when an input data file has more than eight input columns.

2.2. Validation menu

This option must be selected for the validation of the input data (Fig. 2C). If a non-valid character is entered in the input data file, GaS_GeoT will display the typographical mistakes with the precise location of the sample (row and column; see Fig 5). As a result of this mistake, the <Temperature estimate> "*Button (a)*" will be inactive until the mistake is corrected. For example, the "*Error (1)*" was detected because the chemical composition of the gases (in this case CH_4) must have a real number format (Fig. 6). The primary function of the <Data validation> option is used both for the detection and correction of typographical mistakes. The "*Cancel*" button will return to the main window of the GaS_GeoT (Fig. 2A).



San	Geothermal Field	Country	CO2	H2S	CH4	H2
1	well-01	Field-A	Mexico	900.1	60.0	6.429	26.212
2	well-02	Field-A	Mexico	912.5	135.2	A.97	1.937
3	well-03	Field-A	Mexico	857.0	52.6	17.544	12.146
4	well-04	Field-A	Mexico	789.5	137.3	9.046	38.651
5	well-05	Field-A	Mexico	939.2	19.7	15.2	17.7
6	well-06	Field-A	Mexico	972.7	9.2	3.65	13.8
7	well-07	Field-A	Mexico	931.1	10.1	0.187	3.038
8	well-08	Field-A	Mexico	977.0	11.9	1.332	1.926
9	well-09	Field-A	Mexico	817.2	7.8	0.176	22.589
10	well-10	Field-A	Mexico	890.1	32.0	3.429	1.212
11	well-11	Field-A	Mexico	914.5	138.3	4.997	6.937
12	well-12	Field-A	Mexico	859.0	55.6	21.544	17.146
13	well-13	Field-A	Mexico	891.5	135.3	6.046	16.651
14	well-14	Field-A	Mexico	941.2	22.7	19.2	22.7
15	well-15	Field-A	Mexico	974.7	12.2	7.65	18.8
16	well-16	Field-A	Mexico	903.1	10.1	4.187	2.038

Fig. 5 Example of the validation option for checking the format of the input data in the samples.

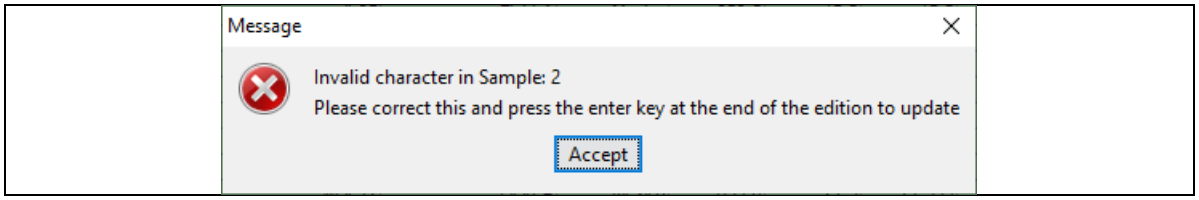
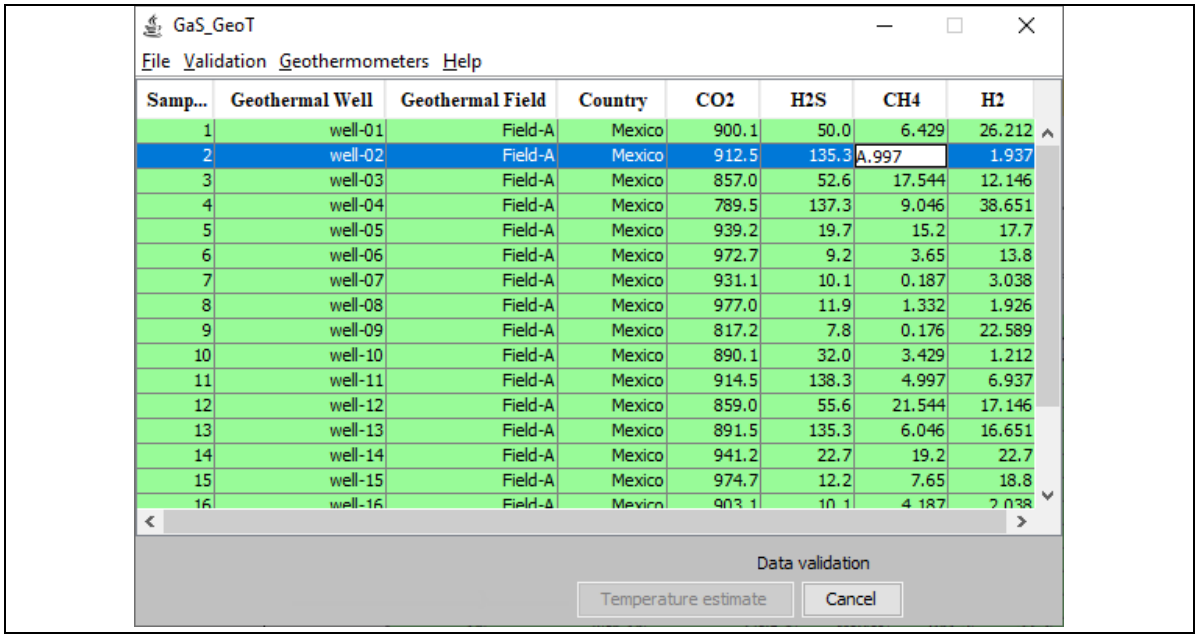


Fig. 6. Error message displayed when an invalid character is detected.

To correct the typographical mistakes (Fig. 5), an edition capability has been programmed in GaS_GeoT. The edition option is directly enabled in the cell that contains the invalid character or mistake, as shown in Fig. 7. Once the typing mistakes are corrected, the enter key must be pressed both to update the input data, and to activate or start the validation process. When the data to be processed has been successfully validated, the <Temperature estimate> will be

enabled, and a frame with a text legend will appear indicating the total number of validated samples (Fig. 8).



Samp...	Geothermal Well	Geothermal Field	Country	CO2	H2S	CH4	H2
1	well-01	Field-A	Mexico	900.1	50.0	6.429	26.212
2	well-02	Field-A	Mexico	912.5	135.3	A.997	1.937
3	well-03	Field-A	Mexico	857.0	52.6	17.544	12.146
4	well-04	Field-A	Mexico	789.5	137.3	9.046	38.651
5	well-05	Field-A	Mexico	939.2	19.7	15.2	17.7
6	well-06	Field-A	Mexico	972.7	9.2	3.65	13.8
7	well-07	Field-A	Mexico	931.1	10.1	0.187	3.038
8	well-08	Field-A	Mexico	977.0	11.9	1.332	1.926
9	well-09	Field-A	Mexico	817.2	7.8	0.176	22.589
10	well-10	Field-A	Mexico	890.1	32.0	3.429	1.212
11	well-11	Field-A	Mexico	914.5	138.3	4.997	6.937
12	well-12	Field-A	Mexico	859.0	55.6	21.544	17.146
13	well-13	Field-A	Mexico	891.5	135.3	6.046	16.651
14	well-14	Field-A	Mexico	941.2	22.7	19.2	22.7
15	well-15	Field-A	Mexico	974.7	12.2	7.65	18.8
16	well-16	Field-A	Mexico	903.1	10.1	4.187	2.038

Fig. 7 Direct correction of a typing mistake in the invalid cell of input data.

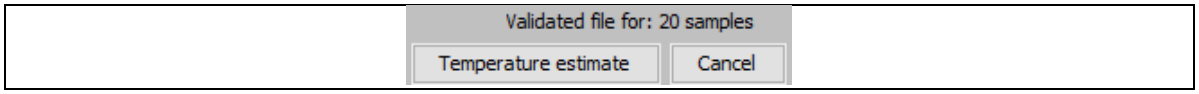


Fig. 8 A typical text legend shown when a successful validation of the input data file is obtained.

2.3. Geothermometers menu

When the input data file has been successfully validated, the Geothermometers menu option will be enabled (Figs. 2D and 9). The GaS_GeoT program allows the estimation of the subsurface geothermal temperatures (in °C) by selecting either all gas geothermometers (first option) or by checking/selecting the geothermometer boxes, and finally pressing the temperature estimate button to proceed with all the calculations of the subsurface geothermal temperatures. After this instruction, the GaS_GeoT program will allow to save the calculation results in an output file using either an output file name defined by the user (filename.xlsx) or a default output file name (*RESULTS_input data.xlsx*) as shown in Fig. 10.

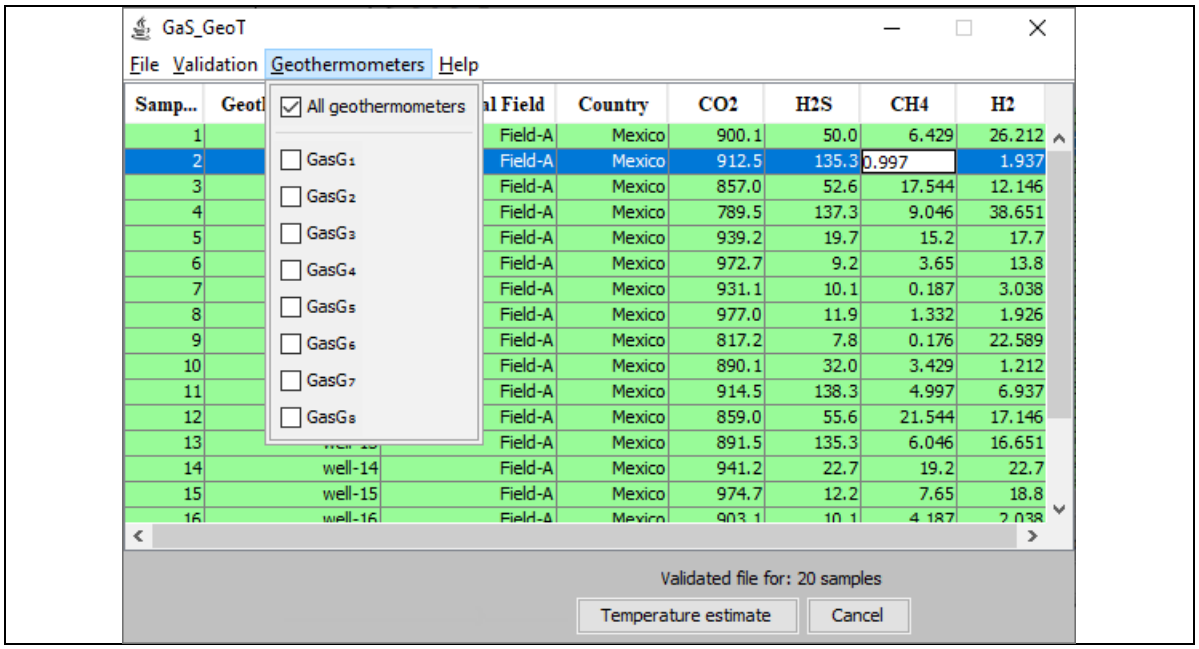


Fig. 9. Selection of the new gas geothermometers for the calculation of subsurface temperatures.

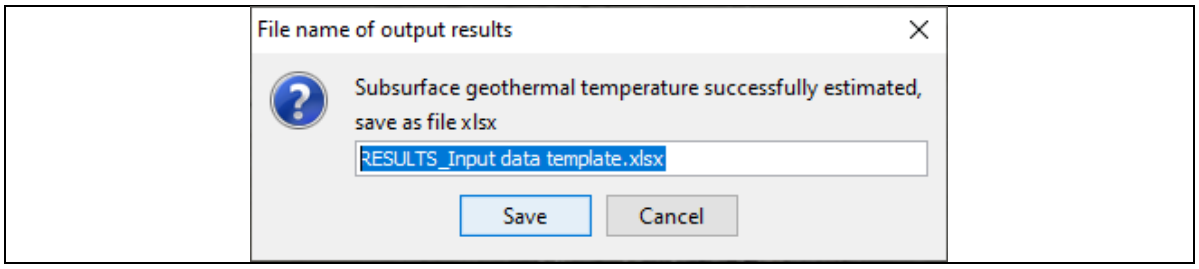


Fig. 10 Save option of the GaS_GeoT is for saving the results either in a new output filename or by using the default output file.

If the user requires to edit the file of output results, the computer program GaS_GeoT will allow this function to be performed (Fig. 11). Otherwise, the output file will be stored in the current directory of the computer. It is important to mention that the option shown in Fig. 11 only works for operating systems of Microsoft Windows.

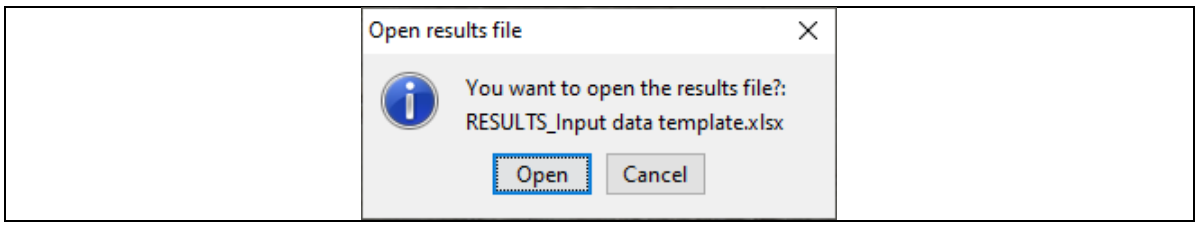


Fig. 11 Edition functions of the GaS_GeoT for analyzing the output file of results.

After executing the computer program GaS_GeoT, a full output report is printed as an Excel output file (with a filename extension: xlsx). The output report will contain both the input data

used (i.e., the chemical composition of the gaseous phase of the geothermal fluids) and the calculation of the subsurface geothermal temperatures (in °C).

Applicability conditions of the GaS_GeoT program.

The validity of the results calculated by the computer program GaS_GeoT is supported by the applicability conditions and temperature constraints defined for the new gas geothermometers developed (see Table 1).

Table 1. Applicability conditions for eight new gas geothermometers.

New gas Geothermometers ($GasG_i$)	Gas concentrations (mmol/mol dry-basis)				Bottom-hole temperature °C
	CO_2	H_2S	CH_4	H_2	BHT_m
	Concentration Intervals [Min, Max]				[Min, Max]
$GasG_1$, $GasG_2$, $GasG_6$, and $GasG_8$	[311, 3206]	[0.1032, 357]	[0.000059, 57]	[0.1084, 477]	[170, 374]
$GasG_3$, $GasG_4$, $GasG_5$ and $GasG_7$	[699, 994]	[0.1032, 197]	[0.000059, 57]	[0.1084, 128]	[170, 374]
	Input variable 1	Input variable 2	Input variable 3	Input variable 4	Input variable 5
$GasG_1$	[-9.17, -0.21]	[-16.56, -2.67]	[-9.07, 0.43]	-	-
$GasG_2$	[2.67, 16.56]	[-0.82, 13.95]	[-2.99, 11.13]	-	-
$GasG_3$	[-9.17, -1.39]	[-16.56, -2.67]	[-9.07, -1.77]	-	-
$GasG_4$	[2.67, 16.56]	[-0.82, 13.95]	[-2.99, 11.13]	-	-
$GasG_5$	[1.77, 9.07]	[-2.90, 6.14]	[-11.13, 2.99]	-	-
$GasG_6$	[5.74, 8.07]	[-2.27, 5.88]	[-9.73, 4.04]	[-2.22, 6.17]	-
$GasG_7$	[6.55, 6.90]	[-2.27, 5.28]	[-9.73, 4.04]	[-2.22, 4.85]	-
$GasG_8$	[-9.17, -0.21]	[-16.56, -2.67]	[-9.07, 0.43]	[-2.27, 5.88]	[-2.90, 6.14]

Input variables for: $GasG_1$ [$\ln(H_2S/CO_2)$, $\ln(CH_4/CO_2)$, $\ln(H_2/CO_2)$]; $GasG_2$ [$\ln(CO_2/CH_4)$, $\ln(H_2S/CH_4)$, $\ln(H_2/CH_4)$]; $GasG_3$ [$\ln(H_2S/CO_2)$, $\ln(CH_4/CO_2)$, $\ln(H_2/CO_2)$]; $GasG_4$ [$\ln(CO_2/CH_4)$, $\ln(H_2S/CH_4)$, $\ln(H_2/CH_4)$]; $GasG_5$ [$\ln(CO_2/H_2)$, $\ln(H_2S/H_2)$, $\ln(CH_4/H_2)$]; $GasG_6$ [$\ln(CO_2)$, $\ln(H_2S)$, $\ln(CH_4)$, $\ln(H_2)$]; $GasG_7$ [$\ln(CO_2)$, $\ln(H_2S)$, $\ln(CH_4)$, $\ln(H_2)$]; and $GasG_8$ [$\ln(H_2S/CO_2)$, $\ln(CH_4/CO_2)$, $\ln(H_2/CO_2)$, $\ln(H_2S)$, $\ln(H_2S/H_2)$].

For an interpretation of these applicability conditions, the following example is described:

After validating the input data file and estimating temperatures, GaS_GeoT verifies if the concentration intervals were exceeded for any gas geothermometer. If this is the case, GaS_GeoT will run without any restriction, however, will indicate the estimated temperature in red font to warn the user should be used with caution (Fig. 12).

Additionally, if the temperature estimate does not comply with the intervals of concentration and temperature used for the calibration of the new gas geothermometers, a text of “n.d.” will be indicated in the temperature calculation cell (which means that the temperature is not determined) and additional information in the column out of range (I column).

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Sample ID	Geotherm	Geotherm	Country	CO2	H2S	CH4	H2	Out of range	$GasG_1$	$GasG_2$	$GasG_3$	$GasG_4$	$GasG_5$	$GasG_6$	$GasG_7$	$GasG_8$
2	1	well-01	Field-A	Mexico	900.099	49.951	6.429	26.212		270.8	308.2	301.7	373.4	293	312.6	307.4	307.4
3	2	well-02	Field-A	Mexico	912.5	200.3	0.997	1.937	$GasG_7$: input-2	298.4	296.8	299.3	227.8	268.7	278.9	295.1	327.2
4	3	well-03	Field-A	Mexico	856.95	52.632	17.544	12.146		325.8	331.1	331.3	334.8	317.1	301	303.3	326.1
5	4	well-04	Field-A	Mexico	789.474	137.336	9.046	38.651		182.9	278.5	271.1	360.7	271.7	251.8	298	280.5
6	5	well-05	Field-A	Mexico	939.2	19.7	15.2	17.7		258.8	254.5	262.8	266.6	253.4	257.2	260.3	249.7
7	6	well-06	Field-A	Mexico	972.7	9.2	3.65	13.8		251.4	251	239.8	240.4	252.4	243.5	239.8	253.8
8	7	well-07	Field-A	Mexico	931.117	10.08	0.187	3.038		277.5	289.9	279.2	291.3	290.9	280.1	284.9	277.2
9	8	well-08	Field-A	Mexico	976.994	11.853	1.332	1.926		265.2	264.7	261	252.1	261.5	261.4	247.1	262.2
10	9	well-09	Field-A	Mexico	817.2	7.81	0.176	22.589		288.8	289	288.8	287.8	288.8	294.1	297.9	297.2
11	10	well-10	Field-A	Mexico	890.099	31.951	3.429	1.212		211.7	177.7	229.5	301.2	206.8	194.1	298	237.5
12	11	well-11	Field-A	Mexico	914.5	138.349	4.997	6.937		288.6	311.2	304.9	312.8	311.1	335.5	362.3	363.6
13	12	well-12	Field-A	Mexico	858.95	55.632	21.544	17.146		311.8	314.3	322.3	315.8	311.9	308.5	305.5	323.9
14	13	well-13	Field-A	Mexico	891.474	135.336	6.046	16.651		317.1	342.1	300.2	321.7	307	301.9	357.4	337.7
15	14	well-14	Field-A	Mexico	941.2	22.7	19.2	22.7		261	266	259.3	267.6	255.8	261.8	254.9	256.9
16	15	well-15	Field-A	Mexico	974.7	12.2	7.65	18.8		254.8	245.7	245.3	243.9	257.3	252.5	238.1	265.2
17	16	well-16	Field-A	Mexico	903.117	10.08	4.187	2.038		295.6	283.1	287.1	243.2	313.5	285.1	294.6	304.7
18	17	well-17	Field-A	Mexico	978.994	14.853	5.332	6.926		265	243.7	258.8	185.6	265.6	246.5	271.9	238.5
19	18	well-18	Field-A	Mexico	819.2	10.81	4.176	27.589		280.2	271.1	282.9	353.6	304.2	281.1	298.1	284.2
20	19	well-19	Field-A	Mexico	904.099	55.951	14.429	36.212		281.5	293.2	300.7	324	285.9	318.9	302.9	297.4
21	20	well-20	Field-A	Mexico	916.5	141.349	8.997	11.937		267.3	304.5	296.9	272.5	306.8	317.7	356.6	362.7

Fig. 12 Typical output filename file (with an Excel file extension: xlsx) showing the results of the estimated subsurface temperatures.

2.4. Help menu

The help menu contains three options:

(i) <Download User's Manual>, which contains a pdf file that describes the operation and all the computational features of the program GaS_GeoT (Fig. 13);

(ii) <Download Input data template>, which contains the input file (Excel file in xlsx format) as a template for helping the potential users to enter the input data (Fig. 14); and

(iii) <README>, which contains a general description of the computer program GaS_GeoT (Fig. 15).

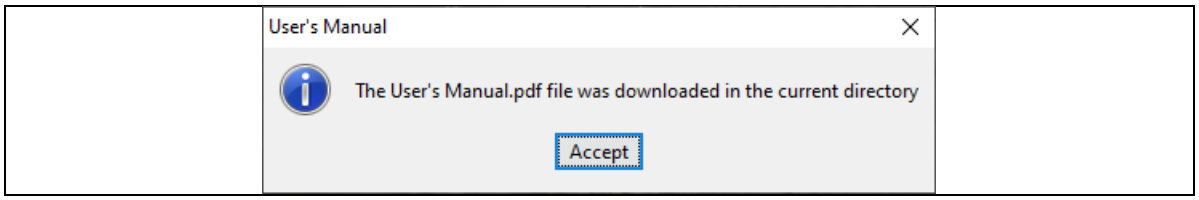


Fig. 13 Display of the message after the program successfully downloads the User's Manual pdf file.

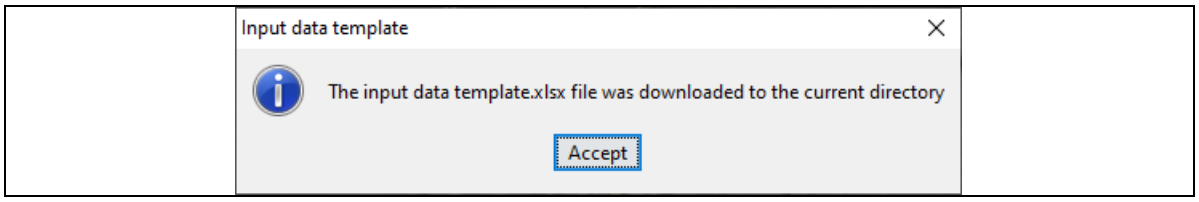


Fig. 14 Display of the message after the program successfully downloads the template Excel file (with the filename extension xlsx) for entering the input data

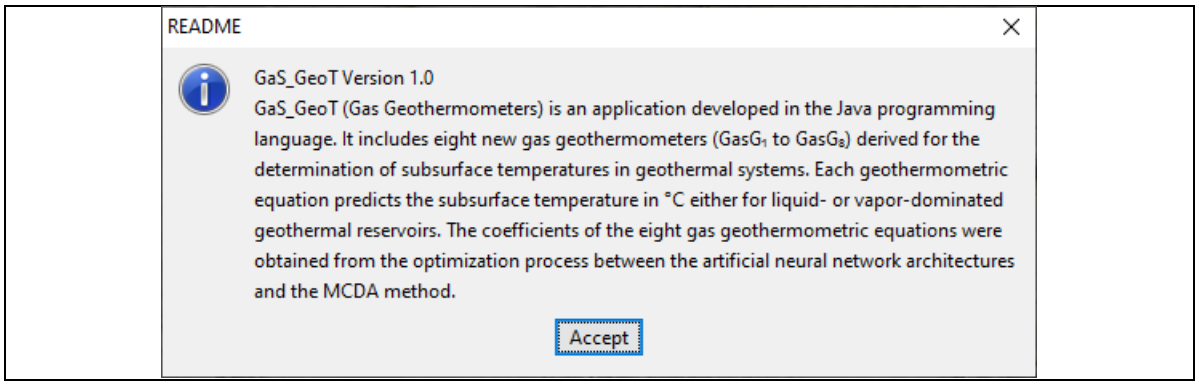


Fig. 15 A general description of the computer program GaS_GeoT

3. Authors and e-mail addresses

If some doubts still exist about the execution of the computer program GaS_GeoT, the users may contact directly to the first or second author of the paper for any additional information.

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