User´s Manual for GasGeo v1.0 the computer program: To be used in the estimation of deep reservoir temperatures geothermal

Computer server site: https://github.com/ANNGroup/GasGeo_v1.0.git

E. Santoyo, Agustin Acevedo-Anicasio, Daniel Pérez-Zárate, Kailasa Pandarinath, Christian Guadalupe García-López and Lorena Díaz-González (2019) New gas geothermometers based on artificial neural network.

A quick user manual is briefly described to estimate the temperature of a geothermal reservoir. Eight new geothermometric equations (gas geothermometers GEOG1-GEOG8) written in the Java language were used to estimate the bottom-hole temperatures (BHT) of geothermal production wells. These new geothermometers use the chemical composition of the gaseous phase of the geothermal fluids as main input data (CO_2, H_2S, CH_4, and H_2) in mmol/mol dry basis.

The installation of the Java virtual machine (free license version 7 or higher) is required to interpret the intrusions of the Jar executable and the Excel spreadsheet (xlsx) for the template that will store the data to be processed. The Jar executable and the template can be downloaded from the public repository: https://github.com/ANNGroup/GasGeo_v1.0.git. To effectively run the GasGeo program, the following hardware specifications are suggested:

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

Computer running instructions. GasGeo program instructions. After running the computer program, a full report is printed as a xlsx file. The report will contain the input data used for the estimation of deep reservoir temperatures geothermal (the chemical composition of the gaseous phase of the geothermal fluids), and the temperature calculated (°C). Thus, the report will include the following parameters:

- Sample (a consecutive number),
- Geothermal well (a string of alphanumeric characters),
- Geothermal field (a string of alphanumeric characters),

- Country (a string of alphanumeric characters),
- CO_2, H_2S, CH_4, and H_2 (integer or decimal numbers),
- Out of range (a string of alphanumeric characters),
- GEOG1 to GEOG8 (integer or decimal numbers).

From these results, an additional information can see in the chemical composition of the gaseous phase according to the range of operation for each new geothermometer, and the temperature estimated (°C). For example, if the value minimum of concentration of the gas CO_2 in geothermometer GEOG1 is 328 mmol/mol, and the user introduce a value lower than that (e.g. 300), the cell with this value appears of colour blue, and the temperature estimated for GEOG1 in red colour.

The following pictures are shown to demonstrate the use of the program GasGeo:

Fig. 1 General environment of GasGeo program

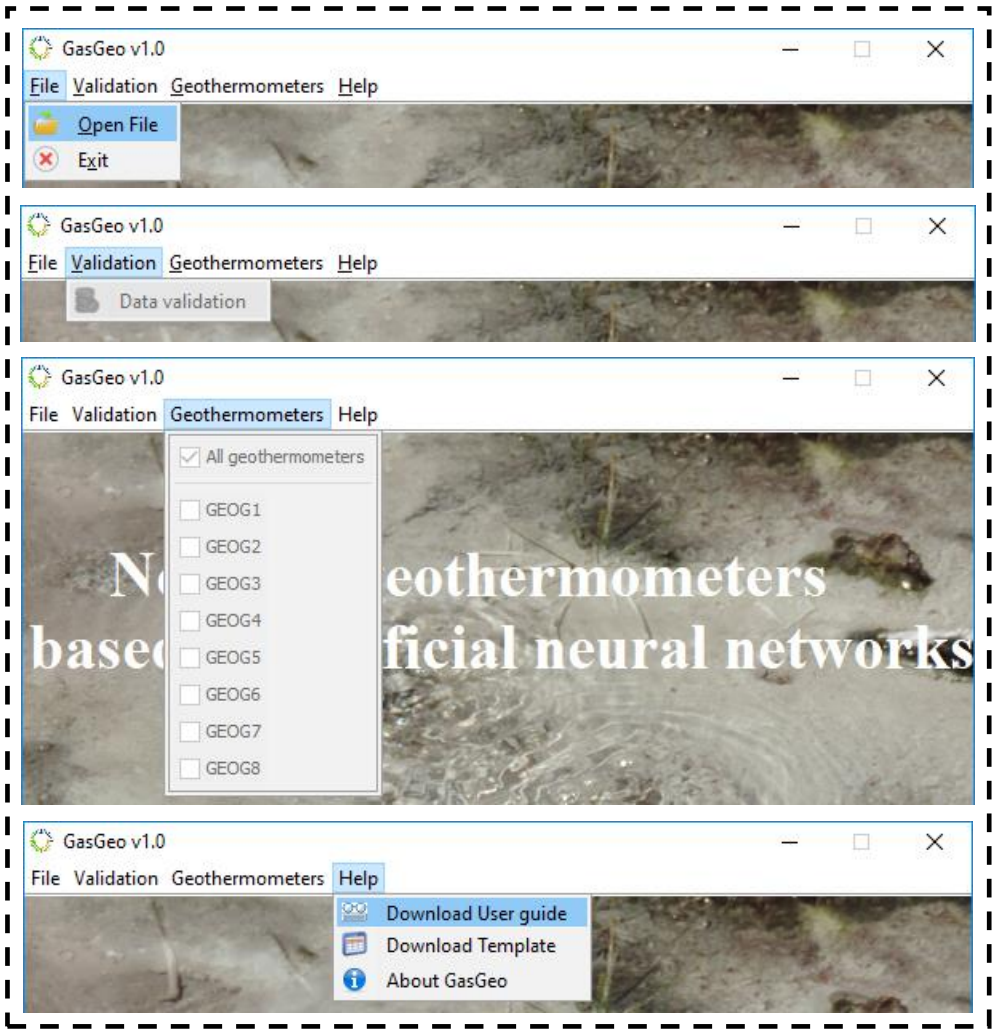


Fig. 2 All the menus displayed

Menu File. It contains two options: (i) "*Open file"*, allows to select the data file (xlsx) to be processed with the following information in each column: Sample, Geothermal well, Geothermal field, Country, CO_2, H_2S, CH_4, and H_2 (Fig. 3); and (ii) "*Exit"*, closes the GasGeo program.

	A	B	C	D	E	F	G	H
1	Sample	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	907.278	50.349	0.997	20.937
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	985.4	5.87	0.324	0.865

Fig. 3 Example with values of a geothermal field of Mexico

As shown in Fig 3, the data file must contain information in 8 columns, in case of having data in more columns, GasGeo displays a message with location of the anomalous sample (Fig. 4).

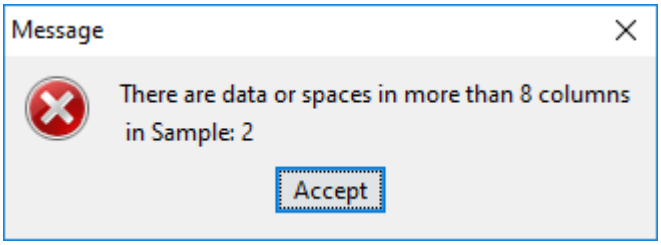


Fig. 4 Data example in more than 8 columns

Menu Validation. This menu is enabled once a data file (xlsx) has been selected, which are displayed in the GasGeo program (Fig. 5).

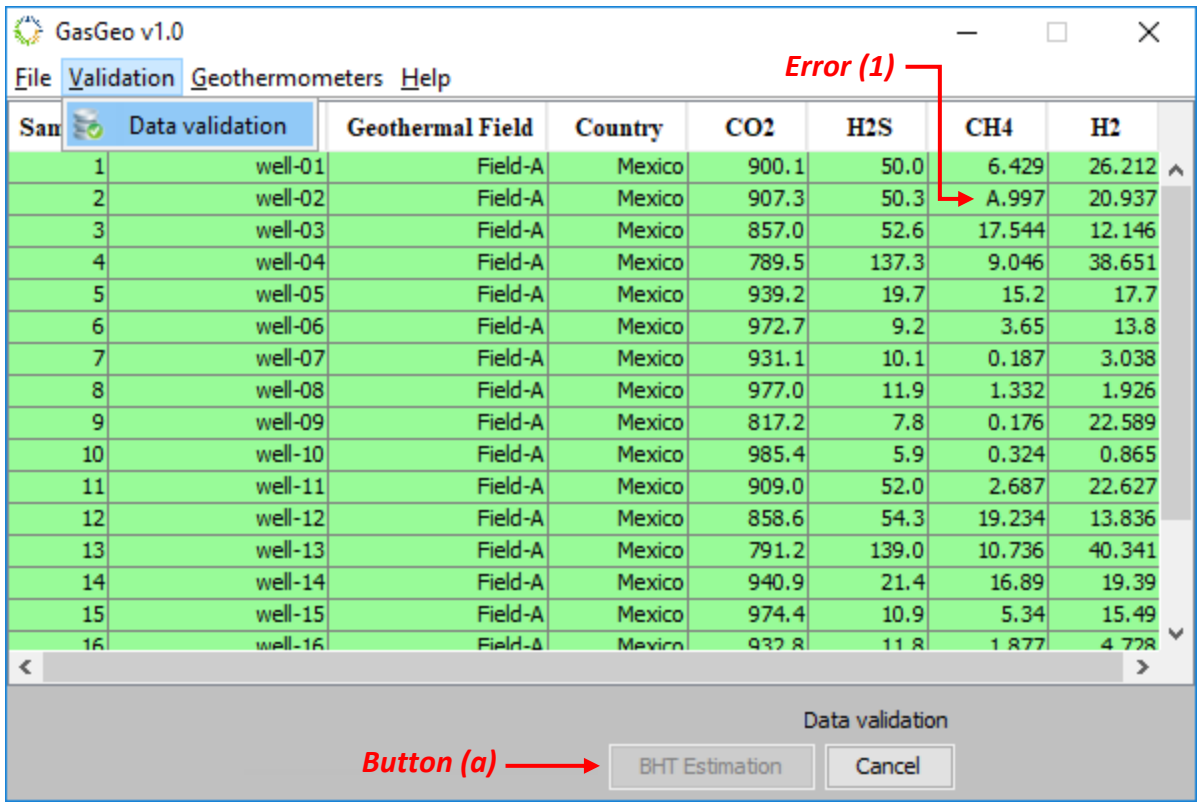


Fig. 5 Example with values of a geothermal field of Mexico displaying in GasGeo program

As shown in Fig 5, the *"Button (a)"* is disabled, since data validation is required to avoid typographical errors. For example, in the same figure, the *"Error (1)"* exists since the chemical composition of all gases (in this case methane CH_4) must be a real number. This is the primary function of the validation menu, detecting and correcting typographical errors

directly from the GasGeo program. The "*Cancel*" button returns to the main window (Fig. 1) of the GasGeo program.

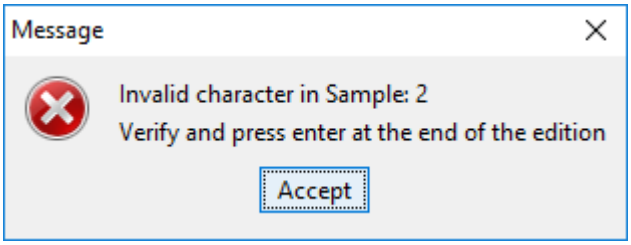
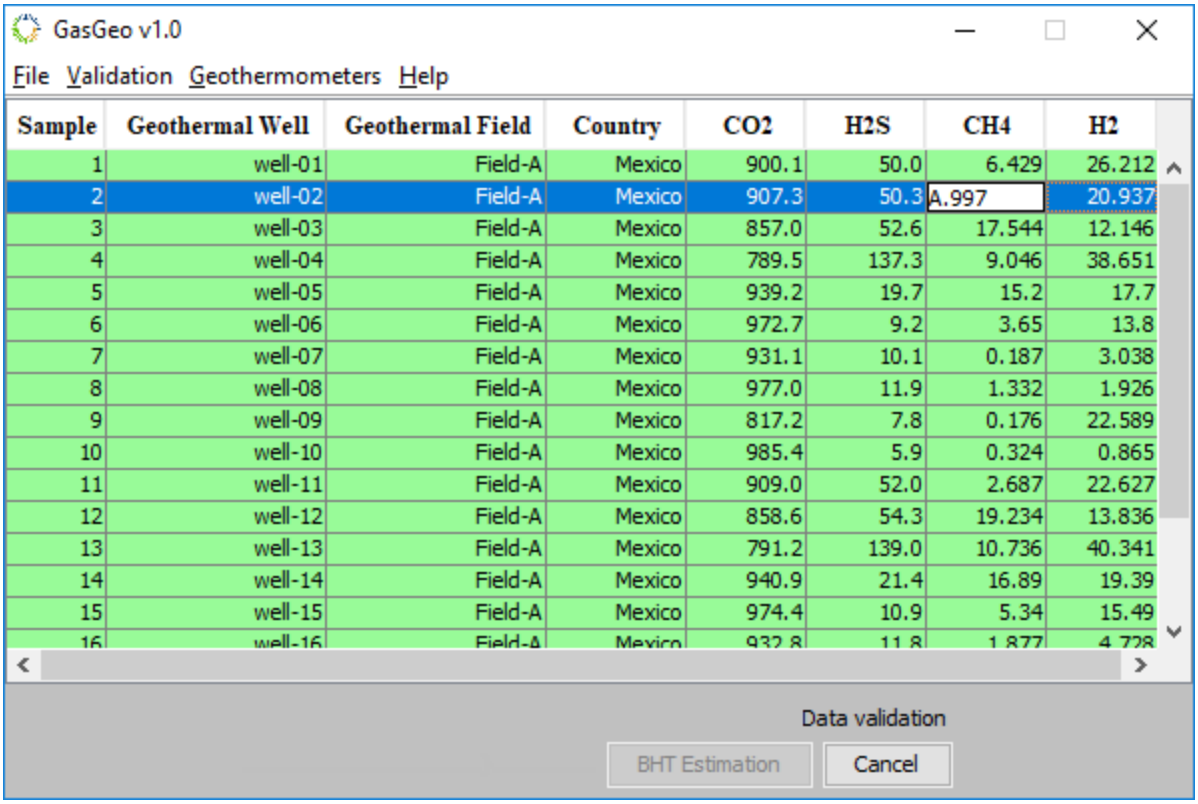


Fig. 6 Message displayed when an invalid character is detected

Later, editing is enabled in the cell that contains the invalid character as shown in Fig. 7. Once the typographical error has been corrected, the enter key must be pressed to update the data to be processed and validate it again.



Sample	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	907.3	50.3	A.997	20.937
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	985.4	5.9	0.324	0.865
11	well-11	Field-A	Mexico	909.0	52.0	2.687	22.627
12	well-12	Field-A	Mexico	858.6	54.3	19.234	13.836
13	well-13	Field-A	Mexico	791.2	139.0	10.736	40.341
14	well-14	Field-A	Mexico	940.9	21.4	16.89	19.39
15	well-15	Field-A	Mexico	974.4	10.9	5.34	15.49
16	well-16	Field-A	Mexico	932.8	11.8	1.877	4.728

Fig. 7 Cell enabled in the sample where an invalid character was located

When the data to be processed is validated, "*Button (a)*" will be enabled and a legend of the total number of samples found in the file will appear (Fig. 8).

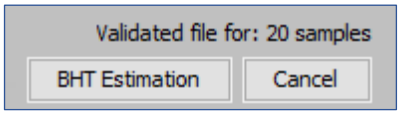


Fig. 8 successful validation

Menu Geothermometers. This menu is enabled once the data to be processed has been validated (Fig. 9).

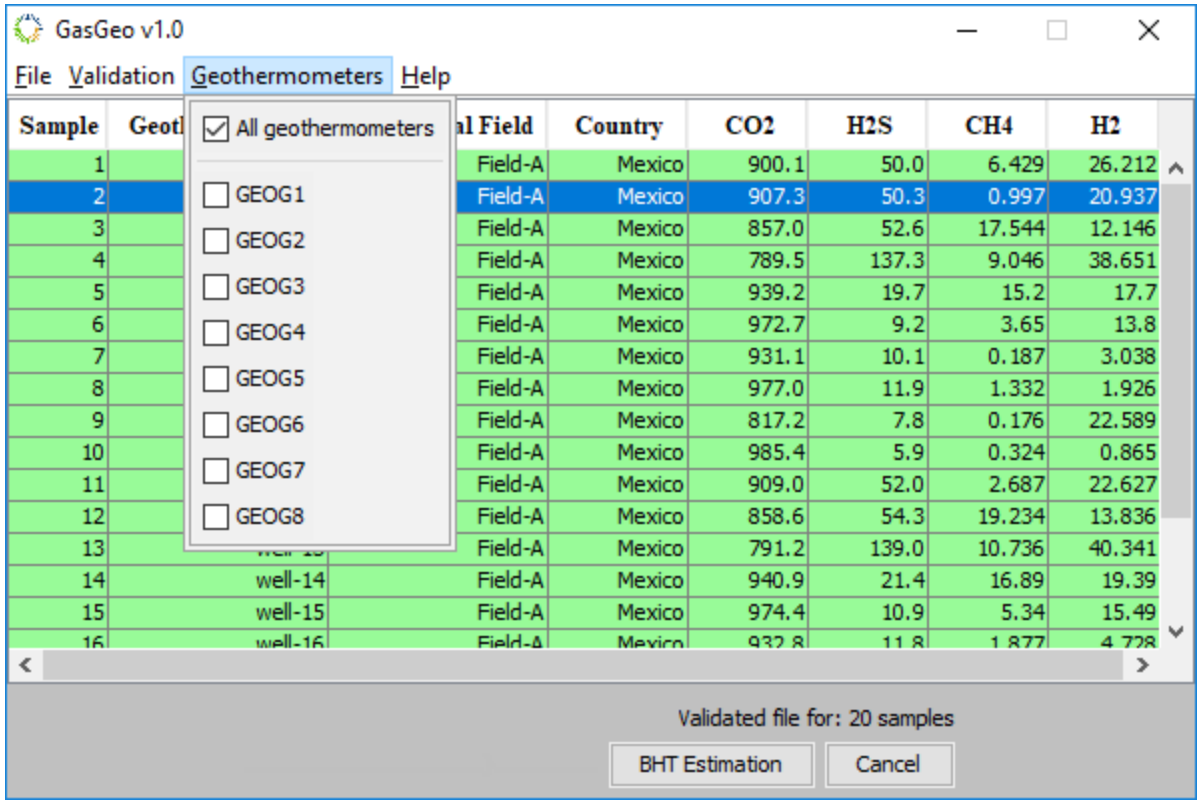


Fig. 9 Example of 8 gas geothermometers available for temperature estimation (° C)

The GasGeo program allows the estimation of the temperature (° C) of all gas geothermometers or only some of them. After clicking on the BHT button, the GasGeo program allows you to save the result file with a user-defined name (*Name.xlsx*) or with the default name (*RESULTS_input data.xlsx*) as shown in Fig. 10

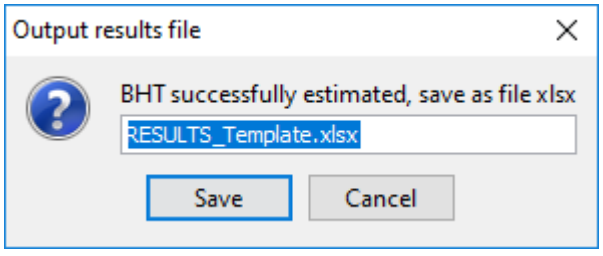


Fig. 10 Save as or by default the output file

Subsequently, the GasGeo program allows opening the results output file (Fig. 11). Otherwise, it will be stored in the current directory. It is important to mention that the option shown in Fig. 11 only works with Microsoft Windows operating systems.

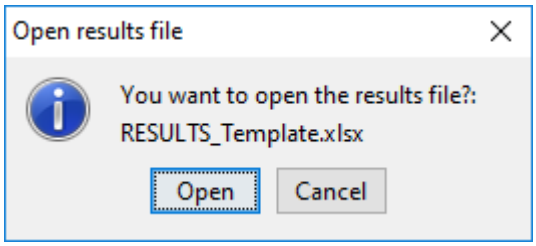


Fig. 11 Open de results file

Finally, an example of the results file is shown in Fig. 12. The first 8 columns (A-H) correspond to the input data, and following 9 columns (I-Q) are the results of the GasGeo program.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Sample	Geotherm	Geotherm	Country	CO2	H2S	CH4	H2	Out of range	GEOG1	GEOG2	GEOG3	GEOG4	GEOG5	GEOG6	GEOG7	GEOG8
2	1	well-01	Field-A	Mexico	900.099	49.951	6.429	26.212		270.7	333.1	320.7	297.7	310.8	312.6	307.4	307.4
3	2	well-02	Field-A	Mexico	912.5	200.349	0.997	1.937	H2S-higher	217.9	331.6	290.1	253	267.6	278.9	295.1	327.3
4	3	well-03	Field-A	Mexico	856.95	52.632	17.544	12.146		293.1	298	322.7	298.6	302.7	301	303.3	326.1
5	4	well-04	Field-A	Mexico	789.474	137.336	9.046	38.651		293.2	305.7	290.1	297.7	289.8	251.8	298	280.5
6	5	well-05	Field-A	Mexico	939.2	19.7	15.2	17.7		270.8	286.3	266	297.5	257.1	257.2	260.3	249.7
7	6	well-06	Field-A	Mexico	972.7	9.2	3.65	13.8		245.8	257.6	256.3	298.6	248.7	243.5	239.8	253.8
8	7	well-07	Field-A	Mexico	931.117	10.08	0.187	3.038		293.1	301.9	255.4	272.2	260.9	280.1	284.9	277.2
9	8	well-08	Field-A	Mexico	976.994	11.853	1.332	1.926		311.3	251.5	247.7	243.3	241.9	261.4	247.1	262.2
10	9	well-09	Field-A	Mexico	817.2	7.81	0.176	22.589		291.9	304.7	256.7	297.7	293.1	294.1	297.9	297.2
11	10	well-10	Field-A	Mexico	985.4	5.87	0.324	0.865		312.1	238	256.7	223.4	226.1	263.4	218.7	246.7
12	11	well-11	Field-A	Mexico	908.968	52.039	2.687	22.627		272.3	332.9	322.3	297.6	315.4	327	314.4	332.5
13	12	well-12	Field-A	Mexico	858.64	54.322	19.234	13.836		293.2	299.1	323.6	297.1	303	306	306.3	325.7
14	13	well-13	Field-A	Mexico	791.164	139.026	10.736	40.341		293.1	305.5	290.1	297.5	290.3	244.5	298.2	279.2
15	14	well-14	Field-A	Mexico	940.89	21.39	16.89	19.39		270.8	284.1	265.8	297.6	256.1	258.9	258.4	251.9
16	15	well-15	Field-A	Mexico	974.39	10.89	5.34	15.49		244.2	255.3	253.3	297.1	248.5	247.1	242.2	257.2
17	16	well-16	Field-A	Mexico	932.807	11.77	1.877	4.728		277.3	298.1	248.4	291.7	280	260.6	240.2	261.9
18	17	well-17	Field-A	Mexico	978.684	13.543	3.022	3.616		293.2	248.9	226.9	272.5	284	257.1	268	269.6
19	18	well-18	Field-A	Mexico	818.89	9.5	1.866	24.279		292.9	304.5	256.1	297.8	288.6	271.2	297.8	282.8
20	19	well-19	Field-A	Mexico	987.09	7.56	2.014	2.555		291.9	235.2	256.7	270.4	252.9	254.7	266.7	268.7
21	20	well-20	Field-A	Mexico	910.658	53.729	4.377	24.317		271.4	332.4	323.3	297.7	312.6	325.6	313.1	329.6

Fig. 12 Example of a results file (xlsx)

In Fig. 12 the sample number 2 appears with information to be considered by the user. The chemical composition of the H_2S (blue background) is above the operating range only of the GEOG7 gas geothermometer. For this reason, the estimated temperature appears in red.

Menu Help. The last menu contains three options: (i) "*Download User guide"*, a pdf file that describes the operation of the GasGeo program; (ii) "*Download Template"*, a file in xlsx format as a template for the input data; and, (iii) "*About this"*, a brief general description of the GasGeo Version 1.0 program.

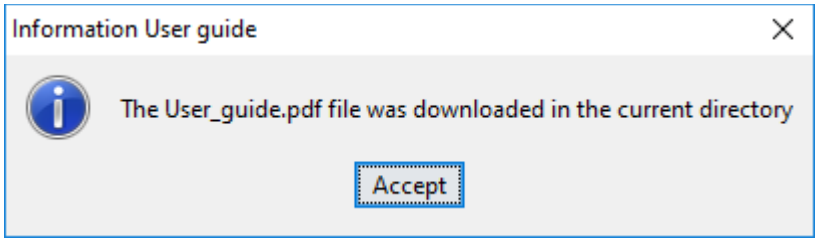


Fig. 13 Subsequent message to download the user guide

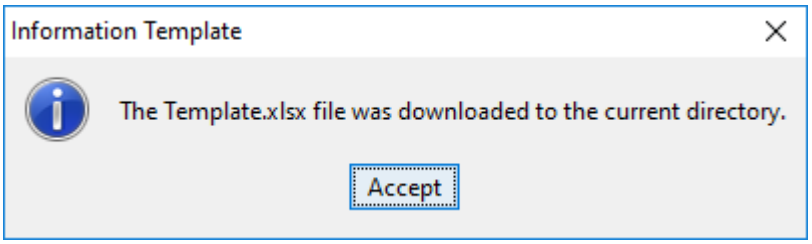


Fig. 14 Message after downloading the template (xlsx) for the input data

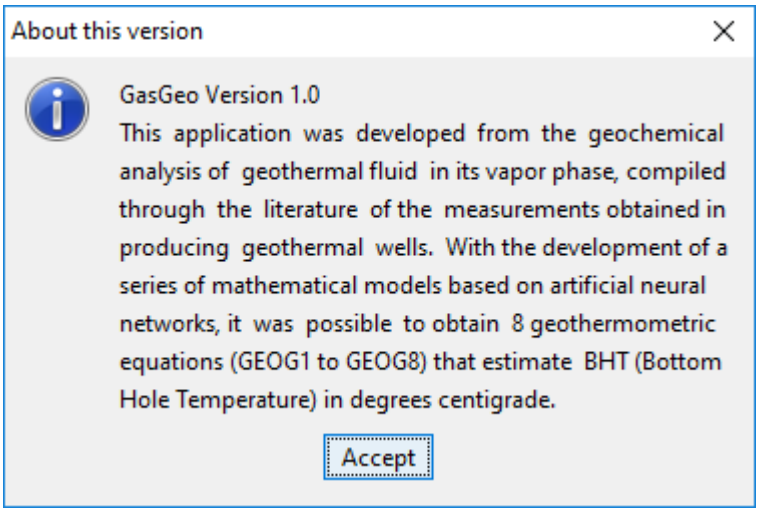


Fig. 15

Developers and contact e-mail address:

If some instructions or doubts are still needed from the users, all the authors of the submitted manuscript are available to provide some additional hints for a successful application of the GasGeo program.

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