

WATCH AUTOMATOR: AN EXCEL BASED DATA PROCESSOR FOR MULTIPLE GEOCHEMICAL SAMPLES

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ABSTRACT

WATCH, originally developed by University of Iceland, is a computer program which is used to combine steam and water samples collected at surface and calculate the down-hole geothermal fluid chemistry such as pH, aqueous speciation, mineral saturations, gas and liquid composition and pressures. However, the manual line by line entry of input parameters and text output make the process of both running the software and reading outputs cumbersome. To address this limitation, WATCH Automator, a Microsoft Excel-based program has been developed to interface with the latest version WATCH (version 2.4., 2010). The Automator speeds up the interpretation of geochemical well data. The input parameters are transferred from an existing geochemistry database to WATCH and key output results, such as saturation indices of calcite and silica, are extracted and plotted. Moreover, the WATCH automator has the capability to process multiple samples, which enables the historical chemical trends of a geothermal well to be efficiently analysed.

1. INTRODUCTION

One of the important factors that can affect the sustained productivity of a geothermal well is scaling. Therefore effective monitoring and predicting the scaling potential is essential in sustaining steam supply to the power plant. WATCH, developed by Arnorrson and Sigurdsson (1982) at the University of Iceland, is a popular computer program among geochemists for calculating geothermal fluid chemistry and composition.

Given the water and steam sample data, WATCH can calculate concentrations of different key chemicals at reservoir condition, which can then be used to analyse the scaling potential of a well. However, WATCH is a console program that requires line by line entry of input parameters, which is time-consuming, cumbersome and error prone. Additionally, the output files generated by WATCH are in text format, which are difficult to extract information from.

To address these limitations, WATCH Automator, a Microsoft Excel-based program, was created to act as an interface to the WATCH console program so that all the operations can be effectively controlled from within an Excel spreadsheet.

2. METHODOLOGY

The WATCH program is composed of two components, an input file generator (wain12.exe) and actual computational analyser program (watch24.exe) which reads the generated input file. Firstly, the WATCH users need to enter all required parameters (e.g., sample IDs, units and

concentration of different chemicals) line by line into the wain12.exe program to generate an input file that can be readable to the analyser program. Subsequently, the users need to repeat a similar line by line laborious process of specifying the required input file and output file name, geothermometer type, boiling steps into the watch24.exe to perform an analysis. The outputs from running the analysis are then stored in a text file. The limitations of running WATCH directly are: 1. It involves laborious work of re-entering information that has been stored in a database. 2. The users have to be meticulous when entering information to avoid correcting information later on by re-entering everything from scratch. 3. Slow to extract key information from output files in text format.

The Excel-based WATCH Automator program runs the original WATCH programs in the background, and it overcomes inefficient line by line command input by replacing it with tabular inputs within Excel (see Figure 4).

Figure 1 shows the relationship between the in-house geochemistry database, WATCH automator and WATCH programs. It should be noted that the development of the WATCH automator does not involve any modification to the original console version of WATCH. Figure 1 also shows the major steps involved in analysing one geochemistry sample.

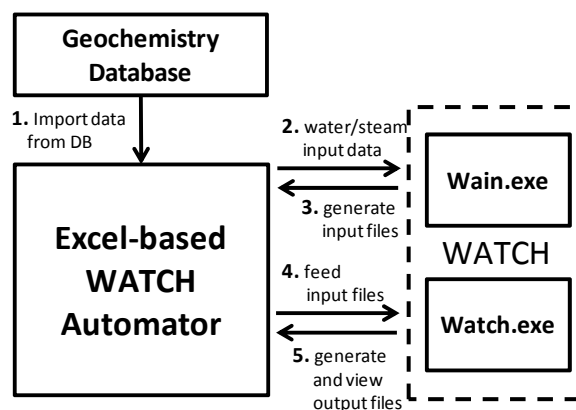


Figure 1: Relationship between WATCH Automator, geochemistry database and WATCH programs.

2.1 Import data from an existing database

One of the features of the WATCH automator is to directly extract input data from Contact's geothermal chemistry database (see Figure 4), effectively avoiding the redundant process of entering stored information (Note that the current implementation can only extract input data from Contact's geothermal database. However, it can be easily tweaked to adjust to generic data structure). Typically steam and water

samples are required for running a simulation. To run the WATCH automator, the concentrations of the following input parameters need to be extracted from a geochemistry database: for water dissolved gases (CO₂, H₂S, NH₃) and B, SiO₂, Na, K, Mg, Ca, F, Cl, SO₄, Al, Fe, Water pH, and for steam CO₂, H₂S, NH₃, H₂, O₂, CH₄, N₂ together with sampling details (separation pressure and discharge enthalpy).

After querying and extracting the relevant information from Contact's geochemistry database, (for example, all the samples taken from well WK070 from 1970 to 2013), we can further refine our sample selection by manually highlighting the ones we would like to analyse.

Since there is inconsistency in units between Contact's geochemistry database and ones used by WATCH, conversion of units to WATCH standard units is performed by an Excel macro. Figure 5 shows the input parameters for a number of samples converted to the WATCH standard units and ready for running analysis.

2.2 Process multiple samples

To study the geochemical trends over time of a geothermal field requires the analysis of data over many years and this could involve calculating thousands of samples. Therefore, purely relying on the console's line by line input is simply not viable.

One of the powerful features of WATCH Automator is that it allows users to analyse multiple samples efficiently by running the selected samples sequentially and automatically. For each sample the process conditions can be individually specified; for example whether to use a specified geothermometer or a measured temperature and what boiling/cooling steps are used. After successful running, hyperlinks to the generated output files will be populated within the spreadsheet, allowing users to easily view the files (see Figure 6).

2.3 Extract key results from output files

All the output files are generated by the original WATCH program and therefore retain the original text format. Extracting key information from these output files is time consuming. Therefore, WATCH Automator also includes a module for viewing key chemical results from all the output files.

Since the output text files for all samples are consistent in format, a feature has been incorporated into the WATCH Automator to import and extract this key information from the relevant output files, and list them in a tabular format in Excel as shown in Figure 7. Any data in the output files can be extracted but only the following mineral species that are of our main interest are extracted: anhydrite, calcite, amorphous silica, chalcedony and quartz.

The current implementation only extract results for the five minerals, however, the program can be modified to include more minerals in the future.

The saturation index (SI) is then given by $SI = \log(Q/K)$, where K is the equilibrium constant and Q is the reaction quotient.

2.3.1 Plotting multiple boiling/cooling steps for a single sample

Limited by the capacity of WATCH, users can specify up to 10 temperature steps of single-stage adiabatic boiling or conductive cooling from the "reference" temperature. Figure 2 shows the charts of saturation index for well WK070 versus boiling temperature generated by the WATCH Automator, given that they are single-stage adiabatic boiling from the reference temperature (240 °C in this case) to 190, 180, 170 and 160°C respectively.

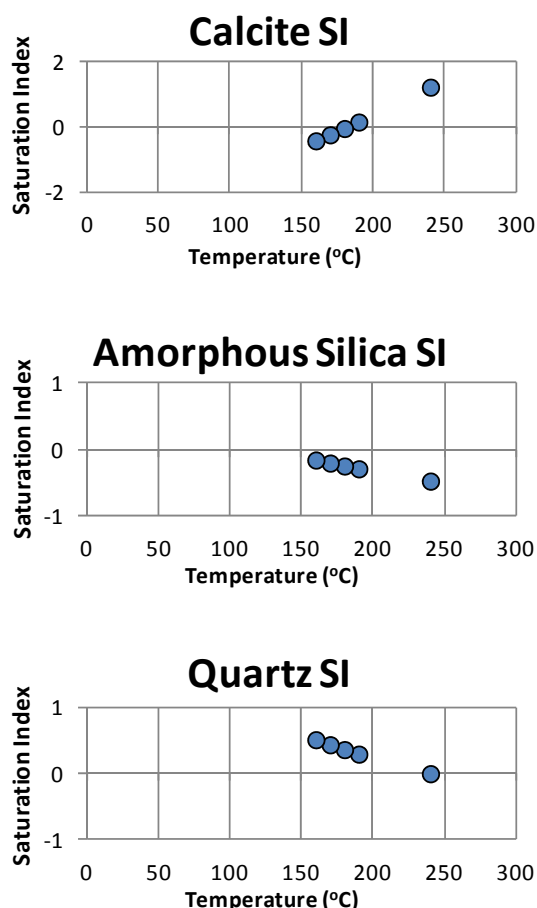


Figure 2: The saturation index (SI) of different minerals for WK070 at different boiling temperatures (°C).

2.3.2 Plotting historical trend of chemistry change

If all samples being analysed by WATCH are from one specific well, we can use the outputs of this group of samples to study the history and predict the scaling potential of this geothermal well. Figure 3 shows the saturation indices (SI) of anhydrite, calcite and amorphous silica for WK070 well from 1974 to 2013. It can be seen from the figure that WK070 has an increasing saturation with respect to calcite. Therefore, it has a higher potential to form calcite scale and therefore other well parameters (e.g., mass flow, wellhead pressure etc) should be closely monitored to identify any decline in output.

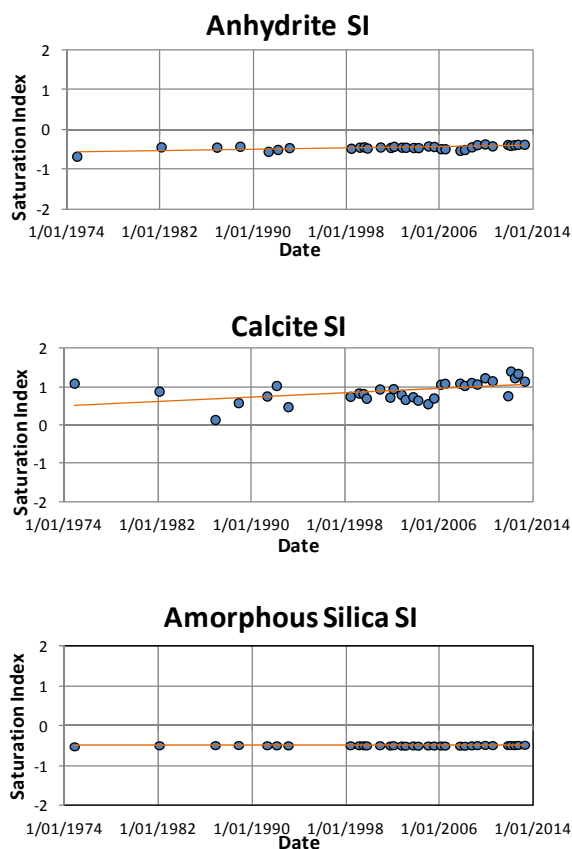


Figure 3: Mineral saturation indices with time for WK070.

CONCLUSIONS

In summary, the Excel-based WATCH Automator has provided the following improvements to the existing console WATCH program:

- Easy to migrate input data for WATCH manually or from an existing geochemistry database.
- Integrate all the WATCH functionalities within Excel, which means there is no need to switch between different programs to generate input files and then run the WATCH program.
- The capability to analyse multiple samples efficiently.
- Extraction of key results from output files and plotting the saturation index of these minerals within Excel.

ACKNOWLEDGEMENTS

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REFERENCES

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- Iceland GeoSurvey (ISOR): The Iceland Water Chemistry Group. *WATCH software*, <http://www.geothermal.is/software> (2013)

APPENDICES

Figures

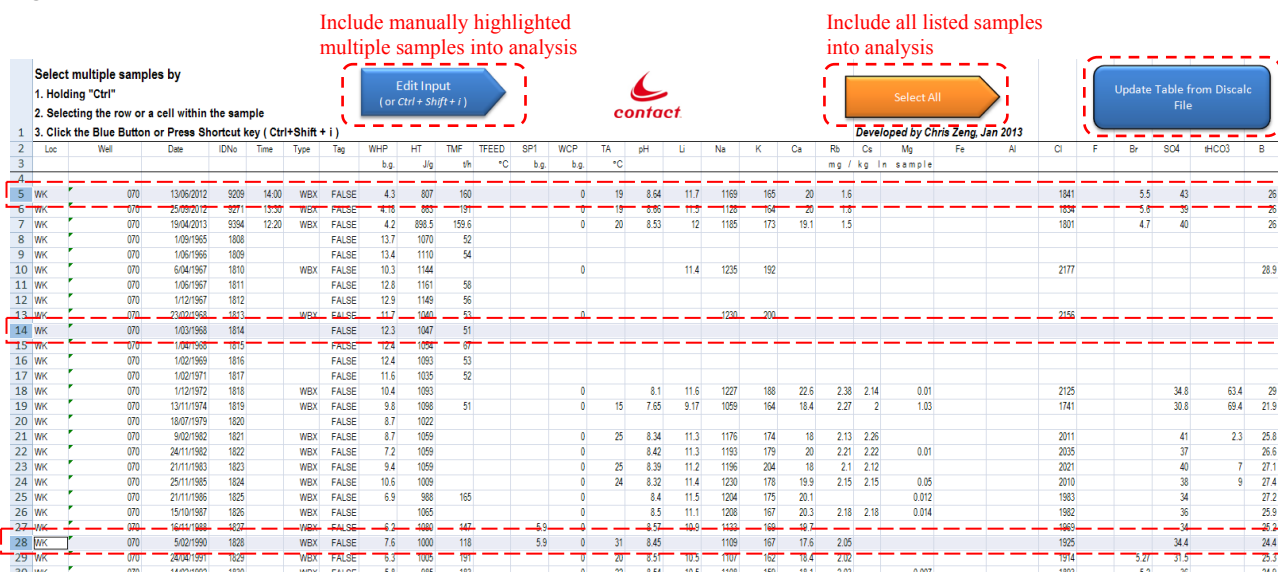


Figure 4: The interface page that can extract information from geochemistry database and subsequently refine sample selection by highlighting the ones of interest.

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Figure 5: Chemical samples for steam and water phases are listed in the main worksheet and can be modified before running the WATCH programs. These are the input parameters for WAIN12.exe.

Analyse all selected samples

Extract and display key results from all analysed samples

Run All (or Ctrl + Shift + R)

Parameters for Running WATCH

Please edit the parameters below before running WATCH

Output file name (please keep the file names with .out extension)	Temperature Type	Boiling Springs Model (Only applicable to single phase water sample)	Degassing Coefficient for boiling springs (Only applicable to single phase water)	After single-stage ADIABATIC BOILING from the reference temp to another	Degassing Coefficient	After CONDUCTIVE COOLING from the reference temp to another	Output file for each sample	Boiling Summary	Cooling Summary	Pick up boil/cool files? (does not apply to RUN ALL)	View all previously created output files
2 Chalcedony geothermometer	To specify an <i>adiabatic or measured temperature</i> , please enter the temperature in	If the fluid is assumed to have boiled and lost steam before sampling, input assumed BOILING TEMPERATURE (C). No boiling = BLANK	Range from 0.01 (little degassing) to 1 (equilibrium degassing). Default <BLANK> is equilibrium degassing.	FORMAT: No. of temp steps, and temperatures separated by commas. i.e., Num of steps, temp1, temp2, ... No boiling = BLANK	Range from 0.01 (little degassing) to 1 (equilibrium degassing). Default <BLANK> is equilibrium degassing.	FORMAT: No. of temp steps, and temperatures separated by commas. i.e., Num of steps, temp1, temp2, ... No cooling = BLANK	Open	View	N/A	Run Duplicate Delete	
3 Quartz geothermometer							Open	N/A	N/A	Run Duplicate Delete	
4 NaK geothermometer							Open	N/A	N/A	Run Duplicate Delete	
5 NaK geothermometer							Open	N/A	N/A	Run Duplicate Delete	
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Generated Summary

Optional

Add new sample

Delete All

Please add or delete samples as

Analyse single sample by clicking a hyperlink

Figure 6: Type of geothermometer or measured temperature to use for the reservoir model is specified. If applicable, boiling/cooling steps, degassing coefficient can also be specified.

Back to WATCH interface page

Key outputs

Sample #	Date	Reference Temp (Celsius)	temp type	Anhydrite			Calcite			Sil. amorph.			Chalcedony			Quartz			
				log K	log Q	S.I.	log K	log Q	S.I.	log K	log Q	S.I.	log K	log Q	S.I.	log K	log Q	S.I.	
WK070_13_11_1974_WHP10	13/11/1974	225.7 (Quartz)		-7.663	-8.343	-0.68	-12.153	-11.06	1.093	-1.724	-2.223	-0.499	-2.097	-2.223	-0.126	-2.223	-2.223	0	
WK070_9_02_1982_WHP9	9/02/1982	239.5 (Quartz)		-7.914	-8.359	-0.445	-12.501	-11.617	0.884	-1.685	-2.157	-0.472	-2.038	-2.157	-0.119	-2.158	-2.157	0.001	
WK070_24_04_1991_WHP6	24/04/1991	239.2 (Quartz)		-7.908	-8.466	-0.558	-12.494	-11.736	0.758	-1.686	-2.158	-0.472	-2.039	-2.158	-0.119	-2.159	-2.158	0.001	
WK070_14_02_1992_WHP6	14/02/1992	238.5 (Quartz)		-7.895	-8.406	-0.511	-12.476	-11.444	1.032	-1.687	-2.161	-0.474	-2.042	-2.161	-0.119	-2.162	-2.161	0.001	
WK070_11_02_1993_WHP6	11/02/1993	238.6 (Quartz)		-7.897	-8.362	-0.465	-12.478	-11.999	0.479	-1.687	-2.161	-0.474	-2.041	-2.161	-0.12	-2.162	-2.161	0.001	
WK070_29_08_1996_WHP5	29/08/1996	236.5 (Quartz)		-7.859	99.999	#N/A	-12.426	-11.535	0.891	-1.693	-2.17	-0.477	-2.05	-2.17	-0.12	-2.171	-2.17	0.001	
WK070_3_04_1997_WHP6	3/04/1997	236.3 (Quartz)		-7.856	99.999	#N/A	-12.42	-11.74	0.68	-1.694	-2.171	-0.477	-2.051	-2.171	-0.12	-2.172	-2.171	0.001	
WK070_5_03_1998_WHP5	5/03/1998	237.7 (Quartz)		-7.88	99.999	#N/A	-12.455	-11.557	0.898	-1.69	-2.165	-0.475	-2.045	-2.165	-0.12	-2.166	-2.165	0.001	
WK070_4_06_1998_WHP5	4/06/1998	238.5 (Quartz)		-7.895	-8.376	-0.481	-12.475	-11.726	0.749	-1.688	-2.161	-0.473	-2.042	-2.161	-0.119	-2.162	-2.161	0.001	
WK070_25_02_1999_WHP6	25/02/1999	239.1 (Quartz)		-7.906	-8.359	-0.453	-12.491	-11.655	0.836	-1.686	-2.158	-0.472	-2.039	-2.158	-0.119	-2.159	-2.158	0.001	
WK070_14_07_1999_WHP6	14/07/1999	239.2 (Quartz)		-7.908	-8.353	-0.445	-12.494	-11.674	0.82	-1.686	-2.158	-0.472	-2.039	-2.158	-0.119	-2.159	-2.158	0.001	
WK070_20_10_1999_WHP6	20/10/1999	236.6 (Quartz)		-7.86	-8.335	-0.475	-12.427	-11.727	0.7	-1.693	-2.17	-0.477	-2.05	-2.17	-0.12	-2.171	-2.17	0.001	
WK070_8_12_2000_WHP6	8/12/2000	238.9 (Quartz)		-7.902	-8.351	-0.449	-12.486	-11.545	0.941	-1.686	-2.159	-0.473	-2.04	-2.159	-0.119	-2.16	-2.159	0.001	
WK070_24_10_2001_WHP5	24/10/2001	235.4 (Quartz)		-7.84	-8.299	-0.459	-12.398	-11.671	0.727	-1.696	-2.175	-0.479	-2.055	-2.175	-0.12	-2.176	-2.175	0.001	
WK070_12_02_2003_WHP6	12/02/2003	234 (Quartz)		-7.813	-8.268	-0.455	-12.362	-11.694	0.668	-1.7	-2.182	-0.482	-2.061	-2.182	-0.121	-2.183	-2.182	0.001	
WK070_9_10_2003_WHP5	9/10/2003	236.3 (Quartz)		-7.856	-8.317	-0.461	-12.42	-11.682	0.738	-1.694	-2.171	-0.477	-2.051	-2.171	-0.12	-2.172	-2.171	0.001	
WK070_18_01_2005_WHP6	18/01/2005	236.1 (Quartz)		-7.852	-8.275	-0.423	-12.415	-11.858	0.557	-1.694	-2.172	-0.478	-2.052	-2.172	-0.12	-2.173	-2.172	0.001	
WK070_21_07_2005_WHP6	21/07/2005	235.9 (Quartz)		-7.848	-8.284	-0.436	-12.411	-11.705	0.706	-1.695	-2.173	-0.478	-2.053	-2.173	-0.12	-2.174	-2.173	0.001	
WK070_21_02_2006_WHP6	21/02/2006	235.5 (Quartz)		-7.841	-8.333	-0.493	-12.4	-11.336	1.064	-1.696	-2.175	-0.479	-2.054	-2.175	-0.121	-2.176	-2.175	0.001	
WK070_28_06_2006_WHP6	28/06/2006	235.2 (Quartz)		-7.835	-8.328	-0.492	-12.392	-11.304	1.088	-1.697	-2.177	-0.48	-2.056	-2.177	-0.121	-2.177	-2.177	0	
WK070_11_10_2007_WHP5	11/10/2007	233.5 (Quartz)		-7.804	-8.338	-0.534	-12.349	-11.257	1.092	-1.702	-2.185	-0.483	-2.063	-2.185	-0.122	-2.185	-2.185	0	
WK070_4_03_2008_WHP5	4/03/2008	234.1 (Quartz)		-7.815	-8.327	-0.512	-12.364	-11.313	1.034	-1.7	-2.182	-0.482	-2.061	-2.182	-0.121	-2.182	-2.182		