

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 Arnorsson 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.

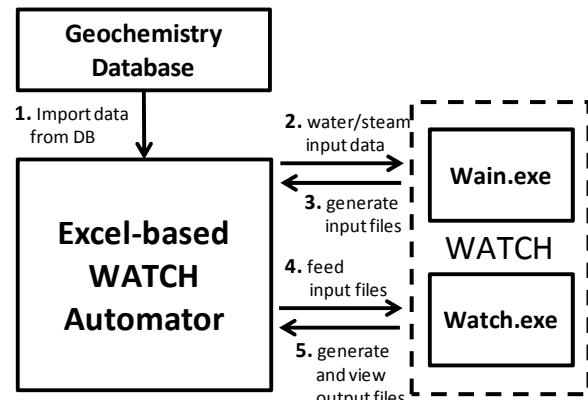


Figure 1: Relationship between WATCH Automator, geochemistry database and WATCH programs.

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.

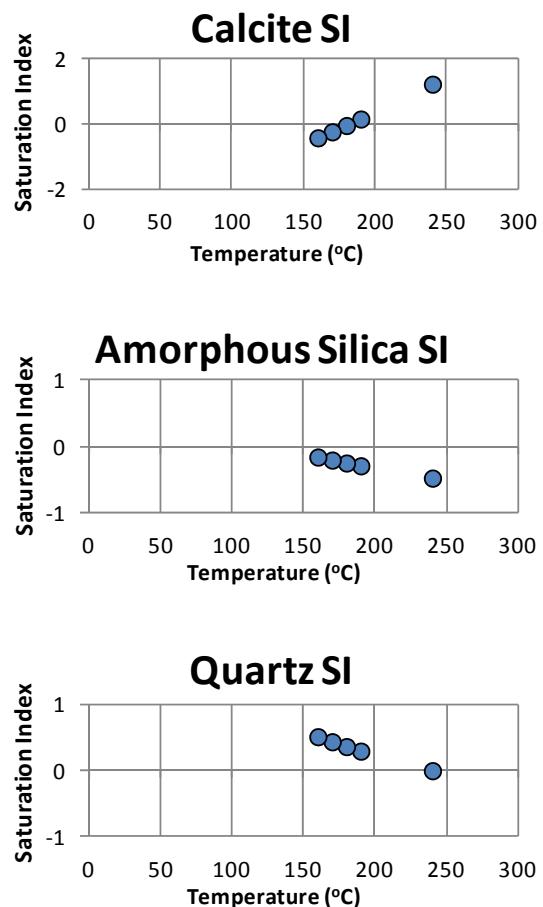


Figure 2: The saturation index (SI) of different minerals for WK070 at different boiling temperatures (°C).

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.

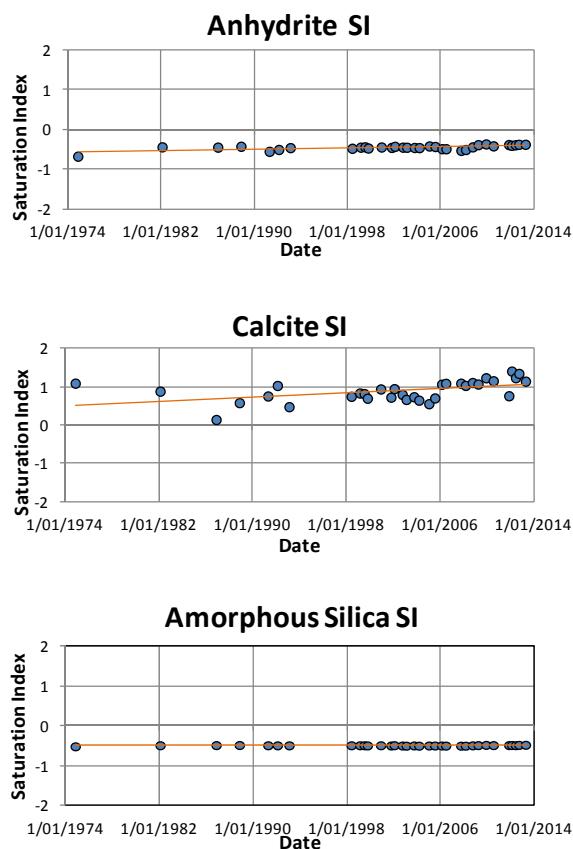


Figure 3: Mineral saturation indices with time for WK070.

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

Include manually highlighted multiple samples into analysis

Include all listed samples into analysis

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Developed by Chris Zeng, Jan 2013

Update Table from Discalc File

Loc	Well	Date	IDNo	Time	Type	Tag	WHP	HT	TMF	TFEED	SP1	WCP	TA	pH	Li	Na	K	Ca	Rb	Cs	Mg	Fe	Al	Cl	F	Br	SO4	iHCO3	B	
1																														
2																														
3																														
4																														
5 WK	070	13/05/2012	9209	14:00	WBX	FALSE	4.3	807	160					0	19	8.54	11.7	1169	165	20	1.5						1841	5.5	43	26
6 TW	070	25/05/2012	1801	13:30	WBX	FALSE	4.3	883	181					0	18	8.56	11.5	1128	164	20	1.5						1834	5.8	39	26
7 WK	070	19/04/2013	9394	12:20	WBX	FALSE	4.2	898.5	159.6					0	20	8.53	12	1105	173	19.1	1.5						1801	4.7	40	26
8 WK	070	1/09/1955	1808																											
9 WK	070	1/05/1955	1809																											
10 WK	070	6/04/1957	1810																											
11 WK	070	1/05/1957	1811																											
12 WK	070	1/12/1957	1812																											
13 WK	070	23/04/1958	1813																											
14 WK	070	1/03/1958	1814																											
15 WK	070	1/04/1958	1815																											
16 WK	070	1/02/1959	1816																											
17 WK	070	1/02/1971	1817																											
18 WK	070	1/21/1972	1818																											
19 WK	070	13/11/1974	1819																											
20 WK	070	18/07/1979	1820																											
21 WK	070	9/02/1982	1821																											
22 WK	070	24/11/1982	1822																											
23 WK	070	21/11/1983	1823																											
24 WK	070	25/11/1985	1824																											
25 WK	070	21/11/1986	1825																											
26 WK	070	15/10/1987	1826																											
27 WK	070	16/4/1988	1827																											
28 WK	070	5/02/1990	1828																											
29 WK	070	24/04/1991	1829																											
30 WK	070	14/02/1992	1830																											

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

Add samples from GeoChem DB

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Run All

INPUTS (for running WAIN12.exe)
Please edit the parameters below before running WATCH

Input File Name	Sample #	Water Phase (mg/kg)												Steam Phase (mmol/mol)																
		Loc	Sampling Temp (°C)	Sampling Pressure (bg)	Fluid Enthalpy (kJ/kg)	Discharge (kg/s)	CO2	H2S	NH3	B	SiO2	Na	K	Mg	Ca	F	Cl	SO4	Al	Fe	Total Solids	Water pH	pH Temp (°C)	CO2	H2S	NH3	H2	O2	CH4	N2
WK070_18_06_2012_WHP4.in	WK070_18_06_2012_WHP4	WK070		0	807	44.44				26	593	1169	165	20	1841	43					8.64	19	0.1	0.01	0.003	0	0	0	0.01	
WK070_25_09_2012_WHP4.in	WK070_25_09_2012_WHP4	WK070		0	863	53.06				26	631	1128	164	20	1834	39					8.66	19	0.11	0.01	0	0	0	0	0	
WK070_19_04_2013_WHP4.in	WK070_19_04_2013_WHP4	WK070		0	898.5	44.33				26	632	1185	173	19.1	1801	40					8.53	20	0.12	0.01	0.002	0	0	0	0.01	
WK070_13_11_1974_WHP10.in	WK070_13_11_1974_WHP10	WK070		0	1098	14.17	50.1			22	500	1059	164	1.03	18.4	1741	30.8					7.65	15	0.19	0.01	0	0	0	0	0
WK070_9_02_1982_WHP9.in	WK070_9_02_1982_WHP9	WK070		0	1059	0	1.66			26	587	1176	174	18	2011	41					8.34	25	0.15	0.01	0.003	0	0	0	0	
WK070_24_04_1993_WHP6.in	WK070_24_04_1993_WHP6	WK070		0	1005	53.06				25	578	1107	162	18.4	1914	31.5					8.51	20	0.28	0.02	0.004	0	0	0	0	
WK070_14_02_1992_WHP6.in	WK070_14_02_1992_WHP6	WK070		0	985	50.83				25	577	1108	159	0.007	18.1	1893	36					8.54	22	0.13	0.01	0.003	0	0	0	0
WK070_11_02_1993_WHP6.in	WK070_11_02_1993_WHP6	WK070		0	1015	56.67				573	1102	163	18.4		1879	36.7					8.53	21	0.15	0.01	0	0	0	0	0	
WK070_29_08_1996_WHP5.in	WK070_29_08_1996_WHP5	WK070		0	1099	37.22				569	1055	153	0.009	19.1	1861						8.79	17	0.17	0.02	0	0	0	0	0	

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.

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.

Key outputs																		
Back to WATCH interface page																		
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_WHPI0	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_WHPI9	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_WHPI6	24/04/1991	239.2	Quartz	-7.908	-8.466	-0.558	-12.494	-11.736	0.758	-1.686	-2.156	-0.472	-2.039	-2.158	-0.119	-2.159	-2.158	0.001
WK070_14_02_1992_WHPI6	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_WHPI6	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_WHPI5	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_WHPI6	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_WHPI5	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_WHPI5	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_WHPI6	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_WHPI6	14/07/1999	239.2	Quartz	-7.908	-8.353	-0.445	-12.494	-11.674	0.82	-1.686	-2.156	-0.472	-2.039	-2.158	-0.119	-2.159	-2.158	0.001
WK070_20_10_1999_WHPI6	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_WHPI6	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_WHPI5	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_WHPI6	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_WHPI5	9/10/2003	236.3	Quartz	-7.856	-8.317	-0.461	-12.442	-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_WHPI6	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_WHPI6	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_WHPI6	21/02/2006	235.5	Quartz	-7.841	-8.333	-0.492	-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_WHPI6	28/06/2006	235.2	Quartz	-7.835	-8.328	-0.493	-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_WHPI5	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_WHPI5	4/03/2008	234.1	Quartz	-7.815	-8.327	-0.512	-12.364	-11.33	1.034	-1.7	-2.182	-0.482	-2.061	-2.182	-0.121	-2.182	-2.182	0

Figure 7: Extracted results of our interest from text files imported into Excel in tabular format.