

**Introduction
to**

AquaChem

So Far - So Good

Site investigation completed

**Hydrogeologic setting
understood**

Sampling plan developed

Samples collected

Lab data evaluated

What Now?

**Evaluate Impacts
Compliance Assessment
Citizen's Complaint
Investigations
Prepare Technical Reports**

How Can I Do This?

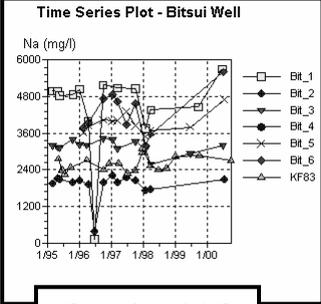


AquaChem

Software package designed specifically for graphical and numerical analysis and modeling of geochemical parameters.

What Can AquaChem Do?





Time Series Plot - Bitsui Well

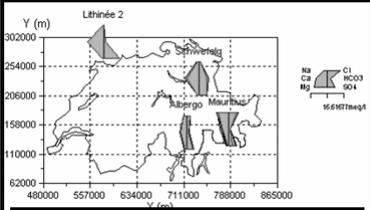
Na (mg/l)

Legend: BT_1, BT_2, BT_3, BT_4, BT_5, BT_6, KF83

SampleID	BITSUI-1	
Date	10/18/1995	
pH	8.9	
Cond 20°C (µS)	17800	
TDS (110 °C, mg/l)	14200	
Cations		
Na+	(mg/l)	(meq/l)
	4.860E+03	2.114E+02
K +	2.000E+01	5.115E-01
Mg++	2.700E+01	2.221E+00
Ca++	5.600E+01	2.794E+00
Mn++	8.000E-02	2.912E-03
Anions		
F-	(mg/l)	(meq/l)
	2.510E+00	1.321E-01
Cl-	1.950E+03	5.500E+01
SO4--	6.850E+03	1.426E+02
HCO3-	1.010E+03	1.656E+01
CO3--	1.080E+02	3.600E+00

GRAPHS

DATA REPORTS



MAP PLOTS

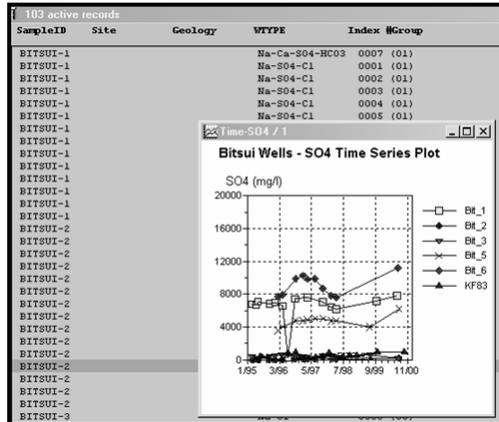
103 samples, concentrations in mg/l						
	Min	Max	Average	St. Dev.	Dev. Coeff	Var
Na	120.0	5700.0	3315.485	1106.742	33.381	98.0
Ca	3.6	570.0	86.735	120.141	138.515	99.0
Mg	1.1	240.0	40.757	56.729	139.188	100.0
Cl	45.7	3160.0	1617.907	877.632	54.245	99.0
SO4	4.5	11400.0	3343.782	3699.8	110.647	100.0
pH	6.6	8.9	7.702	0.923	11.984	26.0

STATISTICS

Temporal Trend Analysis

Time Series

Time Series Plot Changes in Concentration Over Time



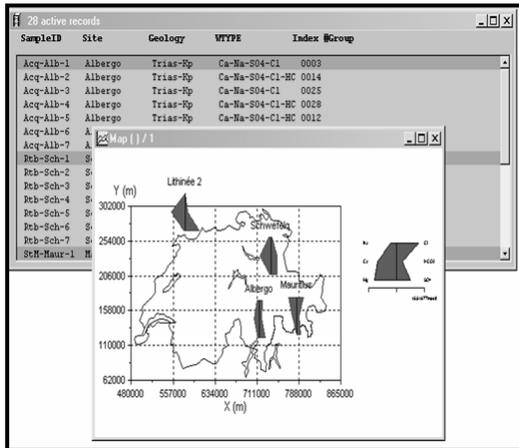
Shows changes in concentration (mg/l) over time.

Current version can only create a plot for one parameter at a time.

Spatial Trend Analysis

Map Plot

Map Plot “Snapshot” in Time



Displays the sampling position in Cartesian coordinates.

Can import and overlay an AutoCAD. Dxf file as a base map.

Can display locations of sample locations.

Can interpret spatial trends in chemical or physical characteristics using proportional symbols or by plotting Pie, Stiff or Piper diagrams.

“Fingerprinting” Water Samples Multiple Parameters

Pie Chart

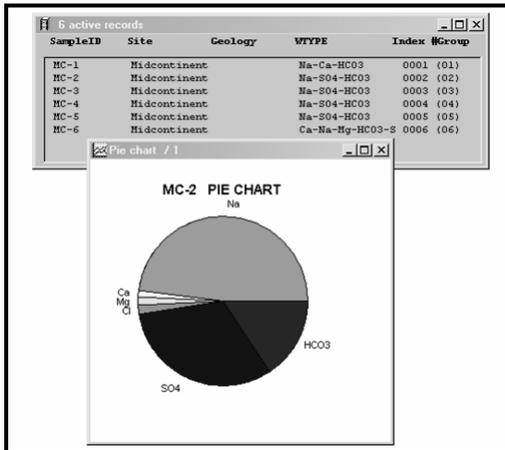
Stiff Diagram

Schoeller Diagram

Ternary Diagram

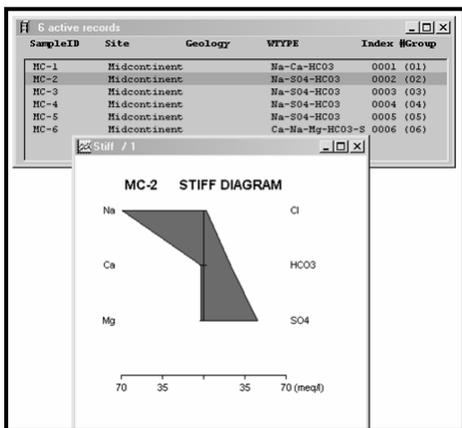
Piper Diagram

Pie Chart “At-a-glance” Relative Concentrations of Each Parameter



Area of the circle represents the total ionic concentration (meq/l).
Subdivisions of the area represent proportions of the different ions.

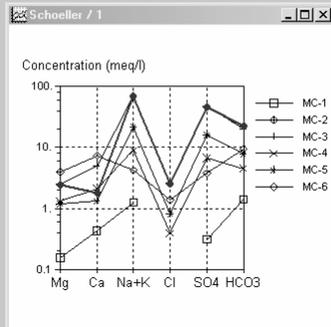
Stiff Diagram Characterizes Water Chemistry



Analyses in meq/l are plotted on four parallel horizontal lines.
Concentrations of up to four cations and anions can be plotted, one each to the left or right of the center zero axis.
Resulting points are connected to give an irregular polygon pattern.
Stiff patterns can be a relatively distinctive method of showing water-composition similarities and differences.

Schoeller Diagram Line Plot That Characterizes Water

MC-1	Midcontinent	Na-Ca-HCO3	0001 (01)
MC-2	Midcontinent	Na-SO4-HCO3	0002 (02)
MC-3	Midcontinent	Na-SO4-HCO3	0003 (03)
MC-4	Midcontinent	Na-SO4-HCO3	0004 (04)
MC-5	Midcontinent	Na-SO4-HCO3	0005 (05)
MC-6	Midcontinent	Ca-Na-Mg-HCO3-S	0006 (06)



Semi-logarithmic diagram that represents major ion analyses in meq/l.

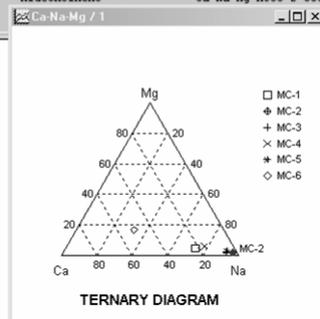
Demonstrates different hydrogeochemical water types on the same diagram.

Number of analyses plotted at one time is limited.

Actual parameter concentrations are displayed.

Ternary Diagram Shows Groupings of Cations or Anions

SampleID	Site	Geology	WTYPE	Index #Group
MC-1	Midcontinent		Na-Ca-HCO3	0001 (01)
MC-2	Midcontinent		Na-SO4-HCO3	0002 (02)
MC-3	Midcontinent		Na-SO4-HCO3	0003 (03)
MC-4	Midcontinent		Na-SO4-HCO3	0004 (04)
MC-5	Midcontinent		Na-SO4-HCO3	0005 (05)
MC-6	Midcontinent		Ca-Na-Mg-HCO3-S	0006 (06)

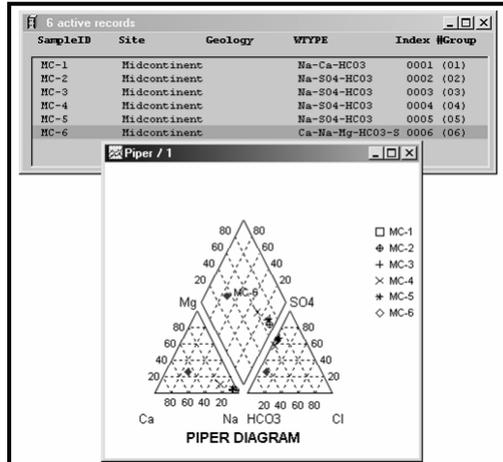


Used to determine the relationship between the concentration of three different parameters in multiple sample records.

Displays relative concentrations of each parameter with respect to the sum of the concentrations of each parameter.

Each vertex represents a concentration of 100%.

Piper Diagram Shows Groupings of Water Types



Major ions are plotted as cation and anion percentages in meq/l in two base triangles.

Total ions are set to equal 100%.

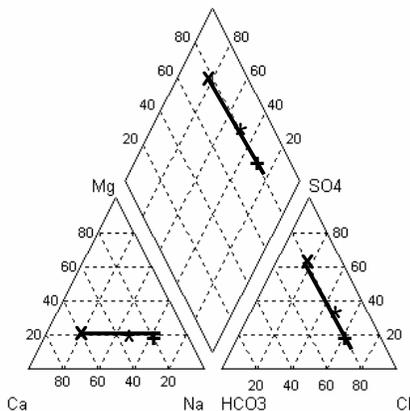
Data points in the two triangles are projected to central diamond.

Allows comparison of a large number of samples.

Shows clustering of samples and water type.

Piper Diagram Binary Mixing

X Mined
* Mined and Background
+ Background



A water sample that is a mixture of two end members (mined and background) will lie in a straight line between both end members on all three parts of the Piper diagram.

Concept has drawbacks. Post-mixing reactions (i.e., dissolution, ion exchange, precipitation) may obscure the mixing trend.

Use with caution.

Database Reports

- Data Report
- Detailed Record Report
- Tabulation Relative to Water-quality Standards

Data Report

```

Database: C:\AquaChem\bitsui.HC3
SampleID           BITSUI-1
Date              1/20/1998
Ph                8.9
Cond 20°C (µS)   24900
TDS (110 °C, mg/l) 15200

Cations            (mg/l)      (meq/l)
Na+               3.750E+03    1.631E+02
K +              1.630E+01    4.169E-01
Mg++             3.250E+01    2.674E+00
Ca++             6.560E+01    3.273E+00
Mn++             2.490E-01    9.064E-03
Fe++             2.000E-01    7.163E-03
Ba++             3.000E-02    4.369E-04

Anions            (mg/l)      (meq/l)
F-               2.490E+00    1.311E-01
Cl-              1.830E+03    5.162E+01
SO4--            6.450E+03    1.343E+02
HCO3-            7.650E+02    1.254E+01
CO3--            1.700E+02    5.666E+00

Uncharged         (mg/l)
Al tot           .27
As tot           .029
H3BO3            9.52
    
```

Detailed Data Report

SampleID	: BITSUI-1			
Location	:			
Site	:			
Sampling Date	: 1/20/1998			
Geology	:			
Watertype	: Na-S04-Cl			
Sum of Anions (meq/l)	: 204.2506			
Sum of Cations (meq/l)	: 169.4952			
Balance:	: -9.30%			
Measured TDS (mg/l)	: 15200.0			
Calculated TDS (mg/l)	: 8306.7			
Hardness	: meq/l	*f	*g	mg/l CaCO3
Total hardness	: 5.95	29.74	16.65	297.4
Permanent hardness	: 0.0	0.00	0.00	0.0
Temporary hardness	: 5.95	29.74	16.65	297.4
Alkalinity	: 18.21	91.03	50.97	910.3
(1 *f = 10 mg/l CaCO3/l l *g = 10 mg/l CaO)				
Major ion composition				
	mg/l	mmol/l	meq/l	meq%
-----	-----	-----	-----	-----
Na+	3750.0	163.114	163.114	43.643
K +	16.3	0.417	0.417	0.112
Ca++	65.6	1.637	3.273	0.876
Mg++	32.5	1.337	2.674	0.715
Cl-	1830.0	51.618	51.618	13.811
S04--	6450.0	67.148	134.297	35.933
HCO3-	765.0	12.539	12.539	3.355

Tabulation Relative to Water Quality Standards

SampleID	: BITSUI-1		
Location	:		
Site	:		
Sampling Date	: 1/20/1998		
Drinking Water Quality Regulations:			
Element	Measured	Recommended	Maximum
-----	-----	-----	-----
pH	8.9	6.5- 8.5	< 9.5
Cond	24900	< 400	< 1250
TDS	15200		< 1500
Na	3750	< 20	< 200
K	16.3	< 10	< 12
Mg	32.5	< 30	
Mn	0.249	< .02	< .05
Fe	0.2	< .05	< .2
F	2.49		< 1.5
Cl	1830	< 25	
S04	6450	< 25	< 250
Al	0.27	< .05	< .2
Irrigation water:			
Conductivity =	24900 uS	(group C4: Very high salinity water)	
Sodium Adsorption Ratio (SAR)	: 94.59		
Exchangeable sodium ratio (ESR)	: 27.43		
Magnesium hazard (MH)	: 44.96		

Table

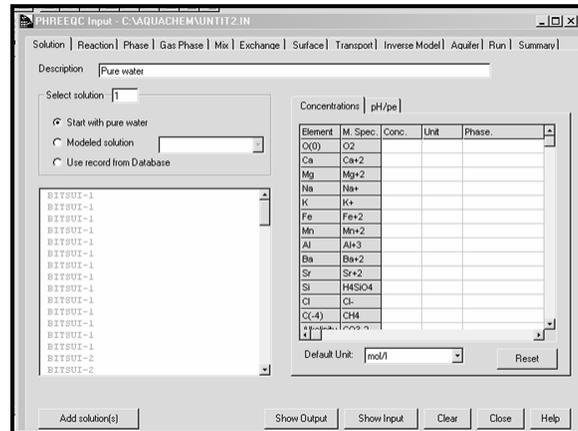
DBIN	SampleID	Date	pH	Cond	TDS	Na	K	Mg	Ca	Mn	Fe	Ba	F	Cl	SO4	NO3	NO2
7	BITSUI-1	6/21/1996	8.5	868		120	2.35	11.7	56.5	.02	.03	.05	.58	58.8	261		
1	BITSUI-1	3/1/1995	8.7	17800	14200	4980	27	28	46	.11	< .05	< .05	2.6	1880	6780		
2	BITSUI-1	4/27/1995	8.8	16100	14200	4970	54	34	56	.094	< .05	< .5	2.64	2050	6680		
3	BITSUI-1	5/19/1995	8.8	25900	14200	4830	23	29	45	.1	< .05	< .5	2.71	2070	7100		
4	BITSUI-1	10/18/1995	8.9	17800	14200	4860	20	27	56	.08	< .05	< .5	2.51	1950	6850		
5	BITSUI-1	1/2/1996	8.8	17800	14700	5040	20	32	63	.1	< .05	.03	4.39	1980	6990		
6	BITSUI-1	4/9/1996	8.9	16600	13200	3980	21.1	119	270	.28	.45	< .5	2.18	1800	6570		
8	BITSUI-1	9/27/1996	8.9	19300	15300	5180	18.4	31.5	51.1	.12	.25	.03	2.62	2310	7460		
10	BITSUI-1	3/12/1997	8.9	19200	15400	5077	22.3	33.6	51.6	.14	.4	.04	2.81	2023	7588		
12	BITSUI-1	10/1/1997	8.8	18500	15000	5050	3	30.7	64.4	.19	.21	.03	2	1980	7040		
13	BITSUI-1	1/20/1998	8.9	24900	15200	3750	16.3	32.5	65.6	249	.2	.03	2.49	1830	6450		
14	BITSUI-1	3/26/1998	8.8	19600	14600	4360	21	28	52	.391	.35	.04	2.74	1750	6200		
15	BITSUI-1	9/16/1999	8.8	17500		4460	21	29.5	86.2	.28	.03	.05	2.51	1750	7150		
16	BITSUI-1	6/16/2000	8.8	18300	14900	5700	45	34	98	.25	.2	.045	2.4	1800	7800		
17	BITSUI-2	3/2/1995	8	8080	5050	1940	7	1.5	3.6	< .02	< .05	2.69	.79	1160	7		
18	BITSUI-2	4/27/1995	8	8110	5020	2110	13	2.7	6.6	< .02	< .05	2.7	1.78	1220	48		
19	BITSUI-2	5/19/1995	8	12100	5010	2090	1.6	3	8.6	< .02	< .05	2.89	1.75	1220	28		
20	BITSUI-2	10/18/1995	8	7730	4910	1990	7	1.9	8.6	< .02	< .05	2.42	1.69	1170	17		
21	BITSUI-2	1/2/1996	7.9	7590	5020	2050	5.1	2.6	6.4	< .02	< .05	2.96	2.66	1150	4.5		
22	BITSUI-2	4/9/1996	8.2	7950	5010	1930	5.87	2.07	6.01	< .02	< .05	2.8	1.81	1250	24.7		
24	BITSUI-2	9/27/1996	8	7990	5160	1980	5.47	1.94	4.61	< .01	.03	2.99	1.74	1260	82.3		
25	BITSUI-2	1/10/1997	7.9	8010	5130	2220	7.43	2.07	5.21	< .01	< .03	2.93	1.68	1270	70		
26	BITSUI-2	3/1/1997	8	8000	5080	2002	6.13	2.1	4.87	< .01	< .03	3.12	1.75	1154	37		
27	BITSUI-2	6/18/1997	8	7900	5100	2150	8	2	5.5	< .005	< .02	2.83	1.71	1150	95		

Why Statistics ?

- Job is to determine spatial and temporal changes in concentration
- But have to deal with:
 - Data noise
 - Measurement Errors
 - Anomalous data points
 - Multiple stresses on the system

Other Features of AquaChem

Geochemical Modeling using PHREEQC Interface



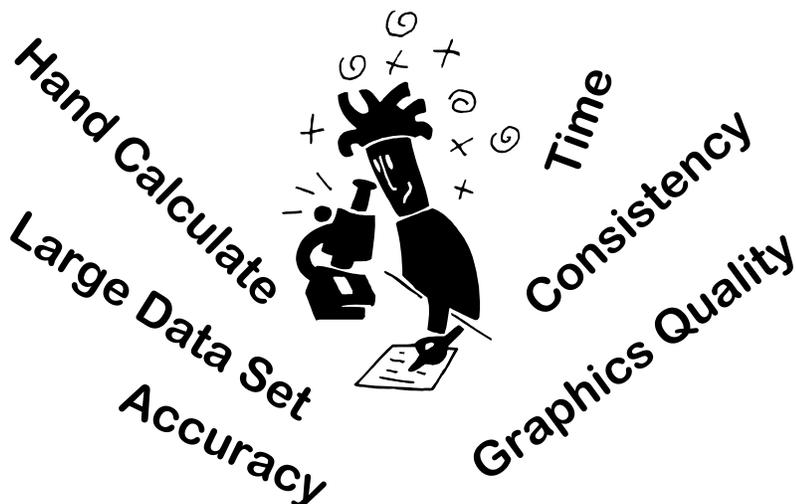
PHREEQC

- Program based on an ion pairing aqueous model and is used to calculate:
 - pH
 - Redox potential
 - Ion exchange
 - Surface reactions
 - Mass transfer (e.g., solution or precipitation of minerals)
- Can also use PHREEQC to perform inverse modeling to estimate the chemical changes that occur as a water sample evolves along a flow path.

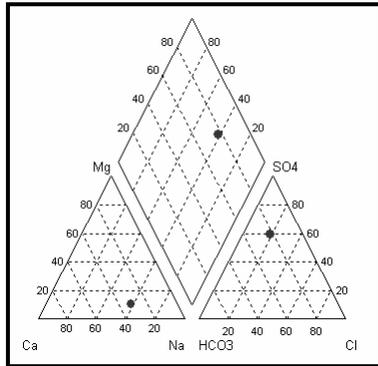
AquaChem PHREEQC Interface

- Comes with the PHREEQC executable file (phreeqc.exe)
- Three thermodynamic database files (phreeqc.dat, wateq4f.dat and minteq.dat)
- **BEFORE** using PHREEQC download and read the detailed users manual
- Users manual and source code may be downloaded from:
<ftp://brrcrftp.cr.usgs.gov> (connect as anonymous)
<http://water.usgs.gov/software/phreeqc.html>
Also see Chpt. 7 in the AquaChem User's Manual

Why Use **AquaChem** ?



Bitsui 1 6/21/96



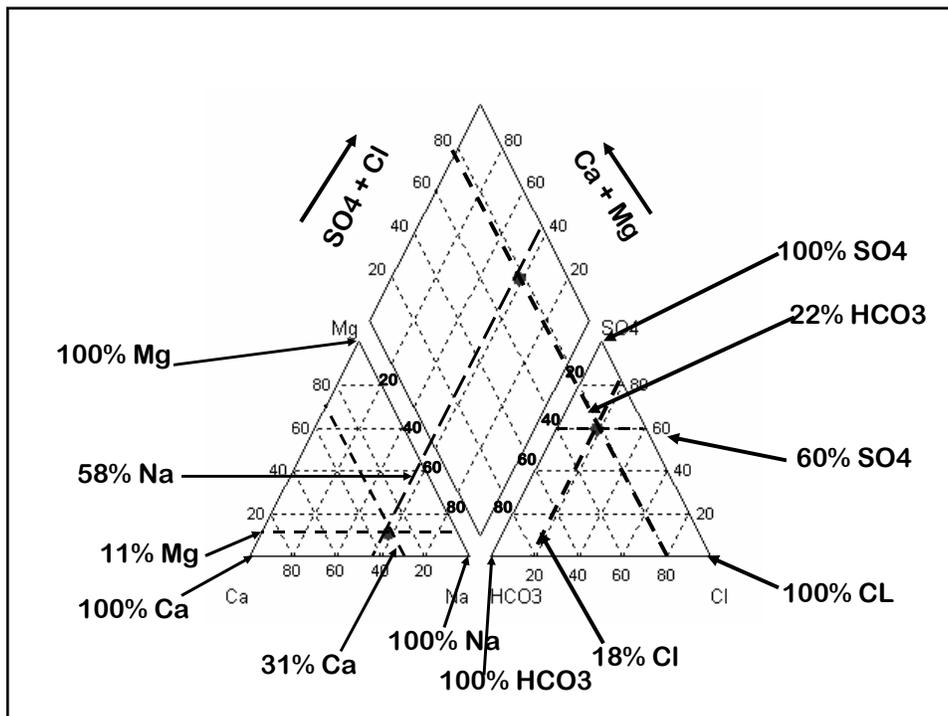
Major ion composition			
	mg/l	mmol/l	meq/l
Na+	120.0	5.22	5.22
K +	2.35	0.06	0.06
Ca++	56.5	1.41	2.819
Mg++	11.7	0.481	0.963
Cl-	58.8	1.659	1.659
SO4--	261.0	2.717	5.434
HCO3-	123.0	2.016	2.016

Cations

	Meq/l	%
Na	5.22	58
Ca	2.82	31
Mg	0.96	11
	9.00	100

Anions

Cl	1.66	18
SO4	5.43	60
HCO3	2.02	22
	9.11	100



Class Exercise

Hand Calculate Piper Diagram



ANSWER KEY – PIPER DIAGRAM

