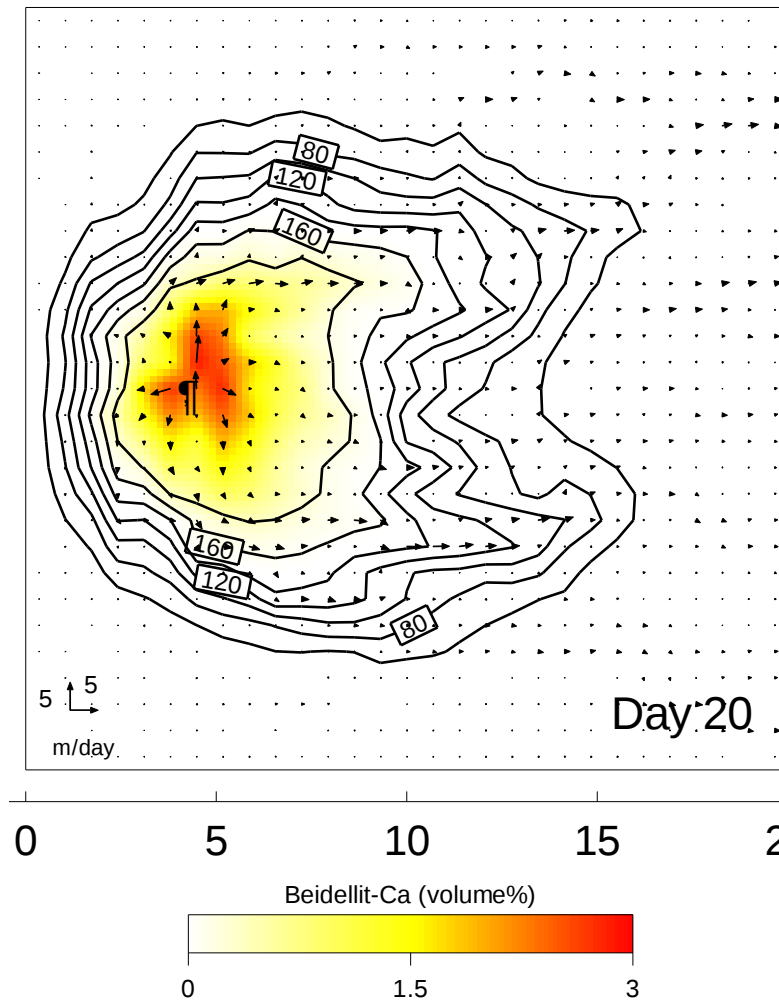




Geochemical modeling

ENV-200 Week 9

Meret Aeppli

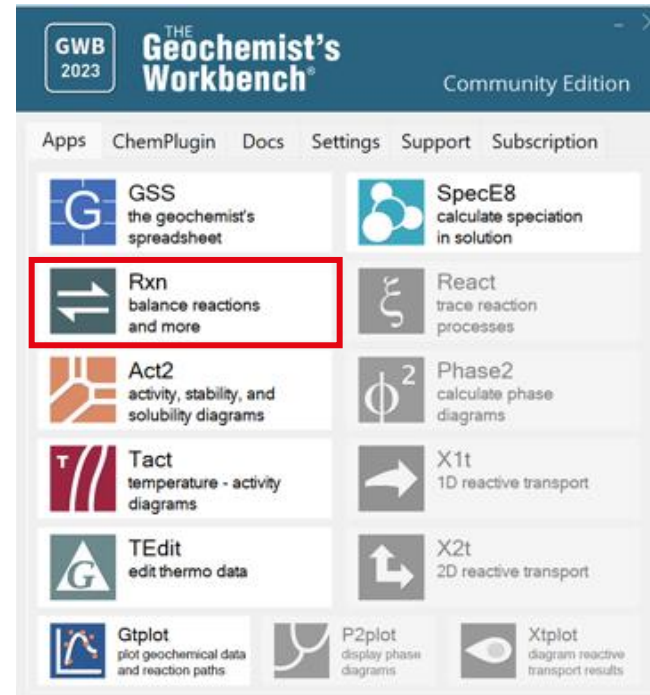
meret.aeppli@epfl.ch

We discussed what geochemical modeling is useful for.

We started exploring the Geochemist's Workbench.

Today, we will continue working with the Geochemist's Workbench.

- Consider the oxidation of $\text{H}_2\text{S}(\text{aq})$ to sulfate (SO_4^{2-}). To balance this reaction, we can use the Rxn App.
- To balance a reaction with Rxn, first set a species, mineral, etc., to appear on the left side of the reaction.
- Then, swap the basis to pull in the various species you want to appear in the reaction.



Rxn: Reaction balancing

Start Rxn and move to the Basis pane. Under “balance reaction for”, select “???” → Aqueous... → H₂S(aq). Set “temperature” to 25 °C

Left side of reaction

The screenshot shows the 'Rxn Community Edition' window with the 'Basis' tab selected. The 'balance reaction for' dropdown is set to 'H2S(aq)'. Below this, the 'in terms of' section lists three species: 'H+', 'SO4--', and 'O2(aq)', each with a stoichiometric coefficient input field and a unit dropdown set to 'activity'. The 'temperature' is set to '25.0' °C, and the 'ionic strength' is set to 'true' with a unit dropdown set to 'molal'. At the bottom, there are 'add' and 'delete' buttons, a 'factor reaction by' input field set to '1.0', and a 'reverse' button. The status bar at the bottom indicates 'Ready'.

Rxn Community Edition - C:\Users\maepli			
File Edit Run Config View Help			
Basis	Command	Results	
balance reaction for			
H2S(aq)			activity
in terms of			
H+			activity
SO4--			activity
O2(aq)			activity
temperature	25.0	C	
ionic strength	true	molal	stoich
add delete			
factor reaction by	1.0	reverse	
Ready			

Rxn: Reaction balancing

- Move to the Results pane and click *Run*. What chemical reaction does the program give? What is its log K?

Rxn: Reaction balancing: Solution

The screenshot shows the 'Rxn Community Edition' application window. The title bar indicates the file path is 'C:\Users\maeappli'. The menu bar includes 'File', 'Edit', 'Run', 'Config', 'View', and 'Help'. The main interface has three tabs: 'Basis', 'Command', and 'Results'. The 'Results' tab is active, displaying the following information:

+ $\text{H}_2\text{S}(\text{aq}) + 2 \text{O}_2(\text{aq}) = 2 \text{H}^+ + \text{SO}_4^{--}$

Log K at 25 C = 131.3943

At the bottom of the window, there is a 'Run' button and a status bar that says 'Ready'.

Rxn: Reaction balancing

Now let's balance the corresponding half-cell reaction. Click on the swap button next to the basis entry for "O₂(aq)" and select Aqueous... → e⁻

The screenshot shows the 'Rxn Community Edition' window with the following settings:

- Balance reaction for:** H₂S(aq) (activity)
- In terms of:**
 - H⁺ (activity)
 - SO₄²⁻ (activity)
 - e⁻ ↔ O₂(aq) (activity) - The swap button between e⁻ and O₂(aq) is highlighted with a dashed box.
 - temperature: 25.0 °C
 - ionic strength: true (molal)
- Buttons:** add, delete, factor reaction by (1.0), reverse

The status bar at the bottom indicates 'Ready'.

Rxn: Reaction balancing

- Move to the Results pane and click *Run*. How has the reaction changed?

Rxn: Reaction balancing: Solution

The screenshot shows the 'Rxn Community Edition' window. The title bar indicates the file path is 'C:\Users\maeppli'. The menu bar includes 'File', 'Edit', 'Run', 'Config', 'View', and 'Help'. Below the menu is a tabbed interface with three tabs: 'Basis', 'Command', and 'Results'. The 'Results' tab is active, displaying the following chemical reaction and its equilibrium constant:

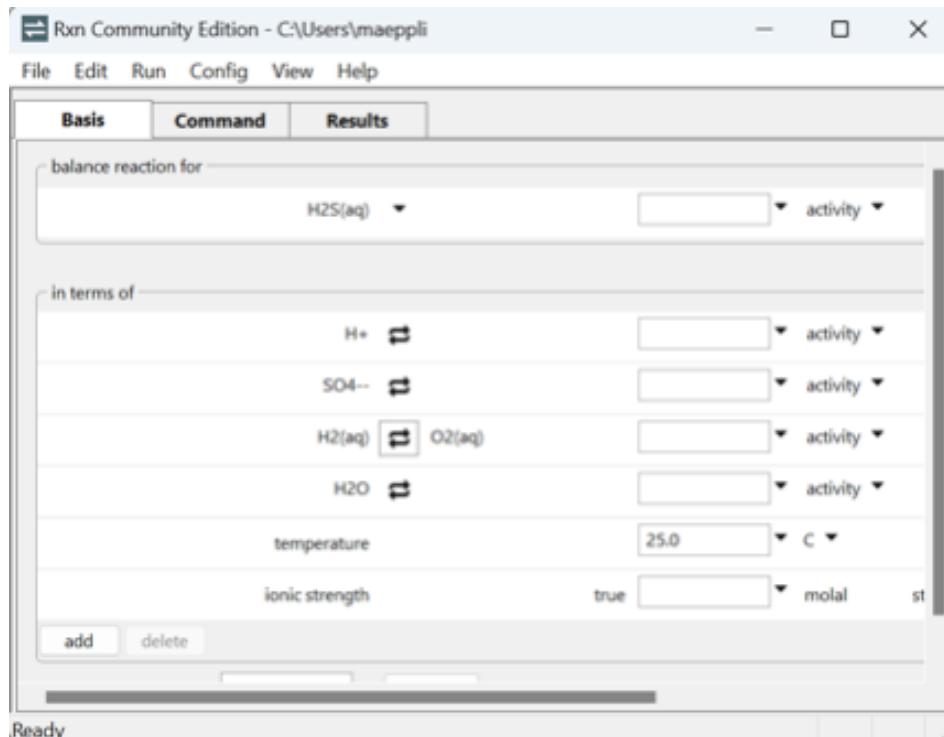
$$\text{H}_2\text{S}(\text{aq}) + 4 \text{H}_2\text{O} = 10 \text{H}^+ + \text{SO}_4^{--} + 8 \text{e}^-$$

Log K at 25 C = -40.6093

At the bottom of the window, there is a 'Run' button and a status bar that says 'Ready'.

Rxn: Reaction balancing

To recast the reaction to liberate dihydrogen, once again click on the swap button next to the basis entry for “O2(aq)” and select Aqueous... → “H2(aq)”



Rxn: Reaction balancing

- Move to the Results pane and click *Run*. How has the reaction changed?

Rxn: Reaction balancing: Solution

The screenshot shows the 'Rxn Community Edition' window. The title bar indicates the file path is 'C:\Users\maepli'. The menu bar includes 'File', 'Edit', 'Run', 'Config', 'View', and 'Help'. The main window is divided into three tabs: 'Basis', 'Command', and 'Results'. The 'Results' tab is active, displaying the following chemical reaction and its equilibrium constant:

$$\text{H}_2\text{S}(\text{aq}) + 4 \text{H}_2\text{O} = 2 \text{H}^+ + \text{SO}_4^{--} + 4 \text{H}_2(\text{aq})$$

Log K at 25 C = -53.0573

A 'Run' button is located at the bottom left of the main window. The status bar at the bottom left shows 'Ready'.

Exercise 1: Iron oxidation



Dissolved ionic iron exists in anoxic (i.e., in the absence of oxygen) ground water as the reduced species Fe^{2+} . When such waters are used from drinking water supplies and the water becomes exposed to the atmosphere, the Fe^{2+} is oxidized by O_2 to Fe^{III} (ferric iron), which is insoluble at neutral pH and precipitates as $\text{Fe}(\text{OH})_3(\text{s})$.

Write the balanced equation for the oxidation of Fe^{2+} to $\text{Fe}(\text{OH})_3(\text{s})$ by O_2 with the help of Rxn.

What is the log K value for the reaction?

This is Exercise 2
from the Redox I
class

Exercise 1: Solution



Basis	Command	Results
balance reaction for		
	Fe++ ▾	▾ activity ▾
in terms of		
	O2(aq) ⇌	▾ activity ▾
	Fe(OH)3(ppd) ⇌ Fe++	1.0 ▾ activity ▾
	H+ ⇌	▾ activity ▾
	H2O ⇌	▾ activity ▾
	temperature	25.0 ▾ C ▾

File Edit Run Config View Help

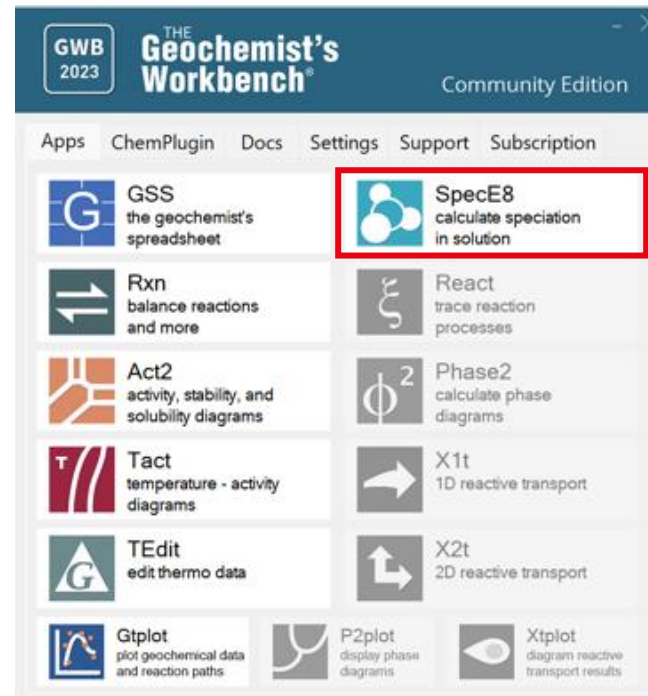
Basis	Command	Results
-------	---------	---------

+

Fe++ + .25 O2 (aq) + 2.5 H2O = Fe (OH) 3 (ppd) + 2 H+

Log K at 25 C = 3.5988

SpecE8 calculates the equilibrium distribution of aqueous species in a fluid, the fluid's saturation state with respect to minerals, the sorption of aqueous species onto various types of surfaces, and the fugacity and partial pressure of gases dissolved in the fluid.



SpecE8: Speciation calculations

The input file “Freshwater.sp8” equilibrates a hypothetical water sample at 25°C. Double-click the file to launch SpecE8, then move to the Basis pane to see the compositional constraints on the hypothetical water.

The screenshot shows the SpecE8 software interface. The 'Basis' pane is active, displaying a list of constraints on the initial system. The constraints are as follows:

Species	Value	Unit	Notes
H2O	1.0	free kg	solvent
Na+	5.0	mg/kg	
K+	1.0	mg/kg	
Ca++	15.0	mg/kg	
Mg++	3.0	mg/kg	
Al+++	1.0	ug/kg	
SiO2(aq)	3.0	mg/kg	
Cl-	15.0	mg/kg	
SO4--	35.0	mg/kg	
HCO3-	50.0	mg/kg	
H+	5.0	pH	
temperature	25.0	C	

At the bottom of the pane, there is a '+ advanced' button and 'add' and 'delete' buttons.

Exercise 1: Hypothetical freshwater



Press the Run button on the Results pane to calculate the equilibrium species distribution in the water.

- SpecE8 produces a dataset as output => “SpecE8_output.txt”.
- Examine the output file. Do you expect any minerals to precipitate in this water? If so, which ones?

Exercise 1: Solution



Click on View Results on the Results pane to see calculation results in tabular form.

```

Temperature = 25.0 C      Pressure = 1.013 bar
pH = 5.000
Ionic strength      = 0.001990 molal
Charge imbalance    = 0.000062 eq/kg (2.634% error)
Activity of water   = 0.999985
Solvent mass        = 1.0000 kg
Solution mass        = 1.0001 kg
Mineral mass         = 0.0000 kg
Fluid density        = 0.996 g/cm3
  compressibility    = 4.446e-05 /bar
  expansivity        = 0.0002428 /C
  viscosity          = 0.009 poise
Chlorinity          = 0.000423 molal
Dissolved solids     = 114 mg/kg sol'n
Elect. conductivity = 149.73 uS/cm (or umho/cm)
Hardness             = 49.81 mg/kg sol'n as CaCO3
  carbonate          = 1.77 mg/kg sol'n as CaCO3
  non-carbonate       = 48.04 mg/kg sol'n as CaCO3
Carbonate alkalinity = 1.77 mg/kg sol'n as CaCO3
Water type           = Ca-SO4
Bulk volume          = 1.00e+03 cm3
Fluid volume         = 1.00e+03 cm3
Mineral volume       = 0.00 cm3
Inert volume         = 0.00 cm3
Porosity             = 100. %
Permeability         = 98.7 cm2
  
```

Exercise 1: Solution



Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
CO2(aq)	0.0007839	34.49	1.0000	-3.1058
Cl-	0.0004225	14.98	0.9513	-3.3959
Ca++	0.0003563	14.28	0.8252	-3.5317
SO4--	0.0003419	32.84	0.8208	-3.5519
Na+	0.0002172	4.993	0.9520	-3.6845
Mg++	0.0001187	2.884	0.8294	-4.0068
SiO2(aq)	4.994e-05	3.000	1.0005	-4.3014
HCO3-	3.544e-05	2.162	0.9523	-4.4718
K+	2.553e-05	0.9980	0.9513	-4.6147
CaSO4	1.723e-05	2.346	1.0000	-4.7637
H+	1.047e-05	0.01055	0.9550	-5.0000
MgSO4	4.664e-06	0.5613	1.0000	-5.3312
CaCl+	6.220e-07	0.04698	0.9520	-6.2276
NaSO4-	3.011e-07	0.03585	0.9520	-6.5426
HSO4-	2.901e-07	0.02815	0.9520	-6.5589
CaHCO3+	1.736e-07	0.01755	0.9527	-6.7814
MgCl+	5.874e-08	0.003510	0.9520	-7.2524
KSO4-	5.097e-08	0.006888	0.9520	-7.3141
MgHCO3+	3.572e-08	0.003047	0.9520	-7.4685
Al+++	1.357e-08	0.0003661	0.6599	-8.0479
AlOH++	1.265e-08	0.0005564	0.8230	-7.9825
NaHCO3	9.391e-09	0.0007888	1.0000	-8.0273
Al(OH)2+	7.412e-09	0.0004520	0.9520	-8.1515
AlSO4+	2.699e-09	0.0003320	0.9520	-8.5902
NaCl	2.090e-09	0.0001221	1.0000	-8.6798
OH-	1.083e-09	1.842e-05	0.9516	-8.9868
H3SiO4-	8.151e-10	7.751e-05	0.9520	-9.1102
Al(OH)3	6.100e-10	4.758e-05	1.0000	-9.2147
KCl	2.523e-10	1.880e-05	1.0000	-9.5981
CO3--	1.860e-10	1.116e-05	0.8219	-9.8157
CaCO3	7.389e-11	7.395e-06	1.0000	-10.1314
Al(OH)4-	6.557e-11	6.220e-06	0.9520	-10.2047

Exercise 1: Solution



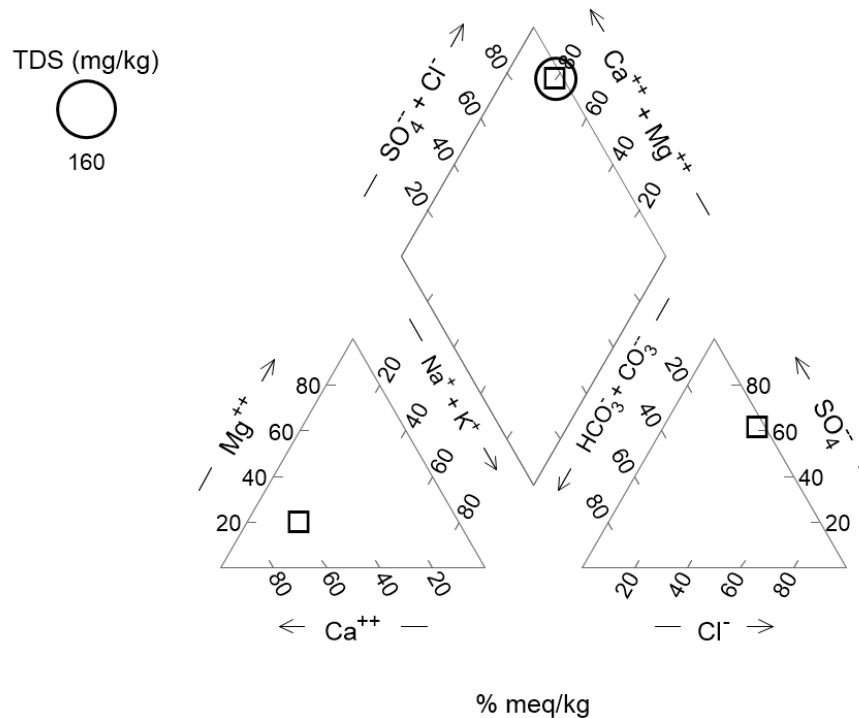
Mineral saturation states	log Q/K		log Q/K
Quartz	-0.3021	Ca(OH) ₂ (c)	-16.1091
Tridymite	-0.4679	Bloedite	-16.2163
Chalcedony	-0.5733	Margarite	-16.4969
Cristobalite	-0.8526	Diopside	-17.1108
Gibbsite	-1.0083	Artinite	-17.4205
Amorph [^] silica	-1.5878	KNaCO ₃ ·6H ₂ O	-18.0936
Diaspore	-1.7997	Clinoptil-Mg	-18.2165
Kaolinite	-2.1279	MgCl ₂ ·4H ₂ O	-18.2561
Gypsum	-2.6403	CaCl ₂ ·2H ₂ O	-18.4197
Boehmite	-2.6441	MgOHCl	-18.4501
Anhydrite	-2.8184	Spinel	-18.4955
Bassanite	-3.4473	CaCl ₂ ·H ₂ O	-18.5545
CaSO ₄ ·1/2H ₂ O(beta)	-3.6159	Clinoptil-Na	-18.5887
Pyrophyllite	-4.3613	Prehnite	-19.3408
Calcite	-4.7164	Ca-Al Pyroxene	-20.3895
Beidellit-Ca	-4.8387	Forsterite	-20.4615
Aragonite	-4.8813	Talc	-20.7888
Beidellit-Mg	-4.8987	Gaylussite	-21.0728
Beidellit-H	-4.9456	Pirssonite	-21.2355
Beidellit-K	-5.5079	Saponite-Ca	-21.2662
Beidellit-Na	-5.5310	Saponite-Mg	-21.3263

Minerals will not precipitation because all saturation states are negative (remember: Q is the ion activity product, when assuming activity = 1 for mineral phases; K is the solubility product. Hence, if log Q/K is negative, IAP < K)

The run also produced a dataset “SpecE8_plot.gtp” that passes more complete information to the graphics program Gtplot.

Click on “Plot Results”.

Create a Piper diagram from the data.



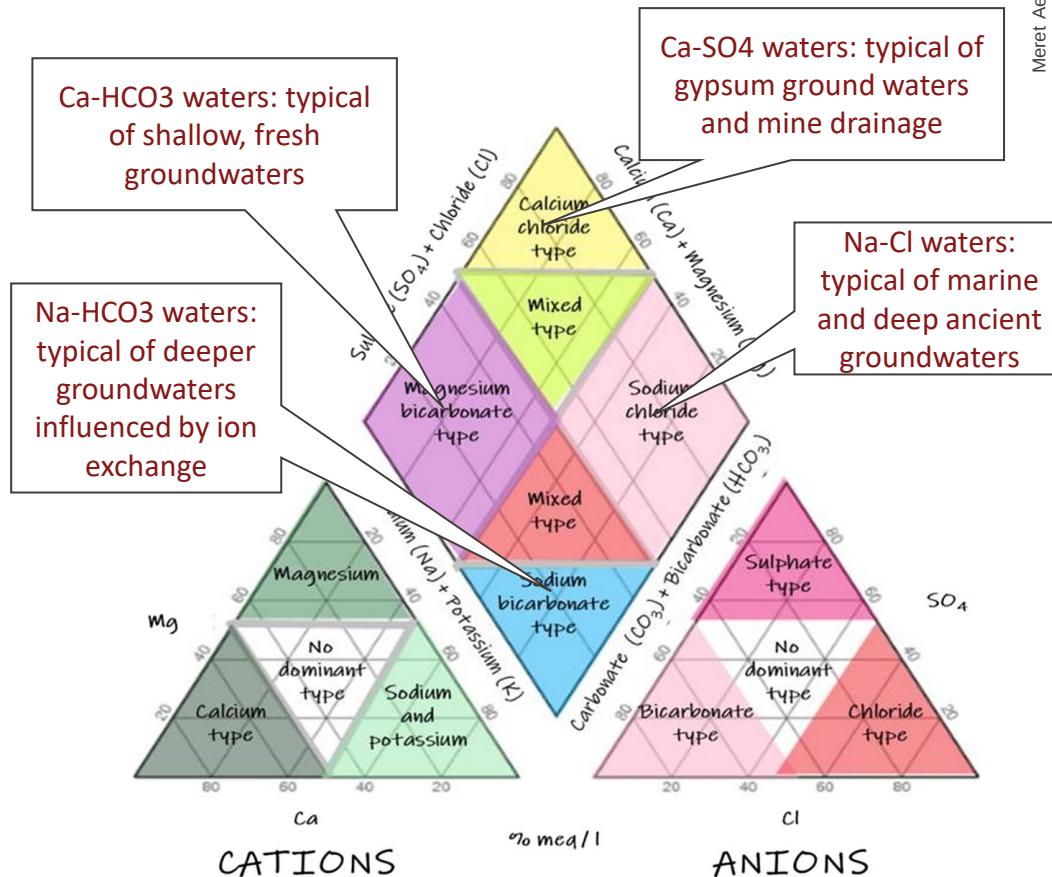
A piper diagram segregates concentrations of the most abundant cations and anions to understand the sources of dissolved constituents in water.

Advantages

- Many water analyses can be plotted on the same diagram
- Can be used to classify waters
- Can be used to identify mixing of waters

Disadvantages

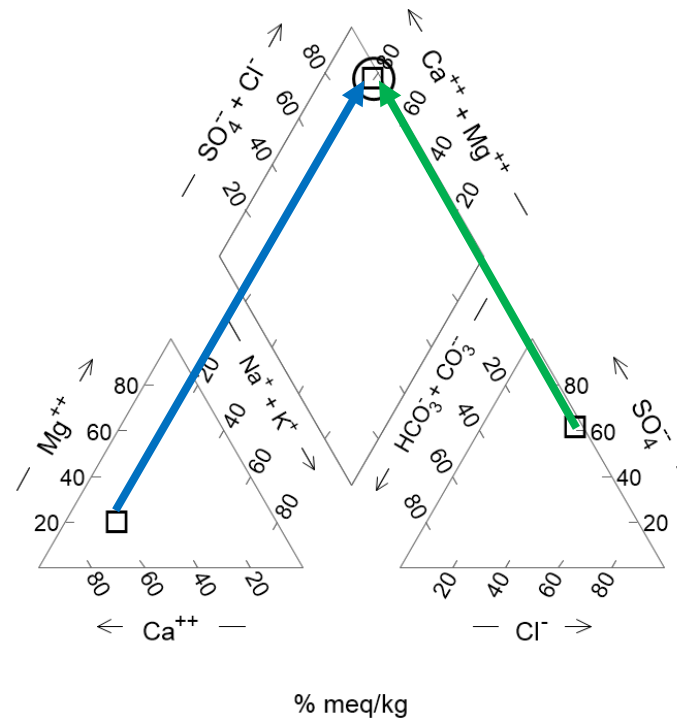
- Concentrations are renormalized
- Cannot easily accommodate waters in which other cations or anions are significant



$$\text{Ca}^{2+} + \text{Mg}^{2+} = 60 \text{ meq/kg} + 20 \text{ meq/kg} \\ = 80 \text{ meq/kg}$$

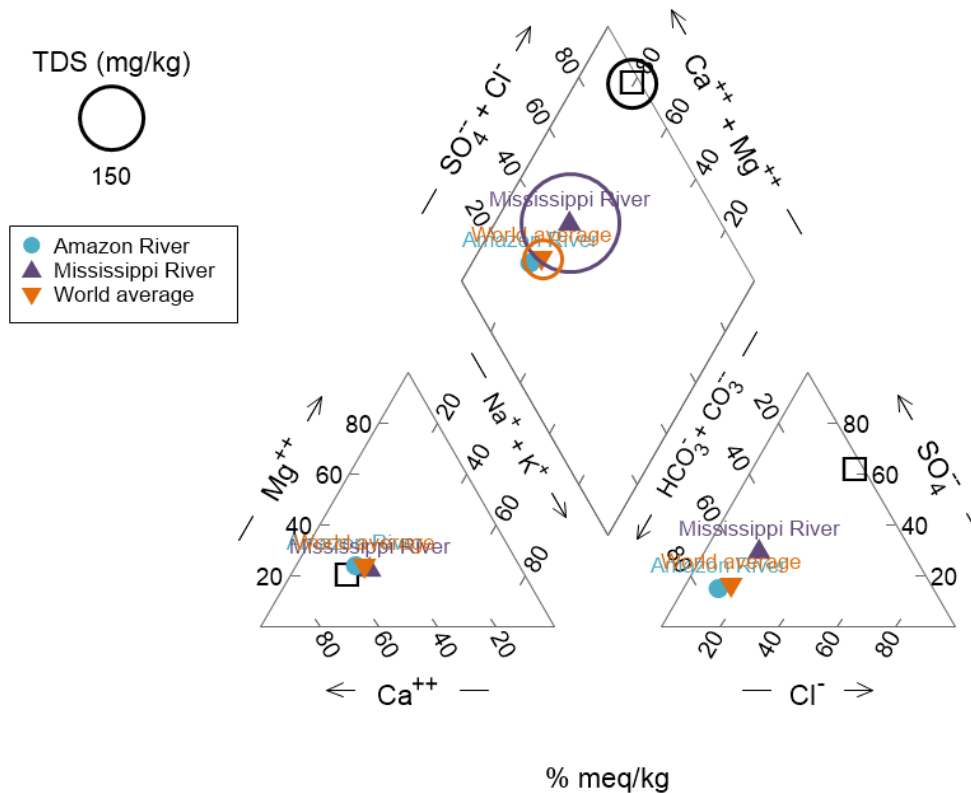
$$\text{SO}_4^{2-} + \text{Cl}^- = 60 \text{ meq/kg} + 40 \text{ meq/kg} = \\ 100 \text{ meq/kg}$$

TDS (mg/kg)



We can add the river data for Mississippi and Amazon from last week: Simply drag and drop the file RiverWaters.gss into Gtplog

What is the main chemical difference between our hypothetical freshwater and the river waters?



TDS = total dissolved solids

Typical tap water concentrations: 150-400

Exercise 2: Iron precipitation



Let's re-examine exercise 1 from Homework 4: A wastewater contains 10^{-4} M phosphate. Fe(III) is added to the system to precipitate phosphate. Is $\text{FePO}_4(\text{s})$ or $\text{Fe}(\text{OH})_3(\text{s})$ precipitated at $\text{pH}=7$?

Use SpecE8 to answer this question. The following information is useful:

- Assume an oxic system ($\text{O}_2(\text{aq})$ at saturation: 9 mg/L)
- Assume an Fe(III) concentration of 10^{-4} M.
- Assume typical wastewater concentrations of
 - $\text{Ca}^{2+} = 6.6$ meq/L
 - $\text{Cl}^- = 3.5$ meq/L
 - $\text{SO}_4^{2-} = 2.6$ meq/L
- Strengite is a FePO_4 mineral.



Basis	Medium	Command	Results
constraints on initial system			
	H2O	1.0 ▼ free kg ▼	solvent
	HPO4-- 	-4.0 ▼ log mol/l ▼	
	Fe+++  Fe++	-4.0 ▼ log mol/l ▼	
	Ca++ 	6.6 ▼ meq/l ▼	
	Cl- 	3.5 ▼ meq/l ▼	
	SO4-- 	2.6 ▼ meq/l ▼	
	H+ 	7.0 ▼ pH ▼	
	O2(aq) 	9.0 ▼ mg/l ▼	
	temperature	25.0 ▼ C ▼	
+ advanced			
add delete			



Mineral saturation states	log Q/K
Hematite	15.8024s/sat
Hydroxyapatite	12.1110s/sat
Goethite	7.4229s/sat
Whitlockite	6.5244s/sat
Magnetite	5.8737s/sat
Ferrite-Ca	5.5997s/sat
Strengite	3.3962s/sat
Fe(OH) ₃ (ppd)	3.0338s/sat

Strengite has a higher saturation state and is therefore expected to form preferentially compared to Fe(OH)₃

SpecE8: Redox disequilibrium

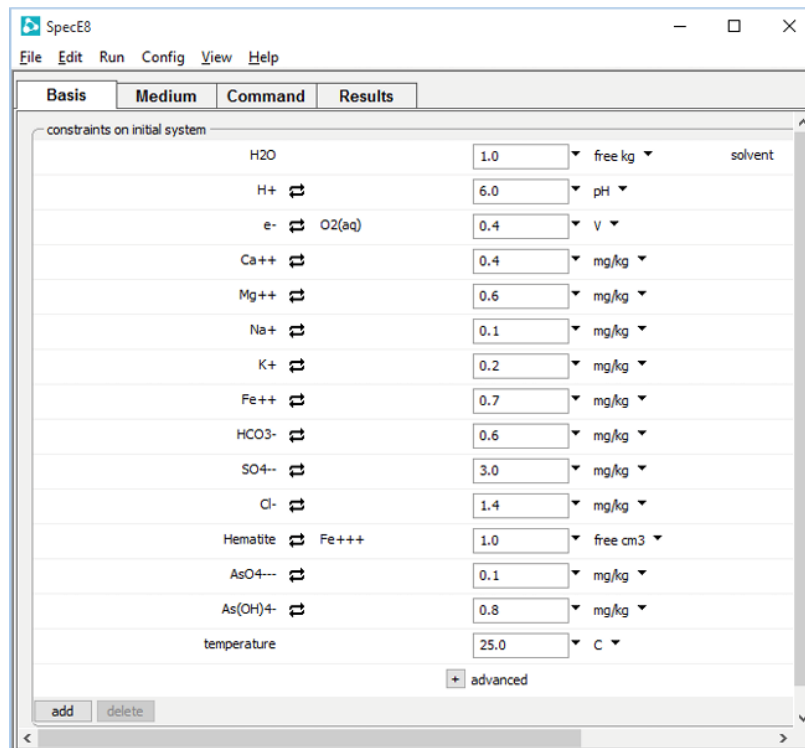
Redox reactions in natural waters, especially at low temperatures, cannot always be assumed to be at thermodynamic equilibrium.

For example, the photo shows part of a river in the Rocky Mountains where waters containing reduced iron come into contact with oxygen-containing waters. As a result, iron is oxidized and iron minerals are precipitating as evidenced from the orange color.

In our modeling efforts, we therefore want to calculate a scenario in which redox reactions are in a state of disequilibrium. Let's see how this works in SpecE8!

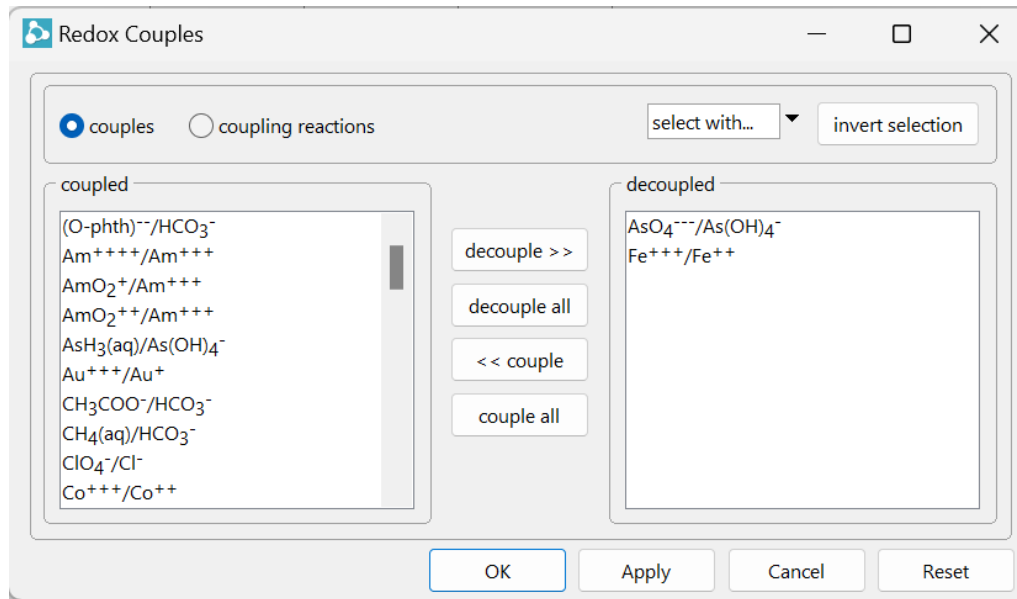


Double-click the “Redox.sp8” input file to launch SpecE8, then move to the basis pane. The input configures a model of a fluid of a certain pH, Eh, and major ion composition.



SpecE8: Redox disequilibrium

Open the Config → Redox couples... dialog and note the decoupled redox pairs. Disabling the redox couples between ferric and ferrous iron and between trivalent and pentavalent arsenic [i.e., basis species AsO_4^{3-} and $\text{As}(\text{OH})_4^-$] causes the program to consider that oxidized and reduced iron and arsenic species exist in quantities not related to the value entered for Eh. Other redox couples, such as between HS^- and SO_4^{2-} , remain enabled and will reflect the specified Eh.



By nature, you need more information to constrain a model of a fluid in redox disequilibrium than you do for an equilibrium model.

As you can see on the Basis pane, separate constraints are required for the oxidized and reduced forms of iron and arsenic (i.e., we give the model different concentrations for each redox species).

SpecE8

File Edit Run Config View Help

Basis Medium Command Results

constraints on initial system

H2O	1.0	free kg	solvent
H+	6.0	pH	
e- ↔ O2(aq)	0.4	V	
Ca++ ↔	0.4	mg/kg	
Mg++ ↔	0.6	mg/kg	
Na+ ↔	0.1	mg/kg	
K+ ↔	0.2	mg/kg	
Fe++ ↔	0.7	mg/kg	
HCO3- ↔	0.6	mg/kg	
SO4-- ↔	3.0	mg/kg	
Cl- ↔	1.4	mg/kg	
Hematite ↔ Fe+++	1.0	free cm3	
AsO4--- ↔	0.1	mg/kg	
As(OH)4- ↔	0.8	mg/kg	
temperature	25.0	C	

+ advanced

add delete

Whenever there are two or more independent redox couples in a run, SpecE8 reports in “SpecE8_output.txt” the theoretical oxidation state of each couple. In this example, the couples and corresponding Nernst Eh and pe values are:

	Eh (volts)	pe
$e^- + \frac{1}{4} O_2(aq) + H^+ \rightleftharpoons \frac{1}{2} H_2O$	0.400	6.762
$2 e^- + 4 H^+ + AsO_4^{---} \rightleftharpoons As(OH)_4^-$	0.081	1.362
$e^- + Fe^{+++} \rightleftharpoons Fe^{++}$	-0.002	-0.035

The first line reflects the Eh specified as an input constraint. The second and third lines show the oxidation states calculated from the activities of arsenic and iron species. The differences in oxidation state reflect the extent of redox disequilibrium in the solution.

Exercise 3: Redox disequilibrium



We just discussed the example on redox disequilibrium. In what speciation would As occur if it equilibrated with the solution at the specified potential of $E_h = 0.4 \text{ V}$?

Use the input file Redox.sp8 and remove the As redox couple from the list of decoupled redox couples. Then, examine the output file. What is the redox state of As and why?

Exercise 3: Solution



As occurs predominantly as H_2AsO_4^- and HAsO_4^{2-} :

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Cl-	3.948e-05	1.400	0.9843	-4.4104
SO4--	3.100e-05	2.978	0.9390	-4.5359
Mg++	2.457e-05	0.5972	0.9401	-4.6364
Fe++	1.248e-05	0.6968	0.9395	-4.9309
Ca++	9.921e-06	0.3976	0.9395	-5.0305
CO2(aq)	6.840e-06	0.3010	1.0000	-5.1649
K+	5.114e-06	0.2000	0.9843	-5.2981
H2AsO4-	4.730e-06	0.6666	0.9844	-5.3320
Na+	4.349e-06	0.09999	0.9844	-5.3684
HCO3-	2.991e-06	0.1825	0.9844	-5.5309
H+	1.015e-06	0.001024	0.9847	-6.0000
HAsO4--	8.655e-07	0.1211	0.9390	-6.0901
MgSO4	1.135e-07	0.01367	1.0000	-6.9448

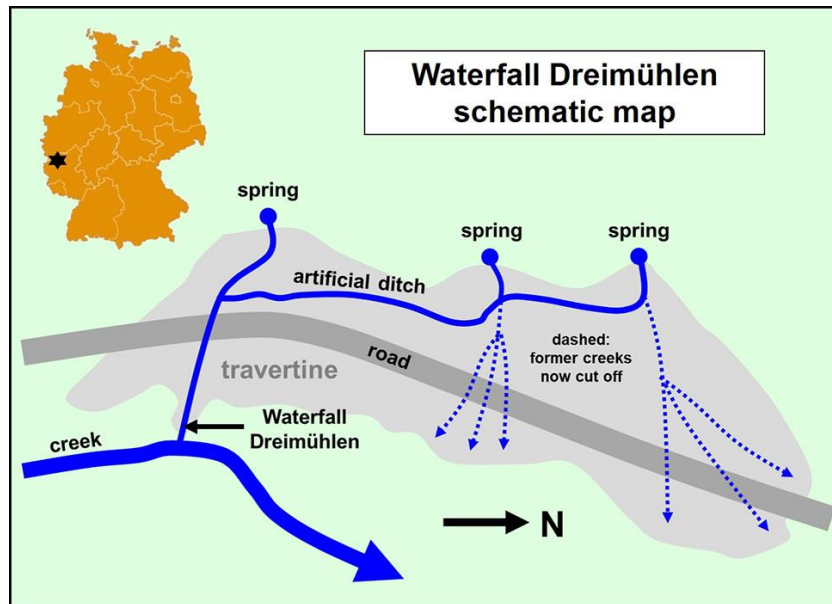
The redox state of As is therefore +V (in As(OH)_4^- ; As has redox state +III). This makes sense because the system Eh is higher than the Eh of the As redox couple in the previous example. When equilibrating the solution to higher Eh, As(III) oxidizes to As(V)

	Eh (volts)	pe
$\text{e}^- + \frac{1}{4} \text{O}_2(\text{aq}) + \text{H}^+ \rightleftharpoons \frac{1}{2} \text{H}_2\text{O}$	0.400	6.762
$2 \text{e}^- + 4 \text{H}^+ + \text{AsO}_4^{3-} \rightleftharpoons \text{As(OH)}_4^-$	0.081	1.362
$\text{e}^- + \text{Fe}^{3+} \rightleftharpoons \text{Fe}^{2+}$	-0.002	-0.035

Environmental engineering challenge

Waterfall Dreimühlen (D): How fast does the waterfall “grow”, i.e., how much calcite is precipitating each year?

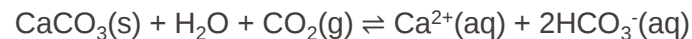




Geology is dominated by limestone

Travertine is a dense, banded rock composed of calcite (CaCO_3)

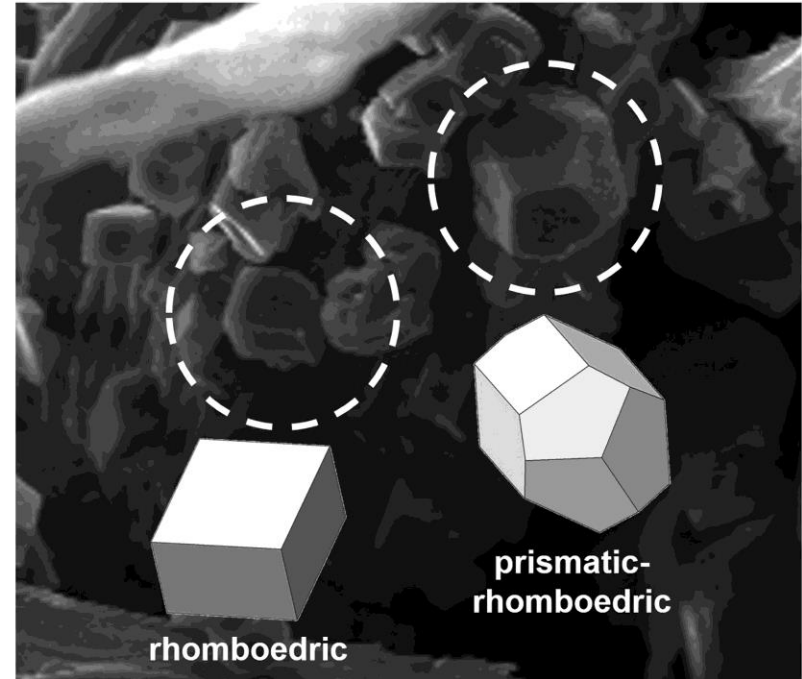
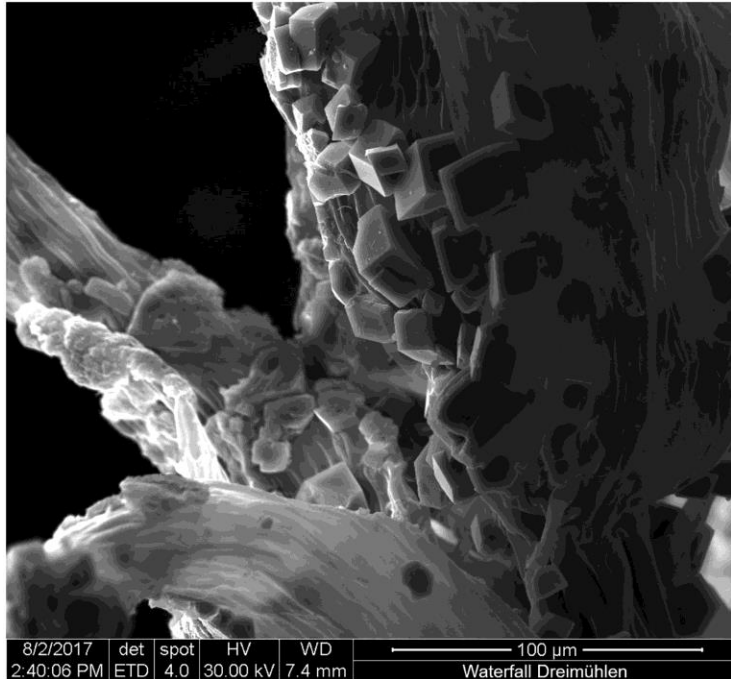
Relevant chemical reaction:



In the underground, high partial pressure of CO_2 ($\gg 400$ ppm) shifts the equilibrium position to the right

When water emerges from the underground, it is oversaturated with dissolved lime (lower partial pressure of CO_2), causing calcite to precipitate

Calcite precipitates as observed under a scanning electron microscope:



How many kg of calcite are precipitating each year?

On your field trip, you measured a flowrate of 60 L/s and the parameters in the table below. Use SpecE8 to calculate the amount of calcite precipitating.

Table 1. Some Averaged Results (Micro-Titrations Only) of All Ten Excursions from 2008 until 2017^a

parameter	head	foot	difference
conductivity ($\mu\text{S cm}^{-1}$)	602		
temperature ($^{\circ}\text{C}$)	8.8		
pH (units)	7.61		
$\beta(\text{Ca}^{2+})$ (mg L^{-1})	108.7		
$c(\text{Ca}^{2+})$ (mmol L^{-1})	2.711		?
$\beta(\text{CaCO}_3\text{aq})$ (mg L^{-1}) (= Ca-hardness)	271.4		
$c(\text{M}^{2+})$ (mmol L^{-1}) (M = Ca, Mg)	3.409		
$c(\text{HCO}_3^-)$ (mmol L^{-1})	5.57		



SpecE8 Community Edition - C:\Users\maepli\OneDrive - epfl.ch\GWB

File Edit Run Config View Help

Basis	Medium	Command	Results
constraints on initial system			
H2O		1.0	free kg
H+	↔	7.61	pH
Calcite	↔ Ca++	108.7	free mg/l as Ca
HCO3-	↔	5.57	mmol/kg
temperature		8.8	C
+ advanced			
add delete			

Ready

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	0.002715	-2.566	0.2717	0.1003
(total)			0.2717	0.1003

0.2717 g/L calcite are precipitating

Using a flow rate of 60 L/s, we obtain 16.302 g/s

$16.302 \text{ g/s} * 60 \text{ s/min} * 60 \text{ min/h} * 24 \text{ h/d} * 365 \text{ d/y} = \underline{514'100 \text{ kg/y}}$

Workflow for thermodynamic modeling

1. Develop a conceptual model: List the processes that likely determine the chemical composition of a system.
2. Make partial equilibrium assumptions: Consider the timeframes in which you wish to understand a system (minutes? years? millions of years?). Decide which of the relevant reactions will reach equilibrium in this timeframe, and which ones will not proceed to any relevant degree.
3. Make sure you have thermodynamic parameters for these reactions.
4. Solve all equations simultaneously with a numerical model.
5. **Interpret the output with respect to your conceptual model.**
6. **Potentially revise the conceptual model and start over.**

Environmental engineering challenge

Waterfall Dreimühlen: Are 514'100 kg/y calcite precipitation a plausible value?



1. We can use the Rxn app in the Geochemist's Workbench to balance reactions.
2. The SpecE8 app is a versatile tool for speciation calculations. Successful implementation of speciation calculations requires a good understanding of the system of interest.
3. Geochemical models are always simplifications of natural systems. They can still provide meaningful clues to understand the functioning and complexities of natural systems.