

Advanced Geochemistry of Natural Waters
GEOL 478/578
CALCULATIONS USING THE MINEQL⁺ COMPUTER PROGRAM

All calculations to be performed here will be conducted using the computer program MINEQL⁺. This program can perform a number of different types of speciation and solubility calculations.

Problem 1:

Sufficient strong acid is added to completely dissolve 10^{-3} moles of $\text{CaCO}_3(\text{s})$ into a liter of water in equilibrium with atmospheric CO_2 . The final pH is measured to be 4.5.

- a) What is the concentration of all aqueous species?
- b) What is the alkalinity?
- c) How much strong acid was added?
- d) Is the final solution saturated with respect to any solids (calculate saturation indices)?

Do parts a)-d) first assuming activity coefficients are equal to zero, and then repeat using activity coefficient corrections.

Problem 2:

Repeat problem 1 assuming that the solution also contains 0.05 M NaCl in addition to the components described above.

Problem 3:

You have analyzed a natural water and found it to contain 4.1×10^{-5} M Ca, 3.1×10^{-5} M Al and 1.3×10^{-4} M SO_4^{2-} . Assuming charge balance, calculate the theoretical pH this system should have, and compare it to the measured $\text{pH} = 3.69 \pm 0.05$. If the calculated and measured pH's do not agree, how do you explain this?

Problem 4:

- a) Calculate the pH of a 0.1 M solution of NaHCO_3 neglecting ion pairs and activity coefficients.
- b) Calculate the pH of a 0.1 M solution of NaHCO_3 including ion pairs and activity coefficients.

Problem 5:

Calculate the solubility of calcite in a 0.07 M solution of NaCl in equilibrium with atmospheric CO_2 at $\text{pH} = 8.0$. How much excess acid is required to obtain these conditions? Include activity coefficients in your calculations.

Problem 6:

Calculate the solubility of calcite and the equilibrium pH for a 0.07 M NaCl solution in equilibrium with calcite and atmospheric CO₂, no added acid or base.

Problem 7:

Calculate the distribution of species and saturation indices for a water of the following composition at 47.9 °C. Evaluate the validity of the analysis of this water.

pH	8.97	SiO ₂	1.012x10 ⁻³
Na	1.167x10 ⁻³	Cl	2.285x10 ⁻⁴
K	1.279x10 ⁻⁵	SO ₄ ²⁻	1.11x10 ⁻⁴
Li	2.018x10 ⁻⁵	HCO ₃ ⁻	7.058x10 ⁻⁴
Ca	2.2x10 ⁻⁵	F	1.527x10 ⁻⁵
PO ₄ ³⁻	1.053x10 ⁻⁷	Sr	9.132x10 ⁻⁷
Ba	7.282x10 ⁻⁸	Pb	9.65x10 ⁻⁸

All analyses are in moles/L.