**GEOL390 Environmental Applications of Geochemical Modeling: HW#2 Answer Key**

**2)** a) Calculate the total concentration of dissolved silica (as ppm SiO2) in equilibrium with quartz at (a) pH 9.0, (b) pH 10.0, and (c) pH 11.0. Use GWB React and add 0.1 molal KCl to the solution for charge balance.

### # React script, saved Wed Apr 10 2002 by Dabieshan

### data = "e:\program files\gwb\gtdata\thermo.dat" verify

### work\_dir = E:\Users\Ayers\GEO320\GWB

### temperature = 25

### swap Quartz for SiO2(aq)

### 1 kg free H2O

### free gram Quartz = 500

### molality K+ = .1

### molality Cl- = .1

### pH = 9

### slide pH to 11

Solubility SiO2(aq) in ppm: a) 7.0 at pH = 9 b) 17.7 at pH = 10 c) 126.8 at pH = 11



b) Use Act2 to construct a solubility diagram for SiO2(aq) from pH = 4 to 14. How do the results compare to those you obtained in (a)? Explain why the solubility of quartz depends so strongly on pH.

# Act2 script, saved Fri Feb 28 2003 by ayersj

data = "c:\program files\gwb\gtdata\thermo.dat" verify

diagram SiO2(aq) on SiO2(aq) vs pH

x-axis from 4 to 14 increment .5

y-axis from -8 to 2 increment 1

Below pH = 9.9 the solubility of quartz is independent of pH and H4SiO4 is the dominant species. Between pH=9.9 and ~12 H3SiO4- is the dominant species. Quartz solubility depends on pH because it dissolves in water to form a weak acid, silicic acid = H4SiO4. Dissociation of H4SiO4 to form H3SiO4- increases the solubility by LeChatlier’s Principle.

3) Kaolinite is often present in soils and sediments affected by acid mine drainage, in which it is the least soluble of the clay minerals. It is probably often the chief source of the dissolved aluminum in acid mine drainage. Use React to calculate the solubility of kaolinite as a function of pH. Assume Na+ = Cl- = SO42- = 0.01 molal, SiO2(aq) = 17 mg/L from pH 4 to 9. Make plots of fluid composition, minerals, and Al species as a function of pH. At what pH is the solubility of kaolinite expressed as ΣAl at a minimum? pH 6-6.25



# React script, saved Wed Apr 03 2002 by Ayers

data = "c:\program files\gwb\gtdata\thermo.dat" verify

work\_dir = C:\

temperature = 25

swap Kaolinite for Al+++

1 kg free H2O

free gram Kaolinite = 100

total molality SO4-- = .01

pH = 4

total mg/l SiO2(aq) = 17

total molality Cl- = .1

total molality Na+ = .1

slide pH to 9



4) Choose a rare earth phosphate (remember to load the extended thermodynamic database thermo.com.v8.r6+.dat). Construct a solubility diagram using Act2 that illustrates the effect of pH on solubility.

# Act2 script, saved Fri Feb 28 2003 by ayersj

data = "C:\Program Files\Gwb\Gtdata\thermo.com.v8.r6+.dat" verify

diagram La+++ on La+++ vs pH

log activity HPO4-- = -1

x-axis from 0 to 14 increment 1

y-axis from -15 to 0 increment 1

