

ENSC/CSES/CHEM 4734
MINTEQA2 Chemical Speciation Computer Program

Equipment: This year we will be using visual MINTEQ. It is a relatively straight forward windows based chemical speciation program. You can download the program at the following URL: <http://www.lwr.kth.se/english/OurSoftware/Vminteq/index.htm>

Follow the directions for downloading. If you have any questions please see me.

Introduction: When pollutants are released into the environment they are involved in a number of competitive reactions that will affect their overall behavior and hence toxicity. These reactions or processes include sorption, precipitation, and complexation. MINTEQA2 is a geochemical equilibrium speciation model capable of computing equilibria among dissolved, adsorbed, solid, and gas phases in an environmental setting. MINTEQA2 requires a chemical analysis of the sample to be modeled which includes total dissolved concentrations of the components of interest and other measurements of interest such as pH, redox intensity (pe), and the partial pressure of one or more gases. MINTEQA2 then uses its extensive thermodynamic data-base to compute the geochemical speciation of the system. MINTEQA2 is an excellent tool for the environmental scientist interested in understanding the physical and chemical processes controlling the behavior of environmental pollutants. However, accurate analytical data must be provided in order to obtain an accurate description of the system of interest. Additionally, MINTEQA2 is based strictly on thermodynamic data and does not allow for kinetic constraints on geochemical reactions. Therefore, the scientist using MINTEQA2 must have an understanding of the chemical principles behind the program's calculations. Otherwise, chemically unreasonable solutions can be arrived at without the program user having the chemical "intuition" to recognize the error.

Objective: To become familiar with the use of computer models used in geochemistry and chemical speciation in aquatic systems.

Problem 1: You are working for a processing industry as an environmental specialist. A technician comes to you with the following data taken from waste-water effluent:

$$\begin{aligned}\text{Ni}^{2+} &= 500 \text{ ppm} \\ \text{Pb}^{2+} &= 800 \text{ ppm} \\ \text{Cu}^{2+} &= 250 \text{ ppm} \\ \text{NO}_3^{-1} &= 1800 \text{ ppm} \\ \text{pH} &= 3\end{aligned}$$

The heavy metal concentrations are in excess of EPA's maximum contaminant level (MCL) and he needs a method or a way to reduce these concentrations. Having extensive knowledge of aquatic chemistry, you tell him that raising the pH to 7 should precipitate most of the heavy metals as metal hydroxides (M(OH)_x). However, to be sure you tell him that you will check it using a computer program and will provide him with the

equilibrated mass distribution between the aqueous and solid phases and the aqueous speciation at both pH 3 and 7. Finally, he almost forgot to tell you that they also want to release some additional waste-water into this effluent stream that contains 15,000 ppm EDTA and 2143 ppm sodium. He doesn't think this will be a problem but wants to make sure. You tell him that you will check this using your computer program.

You will conduct 3 runs: the wastewater data at pH 3 and 7 and the wastewater data at pH 7 in the presence of EDTA and sodium. Input this above data using the MINTEQA2 chemical speciation program and **provide a short report** which includes the percent distribution between aqueous and solid phases and the aqueous speciation of the various components. Additionally, based on the MINTEQA2 results, **explain to the technician** what effect if any the presence of EDTA will have at pH 7.

When you open the Visual MINTEQ program you will need to set some default parameters. Under the parameter menu open default settings and allow oversaturated solids to precipitate but only after the final answer is reached. Also click the button to show organic components. When you enter a component make sure you click "add to the list" otherwise it will not show up on the data list. I believe everything else is pretty straight forward.