Water Chemistry

Notes on the Use of the PC version of

MINEQL⁺

Installation

We are using Version 4.6, which is compatible with Windows 7, 8 and 10[i], Vista and earlier MS platforms. We have noted some problems with Apple operating systems.

Nomenclature

Chemical Species

- **Type-I Species**: soluble species that comprise the basic components of the solution and its solutes. These must be a collection of independent species. Species that are merely combinations of previously specified Type-I species should not be included.
- **Type-II Species**: aqueous complexes that form from the Type-I species.
- **Type-III Species**: solids or other substances with fixed activity (e.g., precipitates that never completely dissolve, atmospheric gases, pH in a pH-controlled environment)
- **Type-IV Species**: precipitates that could become completely dissolved and therefore go from an activity of one to zero
- **Type-V Species**: substances that could precipitate, but do not yet exist as a precipitate
- **Type-VI Species**: substances that are not considered in the calculations

Examples

A. Determine the complete species composition from the addition of 5×10^{-3} moles of NaCN to 1 liter of water.

   1. When you launch the program, it goes directly to the "Select Components for Calculation" screen. If it doesn't, click on "select components" from the "Model" drop-down menu. From here you select the Type-I components by checking the boxes next to desired species. The components you should select are: H2O (almost always a selection), H(+), CN(-) and Na(+). Note that OH(-) is not a selection, because it can be obtained by taking an H(+) away from H2O so that it is not a independent substance. The same is true for HCN (it can be obtained by combining CN(-) and H(+).)

2. Click the "Scan THERMO" button at the top. This selects from the thermodynamic database the equilibrium constants you will need and presents them in a table entitled "Type-II Aqueous Species". If this table does not automatically appear, find it by going to menu bar and selecting: Model>Tableau>Aqueous Complexes. Now move the cursor to the total concentration line at the bottom. Keep H2O and H(+) at zero, but type in 5E-3 for the concentration of CN(-) and the same for Na(+).

3. Escape from the "Aqueous Species" table by hitting the "Close" button. Select "Fixed Entities" (i.e., Type-III species) directly from the tableau switch screen and hit "yes". If the tableau switch screen doesn't automatically appear, you'll need to go to the menu bar and select: Model>Tableau>Fixed Entities. You will now see the "Type III Fixed Entities" screen. Highlight the pH line[1] and click on the "move" key. Choose to move pH to "species not considered (Type-VI)"[2], and click on "Move". This is necessary, because we don't want to force the pH to stay at any particular level. In fact, one of the purposes of this problem is to determine what the final pH will be.

4. Escape from "Fixed Solids" by hitting the "close" button. Now select "No" in the Tableau switch screen if it pops up. The "run time manager" screen may then appear. If it doesn't, you'll need to select it by going to the menu bar adn selecting: Model>Calculate. On the "run time manager" screen, you should type in an "output data name" and select "Run". Keep "µ corrections" (ionic strength corrections) off for now, and keep the temperature at 25°C. Shift over to the "file output" line and select a name for the file where the results of your run will be stored. Then click on "run".

5. After the run is complete (should only take a second or two), the "output manager" screen may automatically appear. If it doesn't, retrieve it by going to: Model>Output Manager. Select your output file name in the drop-down box, if it's not already there. Under "output types" select "component groups". Under "data object" select H(+) and click on "view". A table of species containing an exchangeable proton (i.e., H+) will appear. Copy down the relevant information. Ignore the line labeled "pH". Repeat this process, but this time choose "CN(-)" under the "data object" category. This time you will see data on all species that contain the cyanide group (i.e., CN).

You should get the following concentrations:

Species	Concentration
H⁺	$3.63e^{-11}$
OH⁻	0.000278
HCN	0.000278
CN⁻	0.00472

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[1] Highlighting a line may require that you click on the right-hand scroll bar.
[2] Note that this line may not completely appear on your screen so that it may seem to say "species not considered (Type V)"

[i] For Windows 8 and 10 you may have to change the compatibility settings to be: Windows Vista compatible and then re-run setup