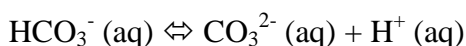
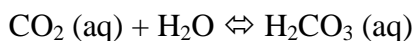


Problem 1

Carbon dioxide dissolved in water at different pH levels.

The following equilibria control the system:



These equilibria are controlled by pH.

Use MINEQL+ to find which species (H_2CO_3 , HCO_3^- , CO_3^{2-}) dominate at the different pH values.

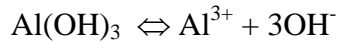
Procedure:

1. Select CO_3^{2-} from the Select components. Do NOT remove H_2O and H^+ as these are needed in aqueous systems.
2. Press **Scan THERMO**
3. Press **Close**
4. Press **No** (- fixed entities)
5. Select folder and write in the name of the output file
6. In the roll down menu **Type of calculation** you select **Titration**
7. Press **Multirun**
8. Select **Fixed Ion**, thereafter **pH**
9. Type in the start and stop value e.g. **0.00** and **14.00**, and how many data points you wish to calculate (e.g. **24**).
10. Press **OK**
11. Now everything is ready to do the calculations,
12. Press **RUN**
13. Select **Graph IT** to show the results as graphs
14. Select the component and species you wish to study: **H_2CO_3 , HCO_3^- , CO_3^{2-}**
15. Select the Y-axis unit **% Total**
16. Press **PLOT**

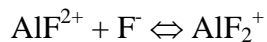
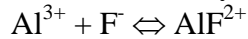
Problem 2

How pH and F⁻ influence the solubility of Gibbsite.

Solubility of gibbsite is commonly used as the mechanism that controls the solubility of Al³⁺.



F⁻ form relatively stable complexes with Al³⁺,



etc...

Use MINEQL+ to show how different concentrations of F⁻ in soil solution influences the solubility of Gibbsite (Al(OH)₃) at different pH values.

Procedure:

1. Start MINEQL+
2. Select the elements that are present in the system (**Al, F**)
3. Press **Scan thermo**
4. Now you get a list with all the species that may be formed and the K-values for the reactions.
Press on **Wizard** type in the Al³⁺ concentration **1·10⁻⁶ M**.
F⁻ concentration shall vary so this will be given later
5. Go to **solid mover** and select **Gibbsite**, move it to **Fixed Solids**. You have now entered the Al³⁺ concentration and selected gibbsite as mineral.
6. Press **OK, Close and No**.
7. Select a name to give to "output file"
8. We are now going to conduct a series of calculations at different F⁻ concentrations and pH values. On "**Type of calculations**" you select "**2-way analysis**".
Press **Multirun**
9. Press on **Select variable**, select "Fixed ion", select pH
Type inn start (**3**) and end values (**9**) and **15** data points. Press **OK**
10. Press **Multirun** Select **Total Conc.**, and "**total concentration of F⁻**".
Type inn start (**0**) and stop values (**5·10⁻⁵**) and **5** data points. Press **OK**.
11. Press **Run** in order to start calculations
12. Select **Graph it** in order to present the results in graphic form.
"Component" is set to Al³⁺ and "units" is set to **Log C**. In the left hand menu you select **Total Al³⁺**. Press **Plot**.

Problem 3

Speciation of Al

We are now going to use MINEQL+ to find which Al species that exist in a water sample. We will also study whether the sample is saturated in respect to certain minerals

Solution:

$$[\text{Al}^{3+}] = 1,0 \cdot 10^{-6}$$

$$[\text{Ca}^{2+}] = 9,0 \cdot 10^{-5}$$

$$[\text{Cl}^-] = 2,8 \cdot 10^{-4}$$

$$[\text{K}^+] = 2,0 \cdot 10^{-5}$$

$$[\text{Mg}^{2+}] = 8,0 \cdot 10^{-5}$$

$$[\text{Na}^+] = 1,3 \cdot 10^{-4}$$

$$[\text{SO}_4^{2-}] = 1,0 \cdot 10^{-4}$$

$$\text{pH} = 5,0$$

Procedure:

1. Select the elements that are contained in the sample, remember to include CO_3^- and press **Scan thermo**.
2. Press **Wizard**, and type in the data in Total and pH, remember to remove (Not considered) all minerals in the folder **Solids mover**.
3. Press **OK** and then **Close** and **No**.
4. You are now ready to run the analysis, select a name on the output file and press **Run**.
5. Select **Component Groups** and **Al(3+)** press on **View**.
6. In order to study the saturation index, select **Special reports** and press **View**.
7. Select **Solids Saturation Index Report**.

Problem 4

Speciation of Zinc and Strontium in seawater.

Sink forms a number of complexes with elements that exists in seawater. What species are formed and what are their concentration?

Procedure:

1. Select the relevant components and press **Scan Thermo**.
2. Press **Wizard** and type inn **concentration** and **pH** values- In the CO2 tablet select 'Closed to Atmosphere' at add the $[\text{HCO}_3^-]$
3. Press **OK**.
4. Press **Close** and **No**.
5. You are now ready to run the calculations. Select a file name for the output file and press **Run**.
6. Select **Component Groups** and **Zn(2+)** and press **View**. Do the same for Sr
7. Select **Graph it**. Select **Zn(2+)** and **plot**. Do the same for Sr
8. In addition you can calculate the alkalinity, select **Special reports** and press **View**.
9. Select **Alkalinity summary**.

Typical seawater concentrations mmol/L:

$[\text{Ca}^{2+}] = 10,4$
 $[\text{Mg}^{2+}] = 53,3$
 $[\text{Na}^+] = 468$
 $[\text{K}^+] = 9,97$

$[\text{Cl}^-] = 546$
 $[\text{SO}_4^{2-}] = 28,1$
 $[\text{HCO}_3^-] = 2,34$
 $[\text{Br}^-] = 0,83$

pH = 8,2

$[\text{Sr}^{2+}] = 0,091$
 $[\text{Zn}^{2+}] = 1,0 \cdot 10^{-3}$