Problem 1

Carbon dioxide dissolved in water at different pH levels.

The following equilibriums control the system:

CO_2 (g) ⇔ CO_2 (aq)

CO_2 (aq) + H_2O ⇔ H_2CO_3 (aq)

H_2CO_3 (aq) ⇔ HCO_3^- (aq) + H^+ (aq)

HCO_3^- (aq) ⇔ CO_3^{2-} (aq) + H^+ (aq)

These equilibriums 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 $\mathbf{CO_3^{2-}}$ 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 inn 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: $\mathbf{H_2CO_3, HCO_3^-, CO_3^{2-}}$
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 Al^{3+}.

$Al(OH)_3 \Leftrightarrow Al^{3+} + 3OH^-$

F^- form relatively stable complexes with Al^{3+},

$Al^{3+} + F^- \Leftrightarrow AlF^{2+}$

$AlF^{2+} + F^- \Leftrightarrow AlF_2^+$

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 Al^{3+} concentration $\mathbf{1 \cdot 10^{-6}}$ 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 Al^{3+} 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 ($\mathbf{5 \cdot 10^{-5}}$) 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 $\mathbf{Al^{3+}}$ and ”units” is set to **Log C**. In the left hand menu you select **Total Al^{3+}**. 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:
$[Al^{3+}] = 1,0*10^{-6}$
$[Ca^{2+}] = 9,0*10^{-5}$
$[Cl^{-}] = 2,8*10^{-4}$
$[K^{+}] = 2,0*10^{-5}$
$[Mg^{2+}] = 8,0*10^{-5}$
$[Na^{+}] = 1,3*10^{-4}$

$[SO_4^{2-}] = 1,0*10^{-4}$

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 inn 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 Zink 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 **[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:

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

[Cl^{-}] = 546
[SO_4^{2-}] = 28,1
[HCO_3^{-}] = 2,34
[Br^{-}] = 0,83

pH = 8,2

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