PRILOG 5.

$CO_2(g) + H_2O(l) \rightleftharpoons H_2CO_3$ $\quad K_H = 10^{-1,47}$

$H_2CO_3 \rightleftharpoons HCO_3^- + H^+$ $\quad K_1 = 10^{-6,35}$

$HCO_3^- \rightleftharpoons CO_3^{2-} + H^+$ $\quad K_2 = 10^{-10,33}$

$CaCO_3(s) \rightleftharpoons Ca^{2+} + CO_3^{2-}$ $\quad K_{so} = 10^{-8,34}$

$[Ca^{2+}] = ?$

Kada je kalcit u ravnoteži s vod. otopinom i CO_2 iz zraka u sustavu su prisutne slijedeće vrste: Ca^{2+}, CO_3^{2-}, HCO_3^-, H_2CO_3, CO_2, H^+, OH^-. Parc. pritisak CO_2 je zadan (0,003 atm) te je preostalo 6 nepoznanica. Trebamo 6 jednadžbi:

1. $K_H = \dfrac{[H_2CO_3]}{p_{CO_2}} = 10^{-1,47}$
2. $K_1 = \dfrac{[H^+][HCO_3^-]}{[H_2CO_3]}$
3. $K_2 = \dfrac{[H^+][CO_3^{2-}]}{[HCO_3^-]}$
4. $K_{so} = [Ca^{2+}][CO_3^{2-}]$
5. $K_W = [H^+][OH^-]$
6. $2[Ca^{2+}] + [H^+] = 2[CO_3^{2-}] + [HCO_3^-] + [OH^-]$

$[H_2CO_3] = 10^{-1,47} \cdot 0,003\,atm = 1,02 \times 10^{-4}\,M$

$[HCO_3^-] = K_1 \cdot \dfrac{[H_2CO_3]}{[H^+]} \cdot \dfrac{[OH^-]}{[OH^-]} = 10^{-6,35} \cdot \dfrac{1,02 \times 10^{-4}\,[OH^-]}{10^{-14}} = 4,56 \times 10^3\,[OH^-]$ ($[H^+][OH^-] = K_W$)

$[CO_3^{2-}] = K_2 \dfrac{[HCO_3^-]}{[H^+]} \cdot \dfrac{[OH^-]}{[OH^-]} = 10^{-10,33} \cdot \dfrac{4,56 \times 10^3\,[OH^-]^2}{10^{-14}} = 2,13 \times 10^7\,[OH^-]^2$

$[Ca^{2+}] = \dfrac{K_{so}}{[CO_3^{2-}]} = \dfrac{10^{-8,34}}{2,13 \times 10^7\,[OH^-]^2} = 2,14 \times 10^{-16}\,[OH^-]^{-2}$

$[H^+] = \dfrac{10^{-14}}{[OH^-]}$

PRILOG 5 (nastavak)

$$2.\ \frac{2,14\times10^{-16}}{[OH^-]^2} + \frac{10^{-14}}{[OH^-]} = 2\cdot 2,13\times10^{7}\,[OH^-]^2 + 4,56\times10^{3}\,[OH^-] + [OH^-] \,/\,[OH^-]$$

$$4,28\times10^{-16} + 10^{-14}\,[OH^-] = 4,26\times10^{7}\,[OH^-]^4 + 4,56\times10^{3}\,[OH^-]^3$$

$$4,26\times10^{7}\,[OH^-]^4 + 4,56\times10^{3}\,[OH^-]^3 - 10^{-14}\,[OH^-] = 4,28\times10^{-1}$$

→ metoda "pokušaj - pogreška" → vidi Excel dokument

$$[OH^-] = 4,54\times10^{-7}\,M \Rightarrow pH = 7,66$$

Sad se vraćamo u jednadžbe na prethodnoj stranici i dobijemo:

$$[CO_3^{2-}] = 2,13\times10^{7} \times (4,54\times10^{-7})^2 = 4,39\times10^{-6}\,M$$

$$[Ca^{2+}] = \frac{2,14\times10^{-16}}{[OH^-]^2} = 1,04\times10^{-3}\ mol/dm^3$$

Ili, ako želimo izraziti topljivost u mg/L:

$$n = \frac{m}{M} \Rightarrow m = n \cdot M$$

$$m = 1,04\times10^{-3}\ mol \times 40,08\ g\,mol^{-1} = 41,6\times10^{-3}\ g$$

$$\gamma = \frac{m}{V} \Rightarrow \gamma(Ca^{2+}) = 41,6\ mg/L$$