GOVERNMENT OF NEWFOUNDLAND AND LABRADOR
Department of Environment and Conservation

# Calculation of the Langelier Index

The Langelier index (LI) is an approximate measure of the degree of saturation of calcium carbonate in water. It is calculated using the **pH**, **alkalinity** (reported as $CaCO_3$ in mg/litre), **calcium concentration** (reported as $Ca^{2+}$ in mg/litre), **total dissolved solids** (reported as *TDS* in mg/litre), and **water temperature** (reported as *t* in degrees Celsius, °C) of a water sample collected at the tap. These parameters are highlighted in **red** in the calculations listed below.

The Langelier Index (LI) is calculated as follows:

$$LI = pH - pH_s$$

where ***pH*** = measured pH of the tap water
$pH_s$= calculated saturation pH of the tap water

$$pH_s = pK_2' + pCa^{2+} - pK_s' - \log(2[Alk]) - \log\gamma_m$$

In order to calculate $pH_s$, $pK_2'$, $pK_s'$ and $pCa^{2+}$ must first be computed. Explanations of how to do these calculations are given below. In addition, concentrations of $Ca^{2+}$ and ***Alk*** must also be converted to moles per litre. These steps are described below.

**1.** To compute $pK_2'$, which is the negative log of the activity constant $K_2'$ $(-\log K_2')$:

**a.** Determine the Ionic Strength (I), in moles per litre (M), of the water:

$$I(M) = (2.5\times10^{-5} moles/mg)\times[TDS(mg/litre)]$$

*where* ***TDS* = Total Dissolved Solids (mg/litre)**

**b.** Determine $\gamma_m$, the activity coefficient of monovalent ions (ions that are able to form only one covalent or ionic bond – having only one valence) using the Davies relationship:

$$\text{If } I < 0.5M, \quad \log\gamma_m = -AZ^2\left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.2I\right)$$

$$\text{If } 0.5M < I < 1.0M, \quad \log\gamma_m = -AZ^2\left(\frac{\sqrt{I}}{1+\sqrt{I}}\right)$$

*where M* = molarity (moles per litre)

$A = 1.82 \times 10^6 (DT)^{\frac{-3}{2}}$

$D = 78.3$, the dialectric constant for water and T = temperature in Kelvins (K). To convert **temperature (*t*)** in degrees centigrade (°C) to Kelvins (K):

[T = ***t***(°C)+273]

*and* $Z =$ the oxidation number of the chemical species in question, which for monovalent ions = 1

$$\text{If } 0.5M < I < 1.0M\ ,\ \log \gamma_m = -AZ^2 \left( \frac{\sqrt{I}}{1+\sqrt{I}} \right)$$

**c**. Calculate $pK_2$ :

$$pK_2 = \frac{2902.39}{T} + 0.02379(T) - 6.498$$

From which we calculate $K_2$:

$$K_2 = 10^{-pK_2}$$

**d.** Calculate $\gamma_D$, the activity coefficient of divalent ions (ions having two valences):

$$\log \gamma_D = -AZ^2 \left[ \frac{\sqrt{I}}{1+\sqrt{I}} \right]$$

*where as defined earlier*;

$A = 1.82 \times 10^6 (DT)^{\frac{-3}{2}}$

$D = 78.3$, the dialectric constant for water, and T = temperature in Kelvins (K). To convert **temperature (*t*)** in degrees centigrade (°C) to Kelvins (K):

[T = ***t***(°C)+273]

*and* $Z =$ the oxidation number of the chemical species in question, which for divalent ions = 2

Then calculate $\gamma_D$:

$$\gamma_D = 10^{\log \gamma_D}$$

**e**. Calculate $K_2'$:

$$K_2' = \frac{K_2}{\gamma_D}$$

**f**. We can then calculate $pK_2'$:

$$pK_2' = \log\frac{1}{K_2'}$$

**2.** To compute $pK_s'$ which is the negative log of the activity constant $K_s'$ $(-\log K_s')$:

**a.** First compute $pK_s$:

$$pK_s = 0.01183t + 8.03$$

*where* ***t* = temperature in degrees Centigrade (°C)**

**b.** Convert the $pK_s$ value to $K_s$:

$$K_s = 10^{-pK_s}$$

**c.** Using the value of $\gamma_D$ calculated earlier, calculate $K_s'$:

$$K_s' = \frac{K_s}{(\gamma_D)^2}$$

**d**. We can then calculate $pK_s'$:

$$pK_s' = \log\frac{1}{K_s'}$$

**3.** To compute $pCa^{2+}$:

a. Convert the concentration of ***Ca$^{2+}$* (mg/litre)** to moles per liter:

$$Ca^{2+}(moles/litre) = \frac{[Ca^{2+}(mg/litre)]\times 10^{-3}}{40}$$

**c.** Calculate $pCa^{2+}$:

$$pCa^{2+} = \log\frac{1}{[Ca^{2+}(moles/litre)]}$$

**4.** **Alkalinity (*Alk*)** is reported as mg/litre $CaCO_3$. It is necessary to convert the given **alkalinity** concentration to moles/litre:

$$[Alk(moles/litre)] = \frac{[CaCO_3(mg/litre)]\times 10^{-3}}{100}$$

**Reference:**


Benefield, L., Judkins, J. & Weand, B. 1982. *Process Chemistry for Water and Wastewater Treatment.* Prentice-Hall, Inc. Englewood Cliffs, New Jersey.