

OLI Tips #73

Converting reported equilibrium constants

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Overview

A change in the concentration basis has been introduced in ESP version 7.0 and OLI Analyzers 2.0. This change in basis from molal (moles/ Kg H₂O) to mole fraction was primarily done to support the Mixed-Solvent Electrolyte (MSE) thermodynamic package. The change in basis was also applied to the Aqueous Electrolyte (AQ) model.

Frequently a user needs to compare an equilibrium constant¹ reported by the OLI software with literature values. Frequently the literature reports equilibrium constants on the molal basis and not the mole fraction basis. Fortunately there is an easy conversion.

Conversion equation

The conversion equation is very simple. Let's define two equilibrium constants. K(m) and K(x). K(m) is the molal based equilibrium constant and K(x) is the mole fraction based equilibrium constant.

The conversion is:

$$K(m) = K(x) * 55.5091^{\Delta n}$$

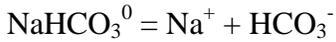
Where Δn is the change in moles across the equation excluding water (H₂O and solids):

$$\Delta n = moles_{prod} - moles_{react}.$$

¹ Also called K-values in the OLI parlance

Example 1: No water

Let's consider this equilibrium reaction:

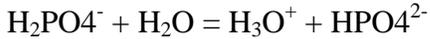


The software calculates an equilibrium constant, $K(x) = 8.43828\text{E-}13$ with $\Delta n = (2 \text{ moles product} - 1 \text{ moles reactant}) = 1$. Thus the conversion is:

$$K(m) = K(x) * 55.5091^1 = 8.43828\text{E-}13 * 55.5091 = 4.68401\text{E-}11$$

Example 2: With water

Now let's consider a conversion where water is present.



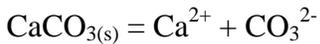
The software calculates an equilibrium constant, $K(x) = 1.1224\text{E-}09$, $\Delta n = (2 \text{ moles of product} - 1 \text{ mole of reactant}) = 1$. Thus our conversion equation is:

$$K(m) = K(x) * 55.5091^1 = 1.1224\text{E-}09 * 55.5091 = 6.23033\text{E-}08$$

Why was there only 1 mole of reactant? In our conversion, we ignore the moles of H_2O (in the molality basis the activity of water is unity for the conversion)

Example 3: With a solid

Now let's consider a conversion where a solid is dissolving:



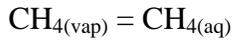
The software calculates an equilibrium constant, $K(x) = 9.66059\text{E-}13$, ($\Delta n = 2 \text{ moles of product} - 0 \text{ mole of reactant} = 2$). Thus our conversion equation is:

$$K(m) = K(x) * 55.5091^2 = 9.66059\text{E-}13 * 3081.26 = 2.97668\text{E-}09$$

Why was there 2 moles of reactant? In our conversion, we ignore the moles of a solid (in the molality basis the activity of a solid is unity for the conversion)

Example 4: With a vapor

Now let's consider a vapor – liquid equilibrium. We will use methane as an example:



The software calculates an equilibrium constant, $K(x) = 2.46184\text{E-}05$,
($\Delta n =$ is 1 mole of product - 0 mole of reactant) = 1.

Although the vapor can be a solution of species we treat it as a single phase. Thus the components in the vapor phase are set to zero for this conversion.

Thus our conversion equation is:

$$K(m) = K(x) \times 55.5091^1 = 2.46184\text{E-}05 * 55.5091 = 1.36655\text{E-}03$$