Total Dissolved Solids and Conductivity

as Calculated by the French Creek Engine

TDS

The French Creek Ion Association Model Engine calculates total dissolved solids(TDS) as follows:

- The Engine iteratively solves for the most likely distribution of species for an analysis based upon 122 ion pair species, as outlined in Table 1.
- TDS is calculated by taking the molal concentration of each species, multiplying each by its molecular weight, and converting to mg/L.
- The calculated TDS is the sum of all species.

This method provides a more accurate estimation of TDS for thermodynamic calculations than taking the individual ions, converting to mg/L, and summing them.

Conductivity

The French Creek Ion Association Model Engine calculates conductivity as molar conductivity as follows:

- The Engine multiplies each specie($\boldsymbol{m}$) by its molar conductivity (Λ^0_m)sums up the individual conductivity contributions to calculate a base specific conductivity (**SC**).

$$\mathbf{SC} = \Sigma\ (\Lambda^0_m\ \boldsymbol{m})$$

- The conductivity calculations used by the French Creek Engine include corrections for activity as ionic strength increases or decreases.
- Calculated molar conductivity will not necessarily duplicate a measured value for conductivity. It is much more accurate than rules of thumb such as

$$\mu = \mathrm{TDS}/0.7$$

Table 1: Example Ion Pairs Used To Estimate Free Ion Concentrations

CALCIUM

[Calcium] = $[Ca^{+2}] + [CaSO_4] + [CaHCO_3^{+1}] + [CaCO_3] + [Ca(OH)^{+1}] + [CaHPO_4] + [CaPO_4^{-1}] + [CaH_2PO_4^{+1}]$

MAGNESIUM

[Magnesium] = $[Mg^{+2}] + [MgSO_4] + [MgHCO_3^{+1}] + [MgCO_3] + [Mg(OH)^{+1}] + [MgHPO_4] + [MgPO_4^{-1}]+[MgH_2PO_4^{+1}]+[MgF^{+1}]$

BARIUM

[Barium] = $[Ba^{+2}] + [BaSO_4] + [BaHCO_3^{+1}] + [BaCO_3] + [Ba(OH)^{+1}]$

STRONTIUM

[Strontium] = $[Sr^{+2}] + [SrSO_4] + [SrHCO_3^{+1}] + [SrCO_3] + [Sr(OH)^{+1}]$

SODIUM

[Sodium] = $[Na^{+1}] + [NaSO_4^{-1}] + [Na_2SO_4] + [NaHCO_3] + [NaCO_3^{-1}] + [Na_2CO_3] + [NaCl]+[NaHPO_4^{-1}]$

POTASSIUM

[Potassium] = $[K^{+1}] +[KSO_4^{-1}] + [KHPO_4^{-1}] + [KCl]$

IRON

[Iron] = $[Fe^{+2}] + [Fe^{+3}] + [Fe(OH)^{+1}] + [Fe(OH)^{+2}] + [Fe(OH)_3^{-1}] + [FeHPO4^{+1}] + [FeHPO_4] + [FeCl^{+2}] + [FeCl_2^{+1}] + [FeCl_3] + [FeSO_4] + [FeSO_4^{+1}] + [FeH_2PO_4^{+1}] + [Fe(OH)_2^{+1}] + [Fe(OH)_3] + [Fe(OH)_4^{-1}] + [Fe(OH)_2] + [FeH_2PO_4^{+2}]$

ALUMINUM

[Aluminum] = $[Al^{+3}] + [Al(OH)^{+2}] + [Al(OH)_2^{+1}] + [Al(OH)_4^{-1}] + [AlF^{+2}] + [AlF_2^{+1}] + [AlF_3] + [AlF_4^{-1}] + [AlSO_4^{+1}] + [Al(SO_4)_2^{-1}]$

Total Analytical Value **Free Ion Concentration**

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