Quantification with the Polyarc®

PA-MAN-QP1

The Polyarc converts all organic compounds to methane, resulting in an equivalent response per mole of carbon. This approximation is illustrated below in Equation 1 as a relative response factor in terms of carbon ($RRF_{mol\ C}$) equal to one:

$$\frac{Area_A/N_A}{Area_S/N_S} = RRF_{mol\ C} = 1 \qquad \text{(Equation 1)}$$

A relative response factor in terms of moles of a compound can be derived from Equation 1 by incorporating the number of carbon atoms per molecule. Equation 2 defines the relative response factor in molar terms (RRF_{mol}):

$$\frac{Area_A/M_A}{Area_S/M_S} = RRF_{mol} = \left(\frac{\#C_A}{\#C_S}\right) \qquad \text{(Equation 2)}$$

A relative response factor in terms of mass can then be derived from Equation 2 by incorporating molecular weights. Equation 3 defines the relative response factor in mass terms (RRF_{mass}):

$$\frac{Area_A/C_A}{Area_S/C_S} = RRF_{mass} = \left(\frac{\#C_A}{\#C_S}\right)\left(\frac{MW_S}{MW_A}\right) \qquad \text{(Equation 3)}$$

Definitions of variables for the equations above are as follows:

N_A = moles carbon of the analyte
N_S = moles carbon of the standard
M_A = Molar concentration of the analyte
M_S = Molar concentration of the standard
C_A = Mass concentration of analyte
C_s = Mass concentration of standard

$Area_A$ = Integrated peak area of the analyte
$Area_S$ = Integrated peak area of the standard
$\#C_A$ = Number of carbon atoms per molecule analyte
$\#C_S$ = Number of carbon atoms per molecule standard
MW_A = Molecular weight of the analyte
MW_S = Molecular weight of the standard

Quantifying in Molar Terms

Equation 2 for quantification in molar terms is solved below for the molar concentration of an analyte. The following equations require the use of an internal or external standard and can be used for any molar concentration units (i.e., ppm molar, mol%, mol/L, mol/g, etc.).

$$M_A = M_S \left(\frac{Area_A}{Area_S}\right)\left(\frac{1}{RRF_{mol}}\right) \quad \text{(Equation 4)}$$

$$M_A = M_s \left(\frac{Area_A}{Area_S}\right)\left(\frac{\#C_S}{\#C_A}\right) \quad \text{(Equation 5)}$$

Quantifying in Mass Terms

Equation 3 for quantification in mass terms is solved below for the mass concentration of an analyte. The following equations require the use of an internal or external standard and can be used for any mass concentration units (i.e., ppm mass, wt%, g/L, µg/mL, etc.).

$$C_A = C_S \left(\frac{Area_A}{Area_S}\right)\left(\frac{1}{RRF_{mass}}\right) \quad \text{(Equation 6)}$$

$$C_A = C_s \left(\frac{Area_A}{Area_S}\right)\left(\frac{\#C_S}{\#C_A}\right)\left(\frac{MW_A}{MW_S}\right) \quad \text{(Equation 7)}$$

Quantifying without a Standard

Additionally, quantification can be done when using the Polyarc without a standard using the following equation, where X_A is the mass fraction of an analyte. Note these equations are only valid when the assumption that everything in the sample is detected by the FID (i.e., no water or solids content in the sample).

$$X_A = \frac{(Area_A \cdot RRF_{mass,A})}{\sum_{i=1}^{n}(Area_i \cdot RRF_{mass,i})} \quad \text{(Equation 8)}$$