How to Calculate a Chloride Equivalent for the Total Chlorine Standard

The hydrogen chloride (HCl) and chlorine gas (Cl_2) standard – also known as the total chlorine standard – of §§63.1203, 63.1204, and 63.1205 is expressed in terms of "parts per million by volume, combined emissions, expressed as hydrochloric acid equivalents, dry basis and corrected to 7 percent oxygen." This document shows how to calculate a chloride ($Cl^{(-)}$) equivalent for the total chlorine standard.

Analytical results using the Method 26 sampling train are often reported in mg/dscm HCl and Cl_2. **Steps 1 and 2** can be used to convert stack gas concentrations from mg/dscm to a $Cl^{(-)}$ equivalent in ppmv assuming the species behaves as an ideal gas.

Step 1: Convert Method 26 Results from mg/dscm to ppmv

Separately convert the HCl and Cl_2 results to ppmv using either Equation 1 or the summary table.

Assumptions:
- Gas at standard conditions (temperature of 20˚C, and pressure of 1 atm)
- Ideal gas molecular volume is 22.4 L/mol at 0˚C and 1 atm
- Stack gas concentration of species being corrected to 7% oxygen

Equation 1:

$$(A\ \text{ppmv}) = \frac{\left(B\ \frac{\text{mg}}{\text{dscm}}\right) \times \left(22.4\ \frac{\text{L}}{\text{mol}}\right) \times \left(\frac{293\ \text{K}}{273\ \text{K}}\right) \times \left(1 \times 10^6\ \text{ppmv}\right)}{\left(M\ \frac{\text{g}}{\text{mol}}\right) \times \left(1000\ \frac{\text{L}}{\text{dscm}}\right) \times \left(1000\ \frac{\text{mg}}{\text{g}}\right)}$$

Where:

M = molecular weight of species. For example, the molecular weight of HCl is 36.5 g/mol; Cl_2 is 70.9 g/mol; and $Cl^{(-)}$ is 35.5 g/mol.

A = concentration in ppmv (at 7% oxygen)

B = concentration in mg/dscm (at 7% oxygen)

Summary Table of Conversion Factors (using Equation 1):

Species (mg/dscm)	To Convert from mg/dscm to ppmv, Multiply by
HCl	0.659
Cl_2	0.339
$Cl^{(-)}$	0.677

Step 2: Calculate Total Chlorine Emissions as a Chloride Equivalent

Convert the HCl and Cl_2 results from Step 1 to a $Cl^{(-)}$ equivalent using Equation 2

Equation 2:

$Cl^{(-)}$ Equivalent (ppmv) = HCl (ppmv) + [2 x Cl_2 (ppmv)]

Alternative Calculation of a $Cl^{(-1)}$ Equivalent

Convert Method 26 analytical results from mg/dscm to a $Cl^{(-)}$ equivalent in ppmv using Equation 3.

Equation 3:

$Cl^{(-)}$ Equivalent (ppmv) = [[HCl (mg/dscm) x (35.5/36.5)] + Cl_2 (mg/dscm)] x (0.677 ppmv / mg/dscm)

Sample Calculation

What is the total chlorine emissions on a $Cl^{(-)}$ equivalent basis if HCl is 100 mg/dscm and Cl_2 is 10 mg/dscm? Both measurements are at 7% oxygen.

Step 1: Convert to ppmv

HCl (ppmv) = (100 mg/dscm) x (0.659 ppmv / mg/dscm) = 65.9 ppmv
Cl_2 (ppmv) = (10 mg/dscm) x (0.339 ppmv / mg/dscm) = 3.4 ppmv

Step 2: Convert to a $Cl^{(-)}$ equivalent

$Cl^{(-)}$ Equivalent (ppmv) = 65.9 ppmv + (2) x (3.4 ppmv) = 73 ppmv

Or, alternatively, using Equation 3:

$Cl^{(-)}$ Equivalent (ppmv) = [[(100 mg/dscm) x (35.5 g/mol / 36.5 g/mol)] + 10 mg/dscm] x (0.677 ppmv / mg/dscm) = 73 ppmv