How to Calculate a Chloride Equivalent for the Total Chlorine Standard

The hydrogen chloride (HCl) and chlorine gas (Cl₂) 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 Cl₂. 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 Cl₂ 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:

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

Where:
- \( M \) = molecular weight of species. For example, the molecular weight of HCl is 36.5 g/mol; Cl₂ 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):

<table>
<thead>
<tr>
<th>Species (mg/dscm)</th>
<th>To Convert from mg/dscm to ppmv, Multiply by</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCl</td>
<td>0.659</td>
</tr>
<tr>
<td>Cl₂</td>
<td>0.339</td>
</tr>
<tr>
<td>Cl⁻</td>
<td>0.677</td>
</tr>
</tbody>
</table>
**Step 2: Calculate Total Chlorine Emissions as a Chloride Equivalent**

Convert the HCl and Cl₂ results from Step 1 to a Cl(-) equivalent using Equation 2

**Equation 2:**

\[
\text{Cl}(-) \text{ Equivalent (ppmv)} = \text{HCl (ppmv)} + [2 \times \text{Cl}_2 \text{ (ppmv)}]
\]

**Alternative Calculation of a Cl(-) Equivalent**

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

**Equation 3:**

\[
\text{Cl}(-) \text{ Equivalent (ppmv)} = \left[\text{HCl (mg/dscm)} \times \left(\frac{35.5}{36.5}\right) + \text{Cl}_2 \text{ (mg/dscm)}\right] \times (0.677 \text{ ppmv / mg/dscm})
\]

**Sample Calculation**

What is the total chlorine emissions on a Cl(-) equivalent basis if HCl is 100 mg/dscm and Cl₂ 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  
Cl₂ (ppmv) = (10 mg/dscm) x (0.339 ppmv / mg/dscm) = 3.4 ppmv

Step 2: Convert to a Cl(-) equivalent

\[
\text{Cl}(-) \text{ Equivalent (ppmv)} = 65.9 \text{ ppmv} + (2) \times (3.4 \text{ ppmv}) = 73 \text{ ppmv}
\]

Or, alternatively, using Equation 3:

\[
\text{Cl}(-) \text{ Equivalent (ppmv)} = \left[\left((100 \text{ mg/dscm}) \times \left(\frac{35.5 \text{ g/mol}}{36.5 \text{ g/mol}}\right)\right) + 10 \text{ mg/dscm}\right] \times (0.677 \text{ ppmv / mg/dscm}) = 73 \text{ ppmv}
\]