GUARDIAN Manufacturing

Ozone Calculation Reference Data

The intent of this document is to provide some basic guidance on calculations and units of measure common in ozone systems.

Reference Conditions:

There are 2 sets of reference conditions commonly used for ozone measurements:

Standard Temperature and Pressure (STP)
Normal Temperature and Pressure (NTP)

These are both defined as 1 Atmosphere, with STP at 0°C and NTP at 20°C.

It is important to understand these reference conditions because flow and concentration measurements are typically 'corrected' to one or the other. The 'correction' is calculated based on a fixed mass of gas.

Flow translation:

Flows referenced to STP (SLPM, SCFH) may have to be converted to NTP. Flows referenced to NTP (most rotometer readings) may have to be converted to STP. The Ideal gas law is used to make the conversion:

If $PV_1 = nRT_1$ describes the fixed mass of gas at one condition, and $PV_2 = nRT_2$ describes the same mass of gas at the other condition then:

P: pressure is the same (1 ATM)
N: Number of molecules is the same
R: Gas Constant is, well, constant
T: defined by the reference conditions (absolute temp)

So:

$V_1/T_1 = V_2/T_2$
Or:

$V_2 = V_1*(T_2/ T_1)$

For the case of a sample at NTP, the volume would decrease by a factor of (273.15)/(20+273.15), Or 0.93

NLPM * 0.93 = SLPM
Mg/NM^3 / 0.93 = Mg/SM^3

The same approach may be used to convert to one of the reference conditions from any other condition (from room temperature, for example)

Flow Measurements:

Rotometers:

Flows in ozone systems are typically measured with 'rotometers' – the 'raw' measurements can rarely be used without significant correction. Sources of 'error' include:

Outlet Temp / Pressure other than NTP (typical of most manufacturers)
Gas composition (most off-the-shelf rotometers are set up for air)

When rotometers are used at conditions other than those for which they are designed, the indicated values must be 'adjusted'. The following corrections are typical:
[Note that absolute Temps/Pressures must be used in all calcs]

Outlet Pressure not equal to calibrated outlet pressure:

Actual flow = Indicated flow * sqrt(P_{ACT} / P_{CAL})

Outlet Temp not equal to calibrated Temp:

Actual flow = Indicated flow * sqrt(T_{CAL} / T_{ACT})

Gas not the same density as Cal gas:

Actual flow = Indicated flow * sqrt(1 / SG)
Where SG = (Density of Actual gas / Density of Cal gas)

Sqrt(1/SG) = 0.95 for actual = Oxygen and Cal = Air

It is (obviously) important to understand the calibration data for the rotometer that one is trying to use. Rotometer direct readings are worthless (for precise calculation) without these corrections.

<u>Mass Flow Meters:</u>

There are a variety of mass flow meters available. They typically 'correct' their outputs to STP. They may be calibrated for any of a number of gases – where a gas other than the calibration gas is used, the manufacturer typically provides a linear correction factor.

<u>Errata:</u>

Calculations for ozone production are typically based on a measured flowrate and a measured concentration. Because ozone is incompatible with so many things, the flow measurement is usually of the feed gas and not of the ozone/oxygen exhaust gas. If the inlet volumetric flow is assumed to be the same as the outlet volumetric flow, a small error is introduced to the calculation; that error grows as ozone concentration increases.

The act of turning O2 into O3 reduces the number of molecules. The 'n' in the ideal gas law is not the same at the inlet and the outlet. The 'error' may be corrected as follows:
(Assume oxygen feed gas)

$FLOW_{OUT}$ = $FLOW_{in}$ * (100/((1.5 * OZ%) + (100 – OZ%))
Where OZ% is the volumetric ozone percentage

For an ozone concentration of 10% (Volume), the correction is 0.95
For an ozone concentration of 5% (Volume), the correction is 0.975
For an ozone concentration of 1% (Volume), the correction is 0.995

Flow Calculations:

Reference Data:

O_3 density at STP: 2.144 g/L

O_2 density at STP: 1.429 g/L

O_3 density at NTP: 1.998 g/L
O_2 density at NTP: 1.332 g/L

Typically, flow and concentration are measured. The following text is intended to demonstrate how everything of any use can be derived from those quantities.

Mass fraction (A.K.A. percent by weight):

All that is required for this calculation is a concentration. The concentration must be in explicit units. It really doesn't matter what the units are, so long as the temperature and pressure are specified. Analyzers that operate at ozone generator concentrations typically use a mass/volume format – g/NM^3 is common.

Mass fraction may be calculated from g/NM^3 as follows:

Mass Fraction = $(g/NM^3) / [(g/NM^3) + (1000-(g/NM^3/1.998))*1.332]$

100 g/NM^3 = 7.32% (mass)

It must be noted that this factor is useful ONLY for the case where the concentration is NTP – it must be modified for all other cases.

Volume Fraction (A.K.A. percent volume):

As in the case of Mass Fraction, only a concentration is required (this calculation is actually a subset of the mass fraction calculation).

Volume fraction may be computed from g/NM^3 as follows:

Volume Fraction = $(g/NM^3 / 1.998) / 1000$

100 g/NM^3 = 5.01% (volume)

Note:

There is apparently a commonly held belief that a constant 'conversion factor' between % mass and % volume exists. This is simply incorrect. The value is in the range of 3(mass) :2(vol) for low concentrations of ozone, but that ratio decreases (approaches 1:1) with increasing ozone concentration.

Mass Flow Rate:

In ozone applications, Mass flows are often expressed in units of 'grams/hour' or 'pounds per day'. The difference between these units is a simple conversion factor. The confusion in these calculations is usually in getting flow and concentration data in consistent units. Specifically, both flow and concentration must be in 'normal' or 'standard' units (any reference condition may be used, but these are the most common).

Given a flow in SLPM and a concentration in g/NM^3 , proceed as follows:

Compute Volume Fraction as described above
Compute ozone volumetric flowrate:

Ozone volume flowrate = SLPM * Volume Fraction [SLPM]

Compute Ozone mass flowrate;

Ozone mass flowrate = volume flow * ozone density (@ STP) [L/min*g/L =g/min]

The ozone mass flowrate will be in units of g/min. Some useful conversion factors:

60 minutes / hour
1440 minutes / day
1000g / Kg
453.6 g / pound

Example:

Given a 10 SLPM flow of 100 g/NM^3 gas, calculate mass flow in LB/Day

The Volume Fraction is .0501 (5.01%)

*The ozone volume flowrate = 10 SLPM * .0501 = .501 SLPM ozone*

*The ozone mass flowrate = .501 SLPM * 2.144 g/L = 1.074 g/min*

Converted to LB/Day:

*1.074 g/ min * 1 LB/453.6g * 1440 min / day = 3.41 LB/Day*

Notes:

If flowrates are given in at normal (rather than ‘standard’) conditions, they may be ‘corrected’ by using the Temperature correction described in the ‘Reference Conditions’ section, above.

Before ANY raw flow measurement is used in the mass flow calculation, it must be evaluated to determine what corrections are required.