TechNote TN-2

Ozone: Different "Concentrations"

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UV radiation at 254 nm wavelength (the mercury line) is ideally suited to measure the density of ozone in air, oxygen, or water, because the extinction spectrum of ozone has its strongest band around 254 nm.

1. g/m³ measured density

A UV photometer practically does not "see" air, or oxygen, or water. UV radiation at 254 nm is partially absorbed, or weakened, only by the ozone present in the cuvette. Thus the UV photometer measures the density [g/m³] (measured density) which the ozone has at the arbitrary temperature and the arbitrary pressure inside the cuvette. Since the ozone is part of a gas mixture this measured density is worthless as long as the temperature and the pressure of the gas mixture in the cuvette are not known. An ozone analyser (for gaseous ozone) thus must have means to additionally measure the temperature and the pressure inside the cuvette. For ozone in water this is not necessary because the density of water (for industrial ozone applications in water) practically does not change with temperature and pressure.

Several different "concentrations" used to describe the ozone content of an ozone gas now can be calculated using the measured ozone density [g/m³], and the temperature and pressure also measured in the cuvette of the UV photometer.

2. g/Nm³ compensated density

The measured ozone density [g/m³] in the cuvette can be compensated for temperature and pressure in order to display the mass of ozone which would be present in one cubic meter of ozone gas at a given standard temperature and a given standard pressure. The standard pressure is agreed to internationally as P_0 = 1 atm (760 mmHg, 1.01325 bar). But the standard temperature is a medieval chaos. Some people recommend 0°C (32°F), others are claiming 15°C (59°F), or 20°C (68°F), or 21.11°C (70°F), or even 25°C (77°F). To escape from this chaos, the SEMI Standard E12-96 decided (for the semiconductor industry) to only use 0°C (273.15 K) as the standard temperature. The standard conditions 0°C / 1 atm should be referred to as "International Standard Conditions". In all ozone measuring instruments made by BMT MESSTECHNIK compensation is calculated to these International Standard Conditions T_0 = 273.15 K / P_0 = 1 atm.

ozone in	mass / volume (temp. / press.)	volume / volume	mass / mass
process gas	$\frac{g}{Nm^3}$ at T_0/P_0	ppm_v	%wt/wt (needs density of "rest")
ambient air	$\frac{mg}{m^3}$ at 20°C / 1 atm	"ppm" = ppm_v	
water	$\frac{g}{m^3}$		"ppm" = ppm_w

Let the (absolute) temperature and the (absolute) pressure measured in the cuvette be T and P. Compensation of the measured ozone density [g/m³] in the cuvette now is made by multiplying with T/T_0 and P_0/P. The compensated ozone density usually is displayed in g/Nm³ (grams per "Normal" cubic meter). This quantity now is a specific property of the ozone gas which does not change with temperature and pressure:

$$[g/Nm^3] = [g/m^3] \cdot \frac{T}{T_0} \cdot \frac{P_0}{P} = [g/m^3] \cdot \frac{P_0}{T_0} \cdot \frac{T}{P} \qquad (1)$$

3. ppm_v for low ozone content

The (compensated) density of pure ozone is 2,143.93 g/Nm³. The volume occupied by one gram of ozone at standard conditions (0ºC / 1 atm) thus is 1 : 2,143.93 = 0.00046643 Nm³/g or 466.43 ppm of one cubic meter.

The dimensions g/Nm³ and ppm_v are proportional to each other:

$$466.43\ ppm_v \triangleq 1\ g/Nm^3 \qquad (2)$$

Attention:

The ozone "concentrations" [ppm_v] and [g/Nm³] are the only two which are proportional to each other. All other "concentrations" are related non-linear, refer to our TechNote TN-1.

Instead of ppm_v (parts per million, volume by volume) the same ozone content could be expressed in %Vol. (percent volume by volume):

$$0.046643\ \%\text{Vol.} \triangleq 1\ \text{g/Nm}^3$$

But this is quite unusual in ozone technology.

4. **%wt/wt** ideal, but be cautious!

To calculate the ratio "mass of ozone/mass of ozone gas" two (compensated) densities have to be known: The density of the ozone, and the density of the "rest" (the ozone carrier gas, or feed gas). Let ρ_O (g/Nm³) be the density of the ozone, and ρ_R (g/Nm³) be the density of the "rest". Now the "concentration" [%wt/wt] can be calculated from the "concentration" [g/Nm³]:

$$[\%wt/wt] = \frac{100 \quad [g/Nm^3]}{[g/Nm^3] - \dfrac{\rho_R}{\rho_O}[g/Nm^3] + \rho_R} \qquad (3)$$

Density of ozone is very well known:
ρ_O = 2,143.93 g/Nm³ (ozone)

Density of oxygen is also well known:
ρ_R = 1,428.96 g/Nm³ (oygen)

Density of dry atmospheric air is about:

$\rho_R \cong$ 1,293.0 g/Nm³ (ambient air)

PSA (oxygen concentration by Pressure Swing Adsorption) removes most of the water vapour and part of the nitrogen from the ambient air. If (theoretically) nitrogen would be removed completely, oxygen content would rise to about 95.6 %Vol.. Practically PSA can reach an oxygen content between 90 and 93 %Vol.. The residual gas is not only nitrogen (molecular weight 28) but also contains other gases, namely argon (molecular weight 40) and carbon dioxide (molecular weight 44). The result is that at about 90 %Vol. the density of the oxygen plus the residual gas (the density of the "PSA oxygen") is exactly like the density of pure oxygen. At 93 %Vol. the density is 0.7 % higher, and at 85 %Vol. it is 0.4 % lower than that of oxygen. Thus it is recommended that for PSA the density ρ_R is set to the density of oxygen:

Density of "PSA oxygen" approx. is:

$\rho_R \cong$ 1,428.96 g/Nm³ (like pure oxygen)

Attention:

The ozone "concentration" [%wt/wt] is the only one which needs information about the density of the "rest". The ozone analyser must be programmed with this density to be able to calculate the [%wt/wt]. If e.g. the density of the "rest" has been programmed for oxygen, but actually is air, the "concentration" [%wt/wt] will be calculated too low (the displayed value is about 10 % lower than the actual value).

In a situtation in which the density of the "rest" is not known, or is in question, the "concentration" [%wt/wt] should not be used!

But [%wt/wt] is ideal for calculating the ozone mass flow rate produced by an ozone generator (the generator's ozone production) if the flow of the feed gas into the generator is measured with a thermal mass flow meter which measures the mass flow rate of the feed gas. The ozone mass flow rate now is calculated by simply multiplying the [%wt/wt] with the mass flow rate of the feed gas (in mass per unit of time).

Attention: Concerning the non-linear relationship between g/Nm³ and %wt/wt refer to our TechNote TN-1.

5. **ppm_v, g/m³** ambient ozone

Ozone content in the ambient air - outside or inside - usually is very low. Ambient ozone measurement is trace analysis. The most commonly used dimension is "ppm" (at the International Standard Conditions: 0°C / 1 atm). Actually it is ppm_v. The dimension "ppm" is not correct [1)].

In the European Community another dimension is used: "mg/m³" at 20°C and 1 atm. The non-standard temperature of 20°C has an advantage in this special case because the relationship between both dimensions now becomes 1 $ppm_v \triangleq$ 1.9976 mg/m³ (20°C / 1 atm), or practically (error only 0.12 %)

1 $ppm_v \cong$ 2 mg/m³ (20°C / 1 atm)

or 1 "ppm" $\cong$ 2 "mg/m³"

6. **ppm_w, g/m³** ozone in water

The density of water is 1000 kg/m³ at 0°C. Density practically does not decrease with increasing temperature: At 90°C e.g. the density of water is only 0.3 % lower than at 0°C. This is the reason why the ozone content in water may be indicated in g/m³ or in ppm_w as well. Example: One gram of ozone in one cubic meter (1 g/m³) means the same as one gram of ozone in one million grams of water (1 ppm_w). The dimension "ppm" is not correct [*)].

*) The molecular weight of ozone is about 50% higher than that of oxygen, and it is about 66% higher than the average molecular weight of air. Thus in ozone applications ppm_v and ppm_w are quite different. The dimensions "ppm" actually mean ppm_v for ambient ozone, and mean ppm_w for ozone in water. To only use "ppm" includes a "mental reservation". But mental reservations have no place in science.