INFICON

TECHNICAL NOTE

Calculating Partial Pressures

Residual Gas Analyzers (RGAs) have been used in vacuum research applications for 25 years. Their role has changed in the last 10 years, as they have evolved from purely a research instrument to a production tool. As a production tool, the RGA can increase productivity, improve product yield, increase throughput and reduce costs, all of which ultimately increases profits.

However, it is up to the user to determine how the tool can best meet the needs of a specific application. This Tech Note is concerned with defining and calculating partial pressures.

HOW DOES AN RGA WORK?

A residual gas analyzer measures the individual partial pressures of gases in a mixture. The RGA system includes a sensor, which operates under high vacuum, the electronics, which operate the sensor, and software, working in conjunction with an external computer to display data and control the electronics.

The RGA sensor consists of three parts:

Ion source: The ion source contains a heated filament that emits electrons. These electrons collide with gas molecules in the vacuum system, giving them an electrical charge, which produces ions:

1. A single electron removed from the molecule produces a parent molecular ion.

2. Multiple charged ions can be formed when sufficient energy of the incident electron releases more than one electron from the molecule or atom.

3. The incident electron has sufficient energy to break chemical bonds and remove an electron(s) forming fragment ions.

Quadrupole Mass Filter: Ions produced in the ion source move into the quadrupole mass filter to be separated according to their mass-to-charge ratio.

Ion Detector: Ions that have been transmitted through the quadrupole mass filter strike the detector, become neutralized, and draw a current that is proportional to and identifies the gas component present.

The RGA electronics module, which incorporates a "smart sensor" design, interprets the output of the sensor for display with the system software and an external computer. This system software is used for process monitoring, statistical process control, and maintenance procedures like mass calibration.

WHAT IS PARTIAL PRESSURE?

RGA instruments can be used to characterize the gas mixture found in a vacuum environment. "Partial pressure" is the absolute pressure measurement for a particular component of this mixture. The sum of all the partial pressures will yield the total pressure for the system. The RGA is designed such that the displayed peak height is proportional to the partial pressure of the substance generating the peak.

HOW IS PARTIAL PRESSURE CALCULATED?

The following will generate the equation for calculating partial pressure and will explain and define the parameters used to get to this equation.

This equation shows the relationship between partial pressure as determined by measuring ion current:

$$PP_A = (MF_{AB} \times A_B) \times I_{AB}$$

Where: PP_A = the partial pressure of substance "A", measured in Torr

MF_{AB} = the material factor for a particular substance

A_B = the analyzer factor

I_{AB} = the ion current at mass peak "B" resulting from substance "A", measured in amps

The material factor MF_{AB} depends on the fragmentation pattern for the particular substance and a reference gas (which is the fraction of total ions from substance "A" having mass "B" and is designated by FF_{AB}) and the ease by which the substance can be ionized relative to a reference gas at the same partial pressure (called the ionization probability and designated by XF_A). This relationship is expressed by:

$$MF_{AB} = FF_{N28} / (FF_{AB} \times XF_A)$$

where FF_{N28} is the fractional abundance of mass 28 ions from the reference gas N_2. Material factors for many gases are calculated and stored as "Material Factors" for use in the Selected Peaks monitoring mode of TranspectorWare and TWare 32™.

Note that fragmentation factors will vary depending on the ionizer, electron energy, and mass calibration tuning and for the best accuracy should be measured with the same instrument under like conditions. Ionization probability factors can be estimated by substituting the relative ion gauge sensitivity for a particular gas. These factors can also be measured by comparing the measured value of a hot cathode ion gauge to a known pressure.

The analyzer factor A_B depends on several factors, namely:

$$A_B = 1/ (TF_B \times DF_{AB} \times G \times S) \text{ where}$$

TF_B is the transmission factor of the quadrupole at mass "B". This is the fraction of ions at mass "B" which pass through the quadrupole, relative to nitrogen ions at mass 28. TF = (28/M) nominal.

DF_{AB} is the detection factor. This is equal to 1 for a Faraday Cup detector. For an Electron Multiplier, DF is a function of the mass of the ion and its chemical nature, measured relative to that of a reference gas (usually nitrogen). In general, as the ion mass increases, the EM detection factor will decrease. TWare 32 uses a $DF_{AB} = (28/M)^{0.3}$.

G is the gain of the Electron Multiplier and is measured as a ratio of the EM output current divided by the FC mode output current. The gain G varies depending on the operating voltage and the condition of the EM. For the FC mode, G = 1.

S is the instrument sensitivity and is measured from the FC mode ion current from a given pressure of pure nitrogen at mass 28, measured in amps/Torr. For an electron multiplier, S varies depending on the operating voltage and condition of the multiplier.

The analyzer factor A_B depends on parameters of the analysis recipe and the analyzer such that TranspectorWare or TWare 32 can calculate A_B internally and use it with the Material Factor for the gas species identified in the Selected Peaks mode to display partial pressure directly.

USER CALCULATIONS FROM RAW DATA

Given the above definitions, the final partial pressure equation of substance "A" indicated by the amplitude (I) of signal at mass "B" is expressed by:

$$PP_A = \{FF_{N28} / (FF_{AB} \times XF_{AB} \times TF_B \times DF_{AB} \times G \times S)\} \times I_{AB}$$

The constants in this equation can be obtained from tables or measured for a particular instrument. Following is a table of factors for some common gases. More factors and constants can be found in the Transpector Operating Manual or other reference materials.

Substance	FF Fragmentation Factor	XF Ionization Probability	MF Material Factor
Argon Ar 40 20	.83 .17	1.2	1.00
Carbon Dioxide CO_2 44 28 16 12	.70 .11 .06 .01	1.4	1.02
Helium He 4	1.00	0.14	7.14
Hydrogen H_2 2	1.00	0.44	2.27
Krypton Kr 84 86 82 83	.45 .13 .10 .10	1.7	1.31
Nitrogen N_2 28 14 29	.93 .06 .01	1.0	1.08
Oxygen O_2 32 16	.95 .05	1.0	1.05
Water H_2O 18 17 1 16	.75 .19 .05 .02	1.0	1.33

Examples can be calculated using these factors and formulas.

EXAMPLE 1

A Nitrogen equivalent vacuum gauge reads a pressure of 2.5E-5 Torr and the residual gas analysis system measures a value of 5E-9 amps for Nitrogen and 7.3E-11 amps for water in Faraday cup (FC) mode. What is the partial pressure of water, in Torr?

Starting with the previously derived equation for partial pressure:

$$PP_A = \{FF_{N28} / (FF_{AB} \times XF_{AB} \times TF_B \times DF_{AB} \times G \times S)\} \times I_{AB}$$

The values of the constants are shown to be:

FF_{N28} = **1.00** as shown in the table for Nitrogen

FF_{AB} = **0.75** as shown in the table for water at mass 18

XF_{AB} = **1.00** as shown in the table for water

TF_B = 28/M = 28/18 = **1.56** for water at mass 18

DF_{AB} = **1.00** for Faraday cup detectors

G = **1.00** for Faraday cup detectors

S = 5E-9 amps / 2.5E-5 Torr = **2E-4 amps / Torr**

I_{AB} = **7.3E-11 amps** as stated in the example

Therefore,

PP H_2O = {1.00 / (0.75 x 1.00 x 1.56 x 1.00 x 1.00 x 2E-4 amps / Torr)} x 7.3E-11 amps

PP H_2O = 3.12E-7 Torr

EXAMPLE 2

Using the same system from Example 1 and assuming the same sensitivity, the residual gas analysis system measures a value of 5E-7 amps for Nitrogen and 5.4E-9 amps for oxygen in Electron Multiplier (EM) mode. What is the partial pressure of oxygen, in Torr?

Again, starting with the previously derived equation for partial pressure:

$$PP_A = \{FF_{N28} / (FF_{AB} \times XF_{AB} \times TF_B \times DF_{AB} \times G \times S)\} \times I_{AB}$$

The values of the constants are shown to be:

FF_{N28} = **1.00** as shown in the table above for Nitrogen

FF_{AB} = **0.95** as shown in the table above for oxygen at mass 32

XF_{AB} = **1.00** as shown in the table above for oxygen

TF_B = 28/M = 28/32 = **0.875** for oxygen at mass 32

DF_{AB} = $(28/M)^{0.3}$ assume to be **1.00** = $(28/32)^{0.3}$ = **0.96**

G = 5E-7 amps / 5E-9 amps (FC ion current from Example 1) = **100**

S = **2E-4 amps / Torr** as determined from Example 1

I_{AB} = **5.4E-9 amps** as stated in the example

Therefore,

$PP\ O_2$ = {1.00 / (0.95 x 1.00 x 0.875 x 0.96 x 100 x 2E-4 amps / Torr)} x 5.4E-9 amps

$PP\ O_2$ = 3.38E-7 Torr

As shown above, the quantitative characteristics of the residual gas analysis system can be used to calculate the partial pressure of a particular component in a gas mixture. This information can be used for accurate process monitoring, useful process control, and guides the user in maximizing RGA equipment potential.

[1] "Mass-Dependent Effects of Channel Electron Multipliers in Residual Gas Analyzers", Journal of Vacuum Science and Technology A 5 (4), Reagan/Frees.

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