

New Folder Name Vacuum System Model

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In response to your telephoned question the other day on the AMU values we listed in the suggested Qualification Test Data Format: we're looking for hydrogen, water, carbon monoxide, nitrogen, oxygen, carbon dioxide, methane, argon, and hydrocarbons (by their fractionation products). This is a good first guess based on our prior experience. By reprogramming, you will be able to allow other AMU values to be measured continuously.

Rai will use these AMU values to solve simultaneous equations for the residual gases. I've attached a copy of a document that explains the strategy. This document is for your interest only, and is not to be construed as direction.

Larry

Appendix 4

Vacuum System Model Gas Solutions and RGA Spectra

The residual gas analyser spectrum of uncalibrated partial pressure (counts at the output of the instrument when set at a particular amu value) can be used to solve for a system gas model providing one has some crude knowledge of the way a particular gas species breaks up between the different amu values in the instrument. The technique described here will always give a solution for the gas model in terms of the relative amounts of each gas in the model that is represented in the residual gas spectrum. The absolute value of a single specie must still be established by calibration. The gas solution is, of course, no better than the model. If a particular gas component exists in the system which has been left out of the model, it may cause the model to be in error. The severity of the error depends on the partial pressure and, especially, on how the unmodeled gas breaks up into different amu values in the instrument. A quick glance at the raw amu data will always show if there is a serious problem. A χ^2 test of the model relative to the amu data (providing the true measurement uncertainties at each amu value are known) shows if there are more subtle problems. The method has been used in the beamtube demonstration project and the results have been given in "RGA air signature analysis" R. Weiss July 11, 1992. The program to carry out that analysis is called `rgaspec.f`

The basis of the method is described by a standard χ^2 minimization. Call the measured count rate at the amu value j AMU_j and the variance in the measurement σ_j . There are m different amu values measured. This is the data.

The model consists of n gas species with unknown count rates. The count rate for the k th gas is designated as gas_k . The model count rate for the j th amu value is designated as amu_j . The model predicts a count rate for j th amu value as

$$amu_j = \sum_{k=1}^n \alpha_{j,k} gas_k$$

The $\alpha_{j,k}$, the partition fraction, of the gas k appearing at amu number j is always made to satisfy the sum rule

$$\sum_{j=1}^m \alpha_{j,k} = 1$$

providing that all the amu values into which the gas breaks up are indeed in the data set (clearly not true for heavy hydrocarbons). The initial values for the $\alpha_{j,k}$ are assumed to be those published in the mass spectrometry literature. Usually the absolute values of the sensitivity for the count rate associated with the gas k when summed over all the $\alpha_{j,k}$ is not known only their relative values. The absolute values require knowledge of the ionization cross section, electron current density in the ionizer and the ion extraction efficiency. These can never be calculated well enough so that, the absolute value for the count rate requires calibration. This ignorance is, however, not an impediment in solving the model for the existence of a particular gas specie, it becomes important when one wants to know the actual value of how much of that gas there is in the system.

The χ^2 for the model/data set is

$$\chi^2 = \frac{\sum_{j=1}^m (AMU_j - amu_j)^2 / \sigma_j^2}{\sum_{j=1}^m 1/\sigma_j^2}$$

The gas solution comes out of the minimization of the χ^2 while varying the values of gas_k . This results in a set of m simultaneous equations for the best values of gas_k and the correlation and error matrices of the model fit to the data. One designs the measurement to have more amu values than gases to keep some degrees of freedom in the χ^2 . Under these conditions the absolute value of the χ^2 has significance and indicates the statistical worth of the result.

In the tests of this procedure in the beamtube demonstration project I found that the published values of the $\alpha_{j,k}$ were often not correct for the specific rga and its state of tuning. The χ^2 and the degree of diagonalization of the correlation matrix could be much improved by allowing the $\alpha_{j,k}$ to vary subject to the sum rule given above. This was incorporated into the modeling program and the consistency of the $\alpha_{j,k}$ from run to run became another measure of the validity of the model.

In the beamtube demonstration project, the data was taken at amu: 2, 12, 14, 15, 18, 28, 32, 40 and 44 and the gases in the model were: H₂, CO, CO₂, CH₄, H₂O, N₂, O₂, and A. The concept was to separate N₂, O₂ and A from the rest as an air signature. It turned out that Oxygen is scavenged by the steel surface and has little value in determining an air signature. The burden fell on nitrogen and the separation of N₂ from CO at amu 28 and N from CH₂ (derived from CH₄) at amu 14. Even with the limited number of amu values used, it was possible to separate CO from N₂ to about 1% of the CO. The partial pressure of N₂ measured was $2 \times 10^{-13} \pm 1 \times 10^{-14}$ torr. The most serious problem was CH₄ for which data at amu 13 and 16 would have been useful. The argon signature was clear in the beam tube demonstration after the bake. Before the bake it was confused by hydrocarbon fractions at amu 40. There are two strikes against using Argon in the beamtube module leak assay; first, it is only 0.93% in the atmosphere by number density and second, it is both a shield and torch gas in the welding. There is bound to be an anomalously large amount of Argon in the beam tube modules.

The programs that carryout the model fits run in less than a 1/4 of a minute on the Sun workstations, the time for solution varies as the square of the number of amu values. The proposed number of amu values for the beamtube leak assay is approximately 50 so with current minicomputers it will take about 6 minutes to get a gas solution.

An alternative to the gas model fitting procedure is to use residual gas analysers with sufficient mass resolution to distinguish gases falling on the same quantized amu value by their nuclear mass defect. CO and N₂ are then directly separable. Boude Moore has been a champion for a commercial cyclotron resonance residual gas analyser with this capability. I know little about the reliability, dynamic range and ultimate sensitivity of these instruments.