Simultaneous monitoring of greenhouse gasses with FT/IR

Introduction

Among gases that affect the global environment, gases that are stable, such as carbon dioxide, methane, halogenated carbon compounds, have a considerable impact on global warming and are termed ‘greenhouse gases’.

On the other hand, nitrogen compounds, sulfur compounds and volatile oxygenated carbon (VOC) gases are quite reactive and thus regarded as air pollution gases that can cause photochemical oxidation, smog and the worsening of indoor environments. Many gases used in the manufacturing processes of semiconductors are also harmful and the strict control and monitoring of these gases are required. It is important to monitor the different classes of gases with appropriate systems to study the impact on the atmospheric environment. One of the features of a newly developed program dedicated for IR gas analysis system is to be able to analyze similar multi-component compounds simultaneously by using a calculation of subtracted spectra. In addition, the Time Course Measurement software makes it possible to perform continuous monitoring of these noxious gases.

Features of the continuous quantitative analysis program for multiple components are:

- Simultaneous quantitative analysis of up to 50 components
- Continuous measurements up to 40 days at a time
- Replaceable calibration curve on an ‘as-needed’ basis
- Open-Path measurement capability

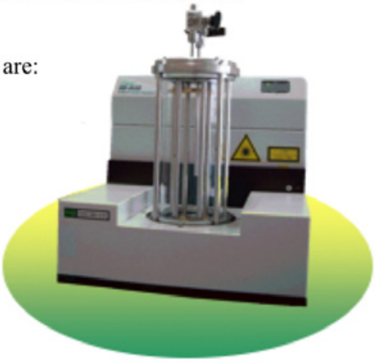

Figure 1: VIR-9500 & 8 m gas cell

Instruments

This program can be used with the VIR-9500 series as well as the FT/IR-4000/6000 series instruments.

The VIR series instruments allows sample monitoring for a wide range of purposes such as outdoor or clean room applications because it can be easily moved and installed due to a small and portable size.

Full vacuum FT/IR systems can provide quantitative analysis of carbon dioxide and water vapor in air with a high degree of accuracy. The gas cells in a length from 10 cm to 20 meters are available and a suitable cell can be selected depending upon the desired analytical gas concentrations.

Measurement example 1

Standard spectra of several perfluorocarbon compounds (PFC), which are targeted as greenhouse gases, are shown as Figure 2. The absorptions in the infrared spectra are observed in a very narrow wavenumber range due to similar chemical structures. Of particular interest is the perfluoromethane compound, with an absorption peak at 1280 cm^{-1}, which overlaps an absorption peak of perfluoropentane. In cases like these, it is difficult to set a single quantitative peak for reliable analysis. For example, when the 5 different gases outlined in Figure 2 are quantified, the quantitative accuracy can be improved by estimating each gas concentration in order from No. 1 to No. 5 as shown in the figure and subtracting a calculated spectrum for each component based on the estimated concentration in series from the measured spectrum. A single analytical peak can be set by the quantitative analysis program at the specific position highlighted by an arrow in the figure, according to the number, which enables quantitative analysis of the perfluoromethane concentration. Quantitative analysis by multivariate statistical technique is possible even in cases where there is no single analyte peak. However, this may not be practical because many mixture samples with known concentrations have to be prepared and the quantitative accuracy may suffer at low concentrations.

By contrast, spectra of hydrofluorocarbons (HFC) have more analyte peaks than spectra of PFC compounds. Therefore, a continuous measurement program for multiple components using a subtracted spectrum can be more effective. It should be noted that conventional methods for quantitative analysis of multiple gases can be difficult and the outlined approach may have more success in these cases.

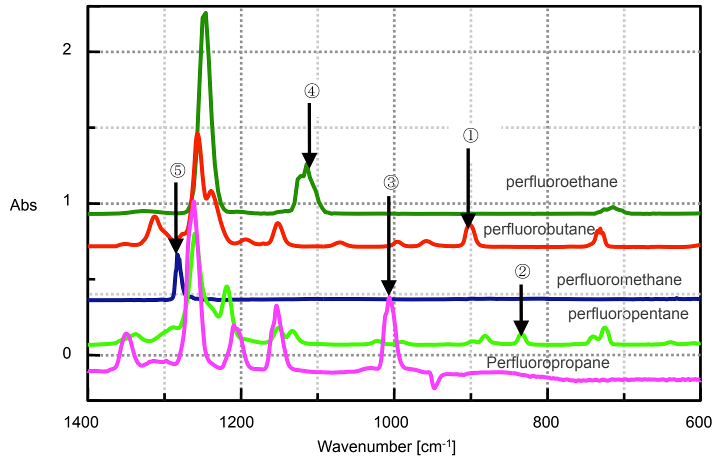

Figure 2: Standard spectra of perfluorocarbon compounds (PFC)

Measurement example 2

Figure 3 outlines spectra of formaldehyde, acetaldehyde, toluene and acetic acid, provided as an example of a measurement example for ‘sick building’ syndrome or simple air pollution. In these gases, the absorption wavelengths for formaldehyde and acetaldehyde overlap each other and the analytical peaks of formaldehyde are hidden behind the broad absorption band for acetaldehyde. In this example, the concentration for the acetic acid (No. 1) is estimated by using the peak at 1290 cm^{-1}. After subtracting the amount of the acetic acid, the acetaldehyde (No. 2) is calculated by using the 1110 cm^{-1} peak. Finally, the ‘hidden’ peak for formaldehyde is determined by using the peak at 1745 cm^{-1}.

For these complicated quantitative determinations, if the order of the components is set in advance, all components can be calculated automatically and simultaneously. The use of the ‘Time Course Measurement’ program makes it possible to perform continuous monitoring and concentration calculations.

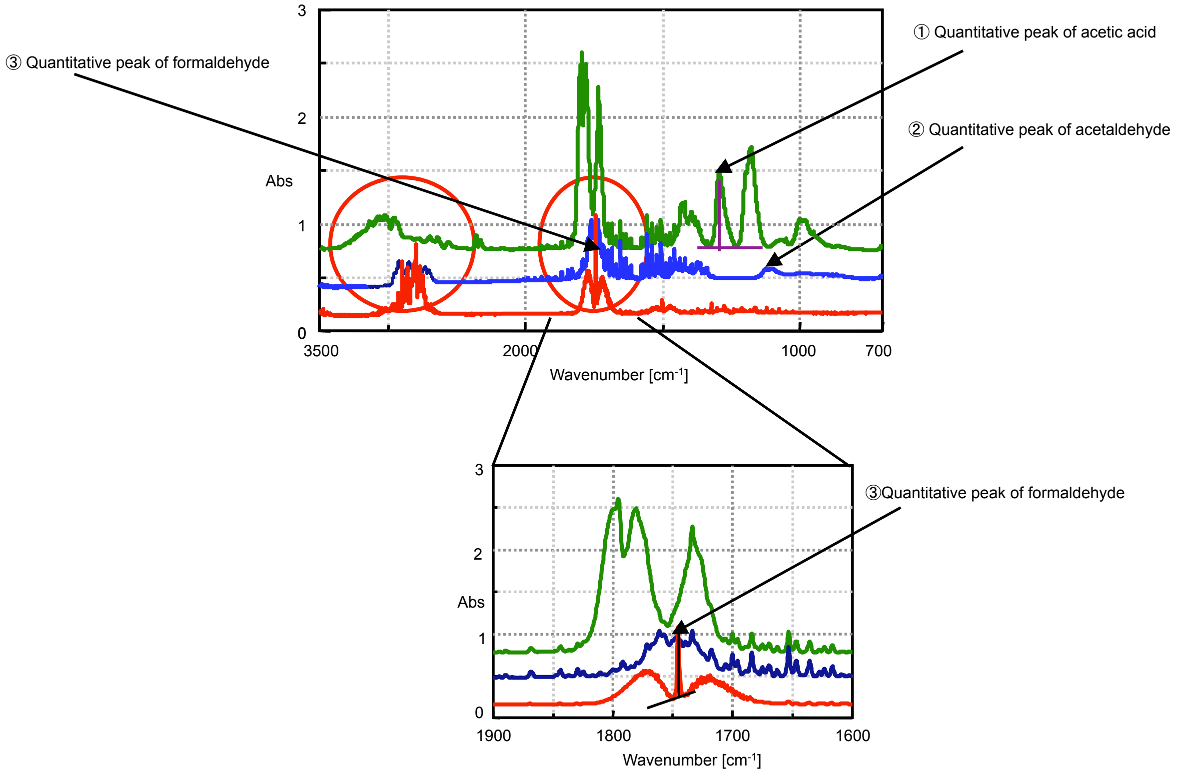

Figure 3: Standard spectra of air pollution gases