Application Note

230-QU-0175

Simultaneous Monitoring Analysis of Multicomponent Gas in the Atmosphere using CLS Automatic Quantitation

<Introduction>

Quantitation method with one wavenumber is a quantitation using height and area of one peak. CLS (Classical Least Square) quantitation is one of the multivariate analyses and calculates quantitatively using all spectral data in the varying area depending on concentration. Therefore, it is an efficient quantitation method in case that it is difficult to find a single peak for quantitation because of overlaid spectra of multicomponent, and simultaneous quantitation of multicomponent is required. One of the advantages of CLS quantitation is high accuracy by noise averaging from calculation using all spectral data in the specified spectral range. The analyses of pure compound (spectrum) obtained in least squares are easy, and this spectrum is similar to pure spectrum of multicomponent. Since it is possible to analyze multicomponent simultaneously, utilization as simultaneous monitoring of multicomponent can be done by use of automatic quantitation program.

<Measurement>

The averaged concentrations of 5 components of gases (CH_4, N_2O, CO, CO_2 and H_2O) in the atmosphere were repetitively monitored using OPEN-PATH FT-IR with optical path length 100 m. Figure 1 shows the quantitative results obtained according to CLS calibration curves model prepared in advance, for specified periods (5 min) for each component, which are shown as time-course curves. The concentration change by time-course is shown.

<Condition>

Accumulation:	200
Resolution:	1 cm^{-1}
Apodization:	Cosine
Optical path length:	100 m (OPEN-PATH FT-IR)
Standard gas cell:	3 m (calibration model)

Figure 1. CLS automatic measurement monitor screen

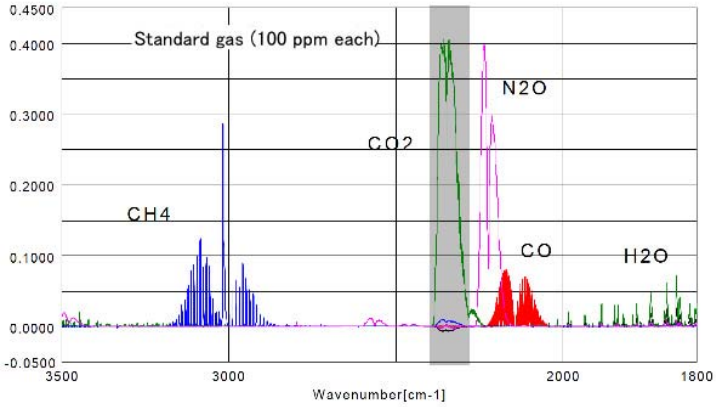

Figure 2. Standard gas (utilizing 3 m cell)

Figure 2 shows measurement result of each standard gas with concentration 100 ppm by standard gas cell (3 m cell). Absorption spectra of gases of CO, CO_2 and N_2O are overlapped. Regarding detection limit, since the concentration 100 ppm of N_2O gas corresponds to absorbance 0.400, indicating that concentration 1 ppm, to 0.004 ABS, quantitation with concentration less than 1 ppm is considerd to be possible.

Figure 3 and 4 show the calibration models (CH_4 and CO gas) measured by standard gas cell (3 m cell). The curves indicates good linearity in the range of 1-120 ppm. The correlation coefficient is more than 0.98. The calibration models of CO_2, N_2O and H_2O gas have been also created even if Figure is not shown. The optical path difference is corrected automatically in the measurement utilizing [OPEN-PATH FT-IR].

JASCO INTERNATIONAL CO., LTD

4-21, Sennin-cho 2-chome, Hachioji, Tokyo 193-0835, Japan
Tel: +81-42-666-1322, Fax: +81-42-665-6512

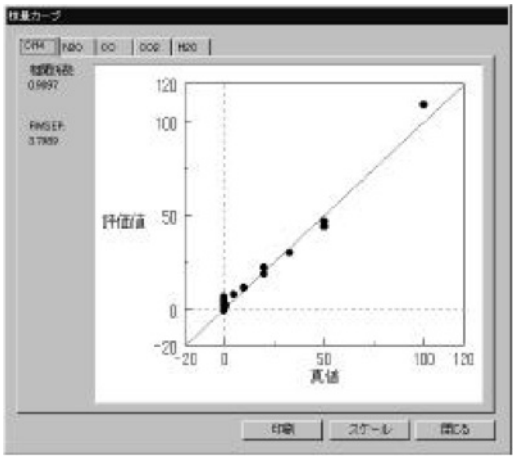

Figure 3. Calibration model: CH_4

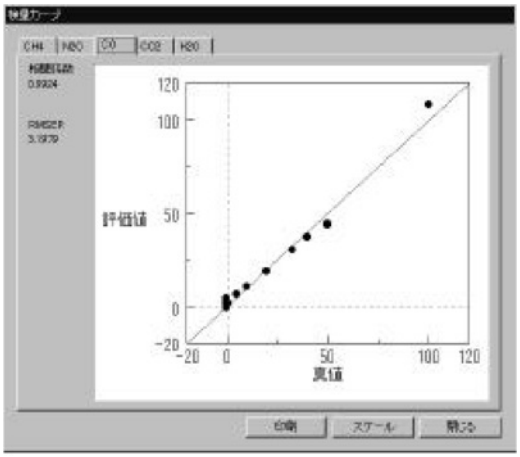

Figure 4. Calibration model: CO

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