Instrument and Software Development for DOAS Measurements of Atmospheric Constituents

A contribution to subproject TOPAS

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A grating spectrograph with a photodiode array as detector has been adapted to perform tropospheric measurements by Differential Absorption Optical Spectroscopy (DOAS), using an optical long path coupled with a Fourier transform spectrometer [1].

The spectrograph is a 1/8 m crossed Czerny-Turner from Oriel (type Multispec) with a F number of 3.7. This instrument has a flat focal field adequate for use with photodiode arrays (PDA) up to 25 mm long. Several entrance slits from 25 to 200 μ width are available. Different gratings can be selected according to the required spectral resolution and the wavelength range of interest. The resolution for a PDA spectrograph is defined over two pixels of the detector. Typically, for this spectrograph, a resolution of 0.4 nm can be reached with a grating of 1200 grooves/mm, an entrance slit of 25 μm and a 1024 elements PDA. In that case, the wavelength range is of the order of 200 nm, between 180 nm and 1300 nm, the interval depending on the blaze angle of the grating. The combination of an entrance slit of 100 μm with a grating with 600 grooves/mm and a 1024 pixel PDA provides a measured Full Width at Half Maximum (FWHM) of 1.2 nm between 270 and 600 nm. In that case, the sampling defined by the size of the pixel (25 μm) and the spatial resolution corresponding to the FWHM is 4. The detector is a Reticon PDA of 1024 pixels which can be cooled down to $-50°C$ by means of a two stage Peltier. This temperature is reached by running methanol at $-5°C$ in a cooling circuit connected to a minicryostat. The detector characteristics are given in Table 1. The read-out electronics made by Princeton Instrument Inc. (PI) provides a dynamic range of 16 bits. The detector head is integrated in a vacuum tight container evacuated by a small pump. The grating position is controlled by a stepping motor having an angular resolution of 16 arcsec per step. Filters can be placed in front of the entrance slit in order to exclude second order overlap. The filter wheel has a closed position used to measure the dark count corresponding to the measurement integration time.

The instrument includes a compatible IBM 386 AT computer, the ST-1000 detector controller and the spectrograph. The detector controller (ST-1000) provides power, thermostating and timing signals to the detector head, coordinates data gathering with the experiment, sets exposure time, digitizes and averages data and transmits it to the computer. For a rapid DMA (Direct Memory Access) transfer, the ST-1000 has free access to the AT's 16 bits bus providing a large dynamic range from 0 to 65536 counts. The data bus is used bidirectionally by the computer to send control information bytes to the ST-1000 and to receive raw data back.

An AT software package named OSMA (Optical Spectrometric Multichannel Analyzer) is provided with the ST-1000 to control the detector and to perform the

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Table 1. Technical specifications of the PDA detector

Number of pixels	1024 pixels
Pixel dimensions	25 μm $\times$ 2.5 mm
Dynamic range	16 bits
Thermoelectric cooling	$T_D \geq -50°$
Quatum efficiency at 700 nm	~ 70°
300 nm	~ 40°
Readout noise	1 count rms
Sensitivity	1 count = 1300 e^-
Dark charge	10 counts/pixels/sec (at −35°C)
Leakage current	3 counts/pixels/sec (at −50°C)
Well depth	7.5×10^7 e^-

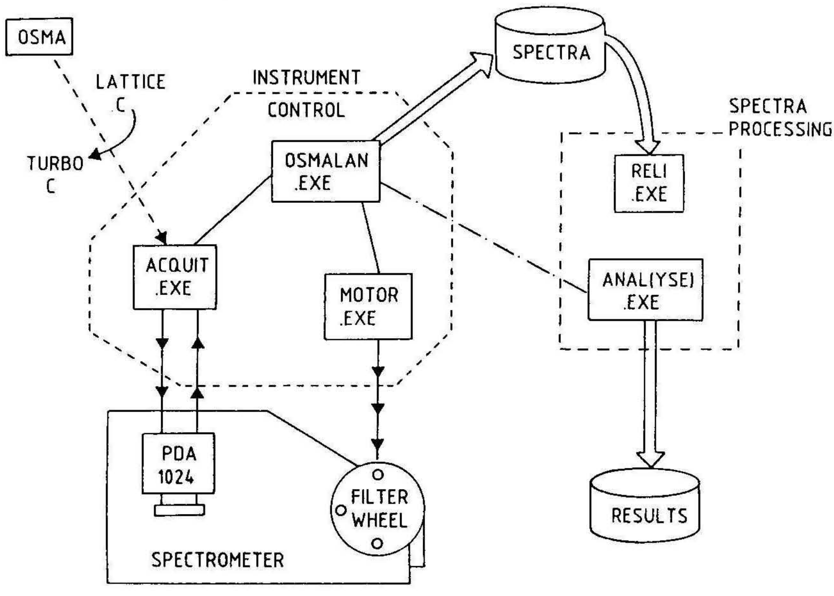

Figure 1. Block diagram showing the organisation of the programmes developed for the automation of a PDA spectrograph.

data acquisition. It also allows real-time viewing of data as it is collected, or replaying stored or modified data. It is possible to obtain multiple graphs in a window in order to display simultaneously real-time data and previously stored data and to zoom on certain features of a spectrum while displaying a time history of another spectrum. All the ST-1000 software is written in C and 8086 assembler utilizing Lattice C Compiler and Microsoft Macro Assembler.

Because the instrument cannot be automated with OSMA, a new software has been written. The main objectives were to take successive spectra with the filter wheel at different positions and with exposure times and numbers of scans computed according to the current signal intensity, and to save the data in a given format.

All the ST-1000 control and spectrum acquisition procedures have hence been

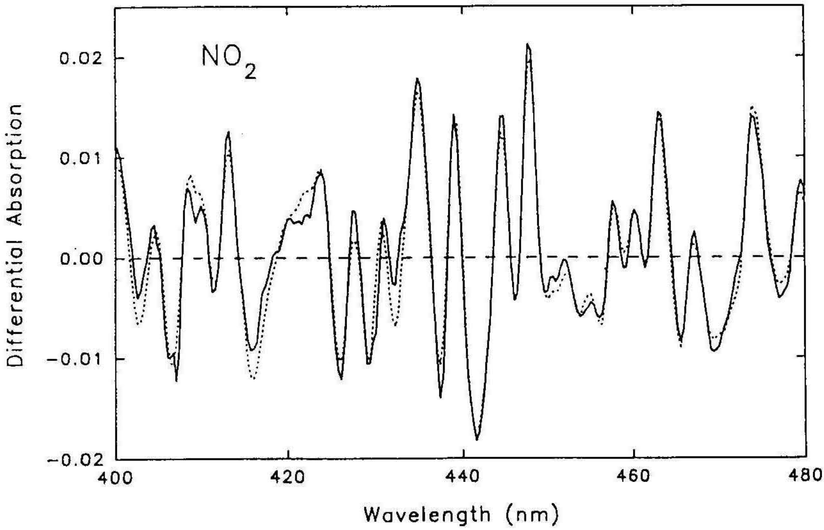

Figure 2. Comparison of the experimental (—) and calculated (····) optical thickness in the 400–480 nm interval where NO_2 is the main absorber.

extracted from the original programme source to be afterwards integrated in a larger programme including not only the experiment automation but also the spectra analysis. Both have been developed in C language.

The principle of measurements is based on the DOAS method. The sun is the present light source in use. In order to eliminate Fraunhofer absorption lines, the raw spectrum is first divided by a reference spectrum obtained with small zenith angle. After wavelength alignment, the resultant ratio spectrum contains only atmospheric absorption features. After transformation into a differential spectrum, the atmospheric concentration is obtained by fitting the differential optical thickness calculated with the absorption cross-sections of atmospheric molecules obtained from the scientific literature or measured in the laboratory, with the observed differential optical thickness. An artificial light source will be utilized for long path measurements in the troposphere.

The experiment automation block diagram is presented in Fig. 1. The complete automation programme has been successfully tested over a period of time of ten days. In addition, some atmospheric observations of NO_2 and ozone have been performed in Brussels for algorithm development and testing (Fig. 2).

This instrument will participate in the intercomparison campaign for DOAS instruments planned for September 1992, in the frame of the subproject TOPAS.

Acknowledgements

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References

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