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by

C. MULLER and J. LAURENT

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3 - Ringlaan
B - 1180 BRUSSEL

FOREWORD

This text will be published in the "Bulletin de la Classe des Sciences de l'Académie Royale de Belgique".

AVANT-PROPOS

Ce texte sera publié dans le "Bulletin de la Classe des Sciences de l'Académie Royale de Belgique".

VOORWOORD

Deze tekst zal in de "Bulletin de la Classe des Sciences de l'Académie Royale de Belgique" verschijnen.

VORWORT

Dieser Text wird in "Bulletin de la Classe des Sciences de l'Académie Royale de Belgique" herausgegeben werden.

SCIENTIFIC PROGRAMS FOR THE SPACELAB ES013 GRILLE SPECTROMETER

by

C. MULLER and J. LAURENT*

Abstract

The ES013 infrared spectrometer, jointly built by ONERA (France) and IASB (Belgium), will perform, late 1983, earth limb observations, in absorption, during sunrise or sunset, and in emission from the "Spacelab" space station. The organization of spectral intervals and observation programs is presented as well as the reasons for the choices made for the first flight.

Résumé

Le spectromètre infrarouge ES013, construit conjointement par l'ONERA (France) et l'IASB (Belgique), effectuera en 1983, des observations du limbe terrestre en absorption au coucher ou au lever du soleil, ainsi qu'en émission à partir du véhicule spatial "Spacelab". L'organisation des intervalles spectraux et des programmes d'observation est présentée ainsi que les raisons des choix effectués pour le premier vol.

* O.N.E.R.A., Boîte Postale 72, F-92322 Châtillon, France.

Samenvatting

De infrarood spectrometer 1ES013, gebouwd in samenwerking tussen ONERA (Frankrijk) en het BIRA (België), zal eind 1983, vanaf het ruimteschip "Spacelab" de kim van de aarde waarnemen, in absorptie bij zonsopgang en ondergang en in emissie. De organisatie van de spectrale intervallen en de waarnemingsprogramma's voor de eerste vlucht worden hier voorgesteld benevens de redenen die aan de grondslag liggen voor deze keuze.

Zusammenfassung

In 1983, wird der ES013 infraroter Spektrometer, der durch ONERA (Frankreich) und IAS (Belgien) gebaut wurde, Beobachtungen des Erdenrandes in Absorption während Sonneaufgang und Sonne-untergang sowie in Emission von "Spacelab" machen. Die Organisation der spektralen Intervallen und der Beobachtungsprogrammen sowie die Gründe der Auswählen für dem ersten Flug sind vorgestellt.

The grille spectrometer, designed for the first Spacelab flight, scheduled for late 1983, is a medium resolution instrument (0.1 cm^{-1}) optimized for the observation of minor atmospheric constituents by limb sounding in the infrared (Besson et al, 1978). The principle of the grille spectrometer was first exposed by Girard (1963) and later this instrument, used on airborne and balloon platforms provided the first vertical distributions of NO and HCl in the stratosphere (Girard et al, 1973, Ackerman et al, 1973, Ackerman et al, 1976) as well as data on most of the stratospheric constituents. This instrument presents the advantage of assigning a defined time and altitude to each point of the observation, this property being very important when compared to interferometers (Park, 1982). It also allows much wider spectral scans than the newly developped heterodyne spectrometers. A complete description having already been given (Besson et al, 1978), only the scientific programming of the instrument will be discussed in this article.

A grating spectrometer scans a part of the spectrum, selected by choosing the grating angles for the beginning and the end and by selecting a diffraction order through an appropriate filter. In the mechanically driven instruments, these parameters are repeated all along the observation. In the Spacelab case, this procedure would have been highly impractical because of the short occultation times and the need for measuring a large number of atmospheric constituents in their optimal lines for an altitude range spanning 150 km. Moreover, because the instrument is successively operated in absorption, emission and calibration modes, an electronic drive of the instrument through a "dedicated experiment processor" (DEP) had to be designed. The complete system of control of the instrument through the DEP and the Spacelab computer is described by Lippens (1982).

The first programming step is the definition of "spectral windows", these are characterized by the limiting positions of the grating, by the code numbers of the optical filters to be placed in front of the In Sb detector (channel 1) and of the Hg Cd Te (channel 2) and finally by the gains on both channels. The gains range from 1 to 624 and are coded from 0 to 15 (Table 1). The filters are coded from 0 to 7 and the grating angles are represented by a resolver code which is the integer part of (6378 - γ) x 30.79 where γ is the grating angle expressed in hundredths of a degree. In the case where the result is negative, the two complement is taken (16 bits words). These conventions, representing the actual coding of the DEP will be used throughout this paper. The simultaneous use of two detectors permit the study of two wavelength regions in the same scan and also extends the spectral sensitivity of the instrument. The InSb detector, sensitive between 2.5 and 5 μm, will be used in addition to the Hg Cd Te, which is used from 2.5 to 10.5 μm but much less performant in the lower wavelength.

The program itself will be a sequence of windows. In the case of a sunset or sunrise, 12 successive altitude zones in which only two successive windows might be scanned are defined. The altitude is computed during the flight by the Spacelab computer and the transitions between zones are managed by the experiment processor. Figure 1 shows the limb sounding geometry, the referred altitudes are in fact the altitudes where the light rays are tangent to a surface parallel to the earth's surface. It has been shown that most of the absorption takes place in this zone for a mixed constituent. In addition to multiplying the optical path by about seventy compared to nadir, this permits a stable inversion of the data in terms of vertical distributions (Ackerman and Muller, 1973). The nominal flight altitude is 250 km and will be the upper limit of the first zone, the next ones are 200, 160, 120, 100, 80, 60, 50, 40, 30, 20 and 10 km. For the first flight, in order to minimize the mechanical operation of the filter wheel and of the fast grating drive, it has been decided to actually change spectral windows only at the transitions of 200, 100 and 50 km. Also, the option of scanning two successive windows in the same zone was avoided, although this procedure would be useful to study two relatively distant

TABLE 1 : Optical parameters of the instrument (wavenumber in cm^{-1})

Filter code	Channel 1	order	Channel 2	order
0	germanium		glass	
1	3663-3817	11	3663-3817	11
2	2910-3050	09	890-1080	03
3	2180-2420	07	2180-2420	07
4	2130-2170	06	2130-2170	06
5	1840-2015	06	1840-2015	06
6	glass		1530-1670	05
7	3921-4010	12	2910-3050	09

Grating : 580.6 lines/cm

Grating angles : 54 to 71 degrees

gain code	total gain
0	1
1	2
2	4
3	8
4	6
5	12
6	24
7	48
8	13
9	26
10	52
11	104
12	78
13	156
14	312
15	624

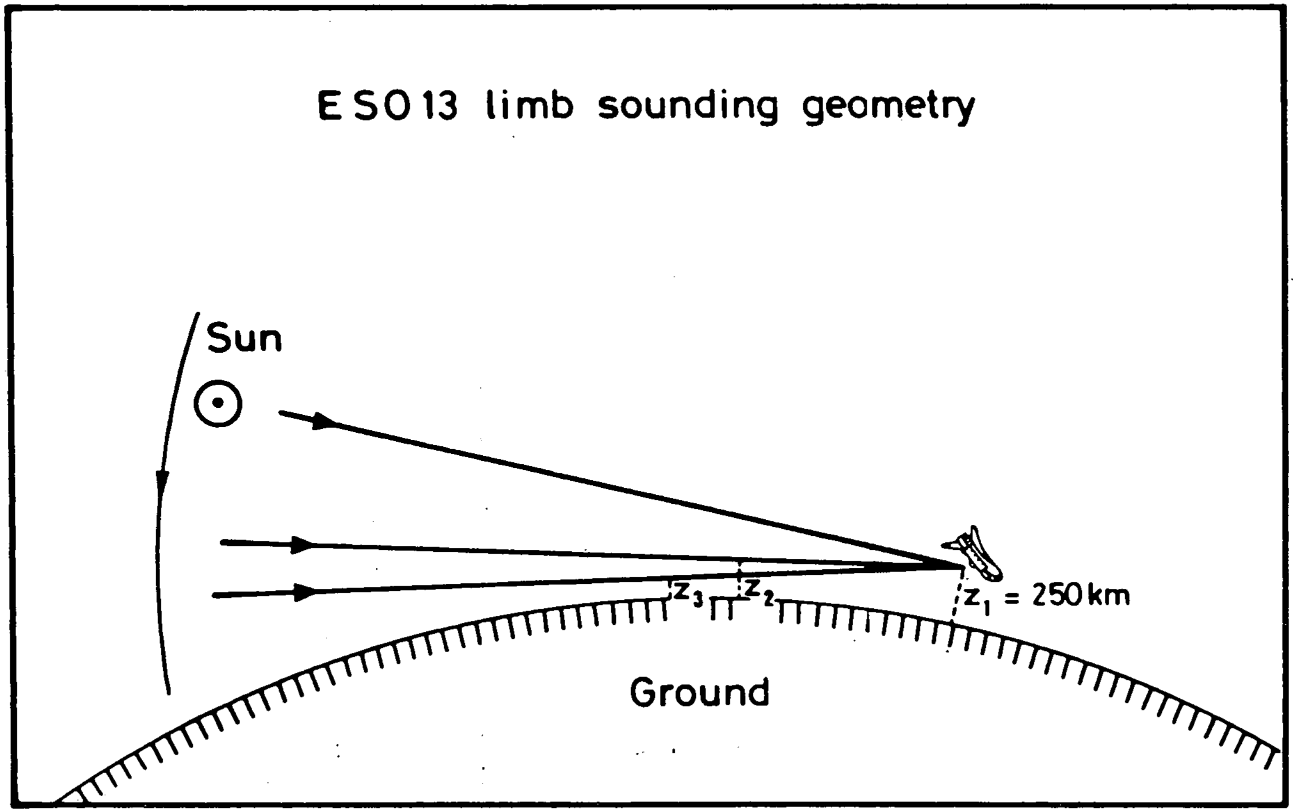

Fig. 1- Observational geometry during a sunset. The spacecraft being at an altitude of about 250 km, the spectrometer heliostat follows the sun as it goes down. At zenith angles greater than 90 degrees, the altitudes Z_2 and Z_3 where the rays are the closest to the earth surface are the zones of main absorption and will be referred to as the altitudes of the observations.

lines of the same constituent in the same scan, rotating the grating fast from one region to the other. A change of filters would be too slow in most cases to permit the retrieval of a profile. In emission, the altitude zones are also determined by the Spacelab computer using several horizon sensors and correspond to the altitudes assigned for absorption.

The total number of spectral windows is 64 of which 40, numbered 24 to 63 are fixed and definitively encoded in the DEP "Read Only Memory"; 24, numbered from 0 to 23 are programmable for use during the test period and later, to accomodate new scientific requirements during the flight. This option allows the loading of new windows and programs from a prepared magnetic tape. It also permits the payload specialist aboard the spacecraft to enter new parameters upon request of scientists or even, if an uplink is possible, would allow the ground team to enter new data directly. There are 20 sunset and 20 sunrise programs numbered respectively from 20 to 39 and from 40 to 59 in which number 20 and 40 are programmable. The emission programs range from 60 to 79, sequence 60 being programmable.

Table 2 gives the parameters of the fixed windows, numbers 24 to 42 represent different spectral intervals while above 42, the gains are varied. Table 3 indicates the molecules for which these windows have been designed. The choice of these intervals, is limited by the range of the filters and the possible grating angles, which had been fixed by an earlier choice of scientific priorities. For example, window 24, observing simultaneously NO and NO_2 has been extensively studied by balloon (Ackerman et al, 1975) under the 40 km altitude, but the vertical distribution of these two molecules above the balloon float altitudes is still largely unknown. Once the most important windows had been chosen, all available combinations of detectors, grating angles and filters were examined to see if other windows could be selected. The constituents which will be studied and which have already been detected

TABLE 2.- Fixed spectral windows.

Window number	θ_{min}	θ_{max}	Filter 1	Filter 2	Gain 1	Gain 2	Channel 1 (cm^{-1})	Channel 2 (cm^{-1})
24	65.24	65.50	5	6	13	15	1914.15 - 1918.13	1595.12 - 1598.45
25	66.78	67.13	3	6	13	"	2205.12 - 2211.21	1575.34 - 1579.44
26	61.20	61.45	2	6	12	"	2974.38 - 2981.49	1652.43 - 1656.38
27	55.10	55.35	4	2	13	"	2117.33 - 2123.75	1058.66 - 1061.88
28	62.45	62.75	7	7	12	"	3918.48 - 3929.13	2938.86 - 2946.85
29	61.20	61.50	3	6	11	"	2312.31 - 2318.94	1651.65 - 1656.38
30	59.90	60.23	2	3	12	"	3010.00 - 3020.00	2341.05 - 2348.84
31	56.60	56.90	1	2	12	"	3811.90 - 3825.01	1039.61 - 1043.18
32	53.65	53.96	4	2	13	"	2154.00 - 2162.50	1077.00 - 1081.25
33	60.63	60.90	2	6	12	"	2990.14 - 2998.03	1661.19 - 1665.57
34	53.65	53.96	4	4	13	"	2154.07 - 2162.62	*
35	60.82	68.00	5	5	13	"	1878.59 - 1995	*
36	59.20	59.60	3	3	11	"	2356.02 - 2365.77	*
37	65.30	65.50	5	5	15	"	1914.15 - 1917.21	*
38	53.65	53.96	4	4	15	"	2154.07 - 2162.62	*
39	60.82	68.00	5	5	15	"	1878.59 - 1995.	*
40	60.06	60.60	3	3	15	"	2332.49 - 2345.05	*

TABLE 2.- (continued).

Window number	θ_{min}	θ_{max}	Filter 1	Filter 2	Gain 1	Gain 2	Channel 1 (cm^{-1})	Channel 2 (cm^{-1})
41	55.10	55.35	4	2	15	15	same as 27	
42	60.63	60.90	2	2	15	"	2990. - 2998.	996.71 - 999.35
43	65.24	65.50	5	6	14	"	same as 24	
44	66.78	67.13	3	6	14	"	same as 25	
45	61.20	61.45	2	6	13	"	same as 26	
46	55.10	55.35	4	2	14	"	same as 27	
47	62.45	62.75	7	7	13	"	same as 28	
48	61.20	61.50	3	6	13	"	slightly wider than 29	
49	59.90	60.23	2	3	13	"	same as 30	
50	56.60	56.90	1	2	13	"	same as 31	
51	53.65	53.96	4	2	14	"	same as 32	
52	60.63	60.90	2	6	13	"	same as 33	
53	53.65	53.96	4	4	14	"	same as 34	
54	60.82	68.00	5	5	14	"	same as 35	
55	59.20	59.60	3	3	13	"	same as 36	
56	66.78	67.13	3	6	12	14	same as 25	
57	61.20	61.45	2	6	7	"	same as 26	

TABLE 2.- (continued).

Window number	θ_{min}	θ_{max}	Filter 1	Filter 2	Gain 1	Gain 2	Channel 1 (cm^{-1})	Channel 2 (cm^{-1})
58	55.10	55.35	4	2	12	14	same as 41	
59	59.90	60.23	2	3	7	"	same as 30	
60	56.60	56.90	1	2	7	"	same as 31	
61	53.65	53.96	4	2	12	"	same as 34	
62	53.65	53.96	4	4	12	"	same as 32	
63	59.20	59.60	3	3	10	"	same as 36	

TABLE 3 : Scientific objectives of the fixed windows.

Window number	constituents	Remarks
24	NO, NO_2, H_2O, CO_2	Covers the 1914.993 NO line
25	N_2O, H_2O	Strongest near infrared lines
26	CH_4, H_2O	Includes a clean CH_4 manifold
27	CO, O_3	Maximum of ozone absorption and strong CO lines, uncontaminated in the upper stratosphere
28	HF, HCl	Covers also non saturating CH_4 lines in the lower stratosphere
29	CO_2, H_2O	Temperature sounding using H_2O lines
30	CH_4, CO_2	Q branch of the CH_4 ν_3 band
31	H_2O, O_3	Strong O_3 region
32	CO, O_3	Uncontaminated CO lines R_2, R_3 and R_4
33	OH, H_2O	Would permit the monitoring of OH
34	CO	CO on both channels
35	Solar CO	Covers a wide interval of the $\Delta v = 1$ CO and NO bands
36	CO_2	Temperature sounding using CO_2 lines
37	NO	Emission, covers the 1914.993 NO line
38	CO	Emission, R_2, R_3 and R_4 CO lines
39	NO	Emission, covers a wide interval in the $\Delta v = 1$ NO bands
40	CO_2	Emission
41	CO, O_3	Emission, strongest O_3 region
42	OH, O_3	Would permit the simultaneous observation of OH and O_3 emissions

in the infrared are NO, NO_2, N_2O, CO, CO_2, CH_4, O_3, HF, HCl, H_2O. The filter choice prohibited the study of $CFCl_3$, CF_2Cl_2, HNO_3 and the sulfur molecules : COS, SO_2, H_2SO_4. All these constituents have their maxima below balloon altitude and thus a spacecraft might not be the best platform to determine their vertical distribution. Except attempts, on one of the channels, to observe OH, all the first flight windows correspond to regions where, at least in the stratosphere, the absorptions are predictable within a factor of two. However, for a possible reflight of the instrument, the "Read Only Memories" could be erased and replaced by more tentative intervals.

The absorption sequences are indicated in table 4 with their scientific objectives, the programs for sunset and sunrise being identical. In the 0 to 50 km range, lines have been chosen which were known not to saturate in stratospheric conditions. The main new scientific information will come in the 35-50 km range, for NO, NO_2, HF and HCl which possibly have a maximum around 40 km. The rate of decrease of CH_4 is also much discussed due to discrepancy between sampling and optical measurements (Ackerman et al, 1977). Also the altitude at which N_2O becomes insignificant and does not contribute any more to the NO_x balance is still to be determined. CO, now known to have low stratospheric values (Farmer et al, 1980) could well present an increase above 40 km related to the CO_2 dissociation at much higher altitudes. The vertical distribution of stratospheric H_2O (Ackerman, 1974; Louisnard et al, 1980) will be measured with the instrument being entirely free of contamination. Finally, the distribution of ozone above its maximum is difficult to access with any other technique.

The region from 50 to 100 km has never been studied at that resolution using an infrared instrument and theoretical models were the main drive in the choice of intervals. The constituents observed will be CO_2, H_2O, NO, CO, O_3 and CH_4, CH_4 being interesting in terms of its decrease with altitude. As no CH_4 production exists in the upper atmo-

TABLE 4 : Absorption sequences
First flight ES013

N°	250-200 km	200-100 km	100-50 km	50-10 km	Main scientific objective
21	27	34	27	32	O_3, CO
22	30	36	30	30	CO_2, CH_4
23	26	34	26	25	CO, CH_4, N_2O
24	35	35	24	24	NO, NO_2
25	31	36	31	31	H_2O, O_3, CO_2
26	28	36	29	28	HF, HCl, temperature
27	33	34	33	33	CO, H_2O, OH
28	46	53	46	51	backup of 21
29	49	55	49	49	backup of 22
30	45	53	45	44	backup of 23
31	54	54	43	43	backup of 24
32	50	55	50	50	backup of 25
33	47	55	48	47	backup of 26
34	52	53	52	52	backup of 27
35	58	62	58	61	CO_2
36	59	63	59	59	CO_2, CH_4, temperature
37	57	62	57	56	CO, O_3
38	63	63	60	60	Temperature CO_2, H_2O
39	60	63	60	60	Temperature CO_2, H_2O

The numbers below the altitude zones designate spectral windows (table 2).

sphere, it is a perfect indicator of the vertical transport. NO, CO and O_3 might have secondary maxima while CO_2 and H_2O could provide the temperature by measuring the intensity ratios of lines (Toth, 1977). In this range of altitudes, the strongest lines have been always used. Above 80 km, the local thermodynamic equilibrium hypothesis which has been used for all predictions may not be valid any more. Departure from "L.T.E" would practically result in having the molecules absorb and emit at temperatures apparently higher than the ambient. One of the objectives of all absorption measurements above 80 km will be, by comparing the relative intensities of lines, to determine when this phenomenon becomes important and to feed this data back in the interpretation of emission spectra.

Above 100 km, only the strongest lines of a very few molecules are expected to be observable, the interval between 200 and 250 km will be used to measure the solar spectrum for spectral windows of stratospheric importance so that the solar lines may be easily eliminated. The long "Solar CO" spectral window is covered once between 250 and 100 km in order to check the solar CO distribution (Muller and Sauval, 1975) and also to verify if any unexpected feature happening in the 1-0 bands of NO did not emerge in the thermosphere.

Table 5 indicates the emission sequences, the lowest altitudes : 60, 40 and 20 will almost certainly present only thermal emissions which are limited by the blackbody at the corresponding temperature, in order to observe a significant signal, about 100 spectra will have to be averaged for each window. The emission observation may be performed at any time and would yeld nighttime ozone values which could be compared with the daytime results of most other techniques.

Above 60 km, the thermal signal will become, in principle, very weak but other effects, already partially observed could take place. Ozone could be produced in a vibrationnaly excited in the meso-

TABLE 5 : Emission programs

code : (Hn, F, p) x
meaning x scans of window p at coded altitude H_n, the altitudes used in the programs being :
H_2 = 160 km, H_3 = 120 km, H_4 = 100 km, H_5 = 80 km, H_6 = 60 km, H_8 = 40 km, H_{10} = 20 km.

Program		Main scientific objectives
61	(H_2, F_{37}) 150 + (H_3, F_{37}) 150 + (H_4, F_{37}) 150 + (H_5, F_{37}) 150 + (H_6, F_{37}) 150 + (H_3, F_{39}) 150	NO in the mesosphere and thermosphere
62	(H_3, F_{38}) 150 + (H_4, F_{38}) 150 + (H_5, F_{38}) 150 + (H_6, F_{38}) 150 + (H_3, F_{39}) 150	CO
63	(H_3, F_{40}) 150 + (H_4, F_{40}) 150 + (H_5, F_{40}) 150 + (H_6, F_{40}) 150 + (H_3, F_{39}) 150	CO_2
64	(H_4, F_{41}) 150 + (H_5, F_{41}) 150 + (H_6, F_{41}) 150 + (H_8, F_{41}) 150 + (H_3, F_{39}) 150	O_3 and CO
65	(H_4, F_{42}) 150 + (H_5, F_{42}) 150 + (H_6, F_{42}) 150 + (H_2, F_{42}) 150 + (H_3, F_{39}) 150	O_3 and OH
66	(H_5, F_{37}) 150 + (H_6, F_{37}) 150 + (H_8, F_{37}) 150 + (H_{10}, F_{37}) 150 + (H_3, F_{37}) 150	NO in the stratosphere and mesosphere

sphere, which instead of loosing its excess energy in a collision could desexcitate itself radiatively (Moreels and Muller, 1976). Programs 64 and 65, performed during daytime, have been designed to observe this emission.

Markov et al (1978) and Gordiets et al (1977) have also observed several high altitude emissions including what they interpreted as a nitric oxide peak around 140 km. This observations has been partially explained by Kockarts (1980) who finds a mechanism of nitric oxide cooling of the thermosphere which would give an emission about a factor of 10 lower than the one reported by Markov et al (1978) but sufficient to give a signal to noise ratio of 6 at 140 km with the grille spectrometer in a single scan. In the case of an auroral enhancement (Stair et al, 1976; Huppi and Stair, 1979), these emissions could still be even higher, by a factor of 100, but the Spacelab orbits will mainly be in the equatorial zones and during a period of low solar activity.

Beside O_3 and NO, CO_2, CO and OH will also be observed in the emission programs, departures from L.T.E. and processes similar to the ones indicated above could also enhance their emissions and bring important mesospheric and thermospheric data. Most of the emission programs end with a scan of a wide window including all the NO band at the 120 km altitude, to check any nitric oxide emission line which could be stronger than the 1914.993 line used in window 37. This long scan also ensures that all the allocated emission time is used.

Finally, the described windows and programs do not close the possibilities of the instrument during the first flight, a space is provided on the Spacelab magnetic tape for eight sets of windows and corresponding programs to be loaded during the flight in the erasable zone of the experiment processor. Also programs will be designed to obtain the highest possible return of sporadic events like a stratospheric warming or a solar proton event.

The flight timeline is still to be defined with this instrument but if twenty occultations and a similar number of daytime and nighttime emission are obtained, the results could be compared in quantity, for the stratosphere only, with all the balloon flights of spectrometers performed since 1965.

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