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AN IMPROVED MICROCARB DISPERSIVE INSTRUMENTAL CONCEPT FOR THE MEASUREMENT OF GREENHOUSE GASES CONCENTRATION IN THE ATMOSPHERE

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I. INTRODUCTION

The MicroCarb mission objective is to better understand the carbon cycle and predict its evolution. For that purpose MicroCarb is designed to measure the carbon dioxide (CO₂) mixing ratio column within 1 ppm (a measurement precision of ~0.3%) from a space observatory in low Earth orbit (LEO) so as to locate and characterise the CO₂ sinks and sources.

Carbon dioxide exhibits strong absorption features in the short wave infrared spectral domain. The solar radiation at these wavelengths reflected by the Earth therefore contains the atmospheric CO₂ signature. The CO₂ mixing ratio is directly linked to the depth of the absorption lines. The MicroCarb mission therefore intends to measure the SWIR spectral radiance at the top of the atmosphere (TOA) in three very narrow spectral windows and at high spectral resolution. Two bands, at 1.6 μm (band B2) and 2.05 μm (band B3), will be devoted to the CO₂ content (see fig.1). An additional spectral band in the oxygen absorption at 0.76 μm (band B1) will additionally provide information on surface pressure atmospheric aerosols and fine clouds. The observation geometry will be nadir over land and towards glint over oceans. The measurement itself is made within discrete sounding footprints of several square kilometres area on the Earth.

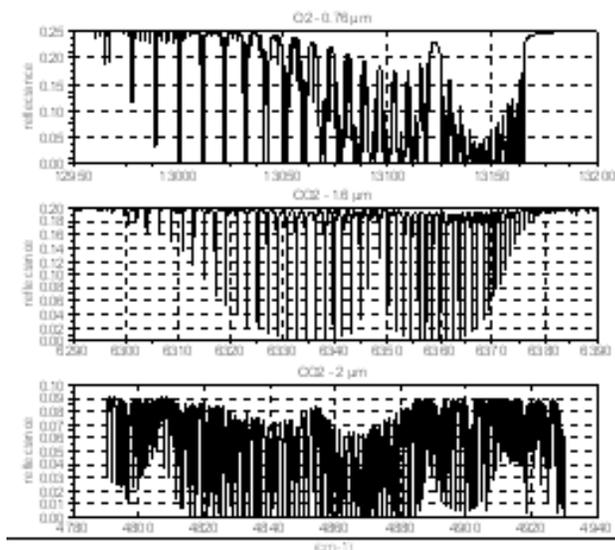


Figure 1. Typical TOA reflectance spectra

These spectral radiance measurements (level 1) will be converted into column-integrated CO₂ mixing ratios (level 2) by inverting the radiative transfer using a Bayesian approach. The level 2 will then be converted into surface fluxes (level 4) by an inversion algorithm that takes into account an atmospheric transport model. The mission high measurement accuracy is driven by the tiny variability in the CO₂ integrated column, variations being around a few ppm out of 380ppm.

The observation system is complemented by a two-dimensional imaging function at a wavelength of 0.76 μm to observe the sounded area. This 2D map of the sounded field accompanies each item of spectral data acquired by the instrument, and will provide data upon clouds.

An in-house CNES research project, preliminary to MicroCarb phase A, focused on an instrument concept using a grating spectrometer for the three spectral bands to meet the mission requirements and the will to fly the instrument on a Myriade microsatellite bus (see fig.2). Grating spectrometer is also the concept chosen, for example, for the instrument aboard NASA's Orbiting Carbon Observatory (OCO) [1]. The main results of this preliminary study, described below, appeared sufficiently credible to pursue this dispersive instrument concept.

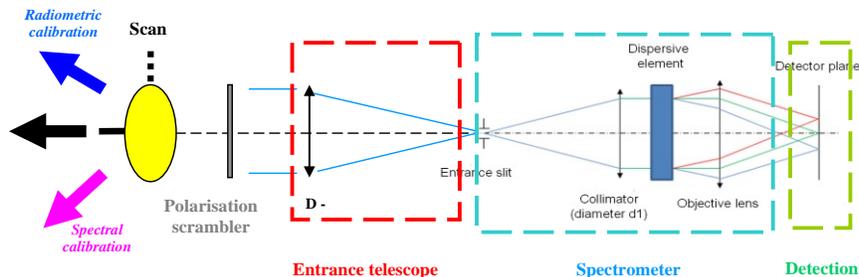


Figure 2. Components of the instrument's functional system

During the MicroCarb phase A, design activities were performed in parallel by two manufacturers, Thales Alenia Space and Airbus Defence and Space. Phase A was concluded by end 2013 with a Preliminary Requirements Review (PRR). Both industrials proposed each an instrumental concept compatible of Myriade Evolution platform resources and compliant with the MicroCarb requirements. The technological pre-development and characterisation of critical devices for mission performances or feasibility as gratings, polariser device and others were completed.

Based on this feasibility, a second CNES internal study was initiated with the objectives to improve the instrumental concept compacity and to add some new capability in particular access to other greenhouse gases (CH₄, CO₂, H₂O). These improvements are the topic of this paper.

II. INITIAL SPECTROMETER DESCRIPTION

A. General principle

The spectrometer studied by CNES was based on a dispersive optical element: the echelle grating spectrometer [2]. The instrument is divided into three parts (see Fig. 2):

- The entrance telescope which collects the flux along a given line of sight and forms a sharp image of the Earth at the spectrometer entrance.
- The spectrometer itself, which analyses the incoming light by dispersing the spectrum onto the detector area
- An imaging system, possibly built into the telescope/spectrometer assembly.

The field at the entrance of the instrument spectrometer section is limited by a physical slit. The spectrometer forms sharp monochromatic images of this slit on a matrix detector array. The three detectors are associated with three spectral bands: B1 (0.76 microns), B2 (1.6 microns) and B3 (2.05 microns). These spectral bands are relatively narrow close to some nanometers, but are observed with a high resolution power, typically $R = 25000$ ($R = \lambda/\Delta\lambda$, where $\Delta\lambda$ is the spectral FWHM (Full Width at Half Maximum) of a monochromatic spectral line).

Using a long slit provides a spatial dimension on each detector which is perpendicular to the direction of spectral dispersion. The information acquired along this axis can be added together (binning) to increase the radiometric resolution. Typically, 50 pixels (Nbin) are summed in this way (Fig.3). The long axis of the slit is itself approximately perpendicular to the satellite speed at nadir. Figure 3 illustrates this geometric configuration and the terminology used in this case (with 3 sounding points).

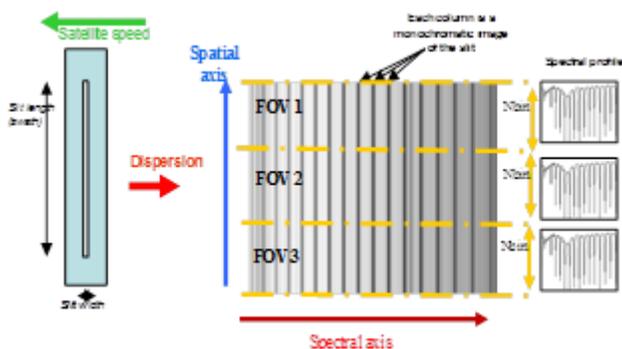


Figure 3. Illustration of spectral axis versus spatial axis

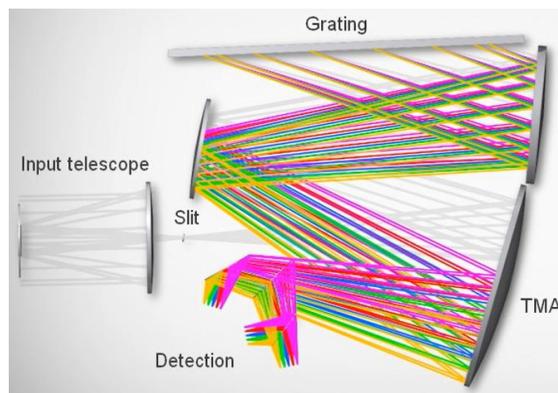


Figure 4. Typical optical configuration. The diffraction orders for the desired spectral bands are separated and sent to the corresponding detectors by a set of dichroic filters

B. Technical approach

The choice of the high spectral resolution (value of parameter R up to 25 000) is justified by the nature of the observed signal: the line depth is a function of the column integrated concentration of the studied greenhouse gazes, here mainly the CO₂. Formally, the line depth or the line strength can be assimilated to its surface or to its Equivalent Width (EW) if this surface is normalized with reference to a totally absorbent line of spectral width EW. A variation of 1 ppm of the integrated CO₂ column concentration (XCO₂) amounts to a variation of the spectral line equivalent width ΔW of 0.25 %. The accuracy of the measurement requires an instrument with very high radiometric and spectral performances. The trade off between these two classes of performances is possible (see the expression of parametric relationship described in paragraph 6). For MicroCarb, we selected an operating point which favored more particularly the high spectral resolution, technically feasible in a restricted volume thanks to the exploitation of the echelle grating properties. The spectroscopy in this case is excellent, in terms of spectral line shape and spectral calibration thanks to a compacted static concept, fully achromatic optics.

This choice enables also to relax significantly the radiometric constraints that are delicate in particular in the SWIR spectral wavelengths and in a such complex instrument like a spectrometer: dramatic effect of residual non-uniformity of detector response, of ghost images, of slit effect (along track, the scene non uniformity in the Earth image projected on the spectrometer entrance slit), of severe blend effect with the ghost lines (H₂O in the B3 band for example), and so on.

An option studied at CNES is the use of the echelle grating with high interference orders k [3]. The profits of this solution are well known: besides the potential high spectral resolution, it offers high degree of spectral multiplexing because the grating diffracts a wide spectral domain in the same direction. In this case, the MicroCarb grating is used in a quasi-Littrow configuration. The blaze wavelength is given by:

$$\lambda_B = \frac{2 \sin \theta_B}{k_n m} \quad (1) \quad \text{with } \theta_B \text{ the blaze angle and } m \text{ the groove density.}$$

It is possible to find different couples (θ_B , m) for which the blaze wavelength corresponds simultaneously in the center of the three MicroCarb bands (B1, B2 and B3) to the diffraction orders k_1 , k_2 , k_3 taking into account the grating technology.

The spectrum segments matched to the orders are separated one from each other by pass-band spectral filters. The manufacturing of the three filters is easy: they can be broad band because of the large free spectral interval in SWIR spectral domain (free spectral interval equals λ_B / k_n).

The spectral resolution power R is given by the following equation in near Littrow conditions:

$$R = \frac{2 d \tan \theta_B}{\phi D} \quad (2)$$

Where:

D = diameter of the entrance telescope

φ = angular width of the slit in radians

θ_B = the grating blaze angle

d = the diameter of the spectrometer internal pupil (linked to spectrometer size)

Diameter d is necessarily small due to the size issue. The value of the entrance pupil diameter D is determined by the radiometric resolution. The spectral resolution power for a given instrument volume will therefore be optimised by increasing the angle of blaze angle θ_B (high value in MicroCarb situation, typically $\tan \theta_B = 2$ or 3).

One of the fundamental characteristics of the MicroCarb instrument is its compactness, because it has to fly on a Myriade Evolution microsatellite bus. For this reason, we chose an optical concept based on double pass Tri Mirror Anastigmat (TMA). Double pass means that the same optical components are used for the collimation function (light rays are made parallel before they arrive at the dispersive component) and for the camera lens function (the rays dispersed by the dispersive component are focused on the focal plane). An initial implementation of this concept (see fig.4) has been studied, taking into account a calibration system and active and/or passive thermal control. The volume is compatible with the one available on a Myriade Evolution bus (H: 412mm x W: 700 mm x L: 864mm).

C. Experimentation of the instrument principle

We set up an experiment to test the principle of an echelle grating spectrometer operating in MicroCarb spectral bands. This breadboard uses a standard (Richardson) echelle grating. The assembly was calculated and set up so as to reach a power resolution of up to $R = 40000$ in the CO₂ 1.6 μm band (i.e. a spectral width of 0.04 nanometres, see Fig.5).

Fig.6 shows the simplified optical configuration used for this feasibility breadboard. The equipment can be used to check the principle behind order selection through bandpass filters, measure the polarimetric specifications of gratings, specify the processing and calibration algorithms, and enhance the modelling of this kind of instrument.

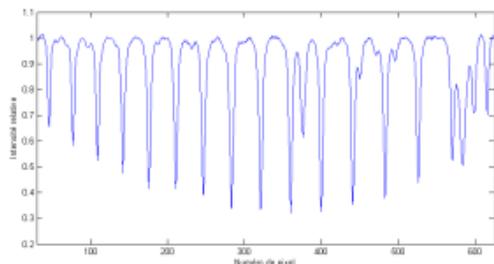


Figure 5. Example of an experiment profile for the CO₂ spectrum in band B2 (uncalibrated)

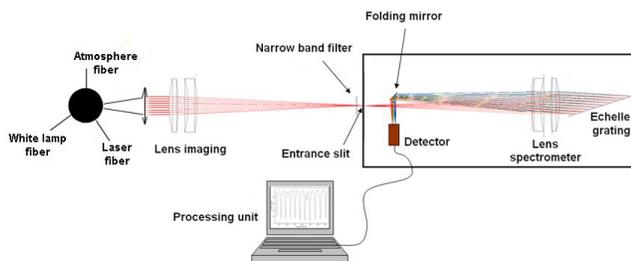


Figure 6. MicroCarb Engineering Breadboard

III. ADAPTATION OF THE DESIGN

CNES pursued the study allowing the increase of the capability of the concept initially studied. The objective is to reduce the instrument volume to make it compatible with an implementation on the Myriade standard platform but also to adapt the concept for other missions like the measurement of the CH₄, H₂O and CO concentration in the atmosphere.

In the design described before, the spectrometer optics is common to the three bands but there are three dedicated detectors: one detector by band. The idea is to reduce the number of detectors needed for the mission. The ideal number is of course a single detector for the three MicroCarb bands. The first gain is a volume reduction but the design is also simplified (fewer detectors to be cooled).

In parallel we studied the possibility to extend the spectral domain of observation to other chemical species than the CO₂ and O₂ gases. This possibility is indeed offered in a almost natural way by the echelle concept. We studied a large number of derived configurations. The most advanced configuration enabled us to accommodate all the spectral ranges enumerated in the table 1 in the surface of two detectors, which gives an idea of the possible field. Bands defined in the mission MicroCarb are reminded in bold.

Spectral Band	Observed gazes	Central wavelength
B1	O₂	763 nm
B1'	H ₂ O	824 nm
B2	CO₂	1605 nm
B2'	CH ₄	1695 nm
B3	CO₂	2034 nm
B4	CO	2346 nm

TABLE I. LIST OF THE MEASURED SPECTRAL BANDS

To illustrate this work, Fig.7 shows on an example on how the various spectral ranges are then projected on the detectors surfaces by the optics (the axis of dispersal is horizontal, strips represent the different spectral ranges).

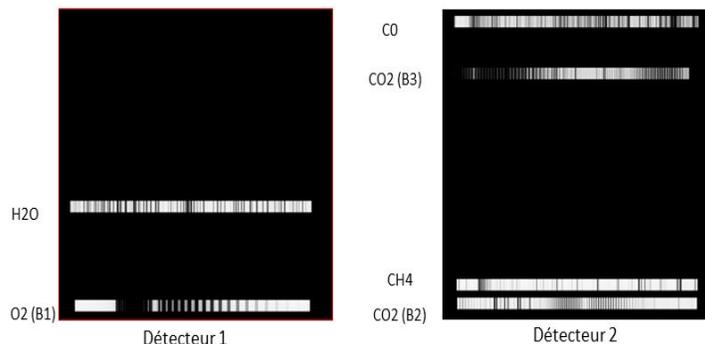


Figure 7. Example of the echelle spectrometer with double multiplexing that allows the observation of 6 bands with only two detectors. The black areas are the sensitive areas of the detectors. The strips are the spectrum associated to each spectral band.

The CO band is located at $\sim 2.4 \mu\text{m}$, in an area of the infrared spectrum where the instrumental thermal signal becomes significant. This part of the spectrum is completely detectable, but the performances can only be reached with a cooling of the whole instrument (towards 250 K estimated). This cooling system complicates the thermal architecture and it is not compatible any more with an implementation on a Myriade standard platform (satellite mass $< 200\text{kg}$). On the other hand, the CH₄ band, located close to 1690 nm, is easily added without impacting the performance of the CO₂ sounding.

A weakly dispersive system is added in the optical plane of Fig.4 to optimize the design. The dispersion axis of this secondary component is perpendicular to the echelle grating. We call it a cross-disperser for this reason. This way, the various orders are angularly separated and can be clearly separated on the surface of a detector. This gives the image shown in Fig.9. Each segment is a portion of the spectrum. There are as many orders of diffraction as segments. Put together, they can constitute a spectrum covering a very large domain of wavelength.

As the spectral bands of the MicroCarb mission are separated (0.77 microns for O₂, 1.55 microns for CO₂), the acquisition of a complete spectrum is not necessary. Only the orders which contain the spectral signature of the considered chemical elements are useful. Consequently, we added a second multiplexing level to the first stage of multiplexing done by the echelle grating itself. This second level uses the cross-disperser grating with the diffraction orders $k' = 1$ and $k' = 2$. Very distant domains of wavelengths (and harmonics) can thus be reached on the same detector because they are diffracted in a very nearby angular direction. We called this new technique the double multiplexing. In MicroCarb, this method is effective in particular to reach the B1 band (0.77 μm) and the B2 Band ($2 \times 0.77 = 1.55\mu\text{m}$). The two bands now can exist on one detector only (see Fig.9).

The complete echelle spectrum is recorded on its full length, which requires a large detector and large field optics. The adequate use of the cross disperser allows to include on the same detector the orders normally very distant one from each other. If necessary, local filters near the detector surface are implemented to avoid the overlapping of the ghost orders.

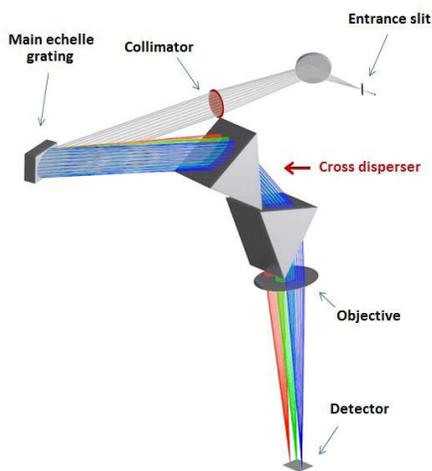


Figure 8. Principal scheme of cross-disperser grating.

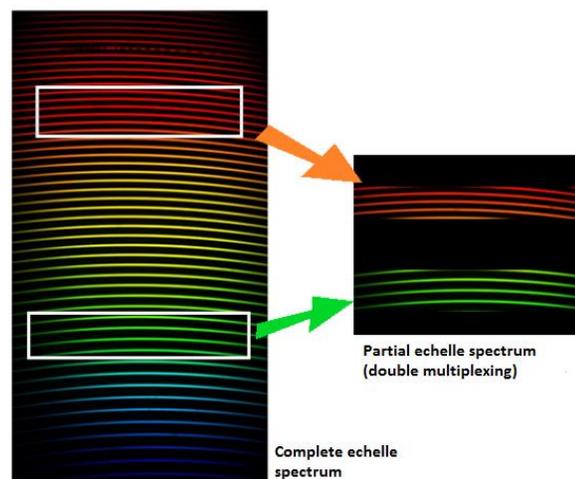


Figure 9. On the left, classical image of echelle spectrum complete. On the right, possibility to group together several narrow spectral band on one detector thanks to the double multiplexing.

IV. FOCUS ON OPTICAL DESIGN

A new adaptation has been designed to fit onboard a Myriade Microsatellite platform. The instrument has a large numerical aperture (F/5.3), which is favourable for a good radiometry. A Dual Babinet polarization scrambler takes place at the instrument entrance, lowering the polarization ratio down to 0.1%. This avoids severe bias due to the scene polarization, especially in presence of aerosols in the atmosphere. A full ICSO 2014 article is dedicated to the polarisation scrambler [4]. A 240mm focal length TMA (Three Mirror Anastigmat) telescope forms the Earth image on a slit which is the entrance of the spectrometer part of the instrument.

Fig.10 illustrates the optical components of the system. The light is collected by the telescope T, and is focused on the entrance slit F. It is then reflected on the mirrors M1, M2, M3 which constitute the collimator of a dispersive spectrometer. The light goes through a transmission grating R1, called cross disperser (or secondary). This weakly dispersive grating works on the diffraction orders with n' such as $n' = 1$ and $n' = 2$ (for example). The R1 grating produces the first multiplexing in the order n' . The light then encounters a classical echelle grating R2. As any echelle grating, it is used with a high incidence and it diffracts in a common direction

all the different diffraction orders n (typically $10 < n < 120$). This R2 grating is at the origin of the dispersion of the spectrum. R2 realizes a second multiplexing of order n . R1 and R2 gratings have perpendicular grooves. The light scattered by R2 goes back to R1 (double passage), then to M3, M2, and M4. These mirrors form the objective of a dispersive spectrometer. The spectrum is focused at the end on the detector D. At this step, the orders n' are demultiplexed either:

- by their position on a common detector, the orders are then separated by a system of filters close to the sensitive area;
- by their arrival on two at least different detectors receiving the involved orders separated enough one from each other;
- by the addition of one or several dichroics which spectrally separate the families of orders n' and send them towards different detectors.

The full instrument, with the polarization scrambler, the entrance telescope and the spectrometer part, fits inside a 450 mm*420mm area. The image quality is diffraction limited, whatever the point in the field, the wavelength in the spectral domain, and the spectral band. The breadboard optical design has been modified to be fully reflective and has been adapted with the double spectral multiplexing. The breadboard is composed of 3 modules: the source, the entrance telescope and the spectrometer (see Fig 11). This new version of MicroCarb breadboard is currently under mounting and will give its first results very soon.

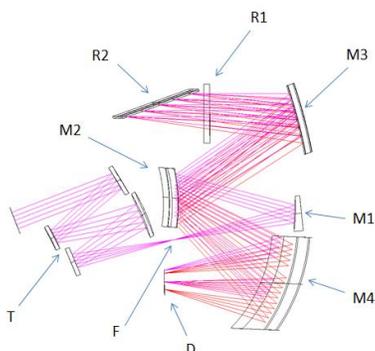


Figure 10. Optical diagram of the spectrometer with cross-disperser

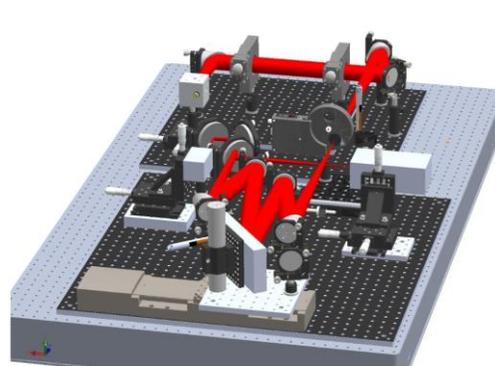


Figure 11. New Microcarb breadboard CAD

V. FOCUS ON DETECTION

A detector with $1k \times 1k$ format is needed in order to meet the size requirement due to the double multiplexing. Moreover, several spectral bands are on a common detector so that the sensitivity must enable the detection from visible to $2.5\mu\text{m}$.

Sofradir is developing a new VISIR $1k \times 1k$ detector which fulfills those requirements in the frame of an ESA program (named Next Generation Panchromatic detector). The first design of the NGP detector has been validated [5] so this detector has been chosen for the MicroCarb improved concept. The quantum efficiency is constant from $0.35\mu\text{m}$ to $2.5\mu\text{m}$ at around 70%. Adding an anti-reflective coating, the quantum efficiency is above 85% on the whole wavelength range. The array is 1024×1024 pixels with $15\mu\text{m}$ pitch. The charge handling capacity is 700 000 electrons. As well as the Saturn detector the readout circuit uses Capacitive TransImpedance Amplifier (CTIA) as input stage which achieves a noise of 140 electrons.

The detector is one of the main contributors for non-linearity pseudo-noise. The measurements performed on the NGP are between 10% and 90% of the full well capacity. The question is to know the non-linearity under 10% of the full well capacity as our application is low signal level. This kind of measurement is difficult because it is mandatory to evaluate the incident flux with a high accuracy even for low fluxes. A solution could be to use calibrate diaphragms to vary the flux and to measure it with a standard.

Next step for this detector is to be tested under spatial environment.

VI. PRELIMINARY ASSESSMENT

A. Parametric relationship (level1)

The level 1 requirements are such that:

- the goal value gives the same level 2 performance as OCO [6]
- The threshold value is such that Level 2 performance is relaxed by 35%.

The signal/noise ratio, spectral resolution and bandwidth are the instrument driving parameters for CO₂ retrieval accuracy. As very different combinations of these parameters might give similarly good level 2 performance, we define a parametric relationship:

$$P = \frac{k}{BW^\alpha SNR^\beta R^\gamma N^\delta M^\delta}$$

Where:

k = coefficient set such that p is equal to the required performance in ppm calculated through linear error estimates for a clear sky without aerosols.

BW = spectral bandwidth

SNR = signal to noise ratio

R = spectral resolution

N = number of across-track FOV

M = number of along-track FOV

$\alpha, \beta, \gamma, \delta$ are optimal values defined for a set of different instrument configurations. A minimum and a maximum value are also specified for each parameter (cf table 2).

This parametric relationship is a specific approach in the MicroCarb requirements that offers a great flexibility for the choice of the instrument functional point. The basic idea is that the degradation of performance due to one parameter can be compensated by the increase of another parameter. It is potentially a way to effectively optimize the compromise between the performance and the complexity of the instrument.

Another driver requirement for the instrument is the quality of the retrieval of the spectral profile of an atmospheric absorption line. A specification implies the knowledge and the stability of the ISRF (Instrumental Spectral Response Function) delivered by the instrument for every spectral channel. This specification also implies the spectral calibration which can induce an error of knowledge of the profile of the lines. Only a global spectral shift in the first order of the moderate spectrum is accepted because this information can be retrieved during the CO₂ concentration estimation.

B. Pseudo-noise (level1)

Along with the key parameters considered in the important function described above, instrument defects will affect the spectrum measured in the spectral bands, and therefore the precision of the estimated CO₂ concentration. Such defects have a similar effect on radiometric noise, which is why the term “pseudo-noise” is used. Different kinds of pseudo-noise include:

- geometric defects such as inter-band and intra-band co-registration...
- spectral defects such as ILS (Instrument Line Shape) knowledge, keystone...
- polarization defects,
- calibration residue,
- non-linearity and non-uniformity defects,

The goal is to design an instrument for which pseudo-noise is limited and noise mainly consists of radiometric noise. In the case of non-linearity defects, one of the main contributors is the detector, especially in the low signal dynamic. It is important to determine whether non-linearity observed at low levels is due to measurement precision, and can be treated as a noise, or if it is a signed response of the CTIA that has to be taken as a bias.

We want to keep the specified objective of not being dominated by pseudo-noise. The design has therefore been studied to increase the signal (integration time and optics diameter). The size of the considered IFOV is an important parameter in the case of polarization by specular-type reflection. For kilometric resolution (MicroCarb or POLDER type), the scattered reflection phenomenon clearly prevails for a view at nadir on Earth. For a view over the sea, however, the polarization rate can be nearly 100% with low winds (specular surface, see Fresnel's Law) due to the glint, which confirms the signal potentially high polarization level when entering the instrument. For MicroCarb, the instrumental polarization is specified so as to ensure that its impact on the signal measured by the detector is negligible compared to the radiometric noise. Other strategies can also be used. The polarization can be measured by the instrument, like for example in the GOSAT instrument. The measurement can also be taken using fixed polarization, as in the case of the OCO instrument. With MicroCarb specifications, the pseudo-noise level is below 1:1000 taking the expected polarization rate values for scenes on entry into account.

The grating is a component which makes up a considerable part of the overall instrument budget i, and special care is taken to ensure good grating polarization performance. This is why we developed a grating polarization model [7] and studied very precise characterisation of the instrument polarization as well as its main contributing factors. Nevertheless, a polarization scrambler (optical depolarising component) needs to be inserted in the MicroCarb design to meet the required specification level.

C. Estimation of CO₂ concentration (level 2)

Estimations of the level 2 performances of the MicroCarb baseline concept have already been published [8]. They revealed to be largely compliant with the random noise and bias requirements on the CO₂ total column mixing ratio, respectively <1ppm and <0.1ppm, for most scenes excluding the impact of aerosols. These performances were obtained using our CO₂ mixing ratio retrieval tool based on optimal estimation methodology [9], which computes the transfer of random error and bias from level 1 to level 2. Random noise is given by:

$$\hat{S} = (K^T S_e^{-1} K + S_a^{-1})^{-1}$$

With \hat{S} the a posteriori variance, K the Jacobian matrix, S_e the instrumental noise and S_a the a priori variance.

Very preliminary estimations of the level 2 random error of these new compact concepts have been computed using the same retrieval tools. Up to now it was applied only to one scene, a tropical atmosphere with Solar Zenith Angle of 30°, albedo of 0.5 and no cloud or aerosol. The performance of the reference three-band concept studied by the industry during MicroCarb phase A for this scene is 0.23 ppm.

Table II gives the level 1 performances of this new compact concept, including the O₂ band, the weak and the strong CO₂ bands, and the additional CH₄ and CO bands. The volume mixing ratio random error of CO₂ exhibits a random error of 0.20 ppm, which shows that the new concept keeps the high level of CO₂ precision. We are also able to retrieve the CH₄ volume mixing ratio with a random error of 6.21ppb, which is compliant with the objective requirement of Merlin (< 8ppb) or Carbonsat (<10 ppb). Finally, this concept enables the retrieval of CO with a random error of 8.69ppb.

BANDE	ESPECE CHIMIQUE	DOMAINE SPECTRAL (nm)	LUMINANCE (W/cm ² /sr/μm)	ORDRE RESEAU	DETECTEUR	RESOLUTION	SNR (par FWHM)	SNR L / 10
B1	O2	751 - 772	8,64 x 10 ⁻³	40	#1	23000	1300	280
B1'	H2O	812 - 835	7,20 x 10 ⁻³	37	#1	23000	1290	270
B2	CO2	1582 - 1627	1,20 x 10 ⁻³	19	#2	23000	780	92
B2'	CH4	1670 - 1717	0,98 x 10 ⁻³	18	#2	23000	720	84
B3	CO2	2004 - 2061	2,79 x 10 ⁻⁴	15	#2	23000	324	35
B4	CO	2312 - 2378	0,93 x 10 ⁻⁴	13	#2	23000	150	16

Table II: Level 1 performances of the new compact concept

VII. CONCLUSION

The use of a cross disperser grating in the MicroCarb concept studied by CNES gives the ability to reach high-quality CO₂ measurements with a very compact concept. This compact design approach will allow CNES to offer a low-cost solution adapted to the mission purposes. Another interest of the cross disperser grating is also to adapt the concept for others missions like the measurement of CH₄, H₂O and CO concentration in the atmosphere. This extension of spectral bands is very interesting especially as the CO₂ concentration performances are not decreased.

All the studies and breadboard made during MicroCarb Phase A consolidate the feasibility of this concept. The instrumental concept thus relies on fully mature technologies (TRL > 5).

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