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Spectral Calibration of the Spectrometer on Board the Colombian FACSAT-2 Satellite Mission

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Abstract: This paper presents the results of the integration, commissioning, and in-orbit calibration of the ARGUS 2000 SWIR wavelength spectrometer onboard the Colombian FACSAT-2 satellite, Colombia's first satellite used for the measurement of greenhouse gases (GHG). The satellite has been in orbit for approximately one year, gathering spectral signatures in order to characterize the data and perform calibration. The calibration represents a certain behavior following a second-order adjustment. For data analysis, retrieval algorithms have been developed to obtain synthetic spectra using the Genspect 1.2 software code. These synthetic spectra were obtained from the spectroscopic data associated with atmospheric gases (H_2O, O_2, CO, and CO_2), which are stored in the HITRAN database. Attempting to achieve a more accurate simulation of the experimental spectrum, certain instrumental parameters have been incorporated into the synthetic spectrum, including the resolution of the spectrometer, the field of view (FOV) angle of observation, the limited quantum efficiency of detection, and the slit function. As a result, six slit functions were tested, with the Gaussian and the diffraction functions proving to be the most effective. Finally, a profile of Total Carbon Column Observing Network (TCCON) concentrations was used for comparison with a spectral signature acquired by FACSAT-2, resulting in a close match between the synthetic spectrum and the measured spectrum.

Keywords: greenhouse gases; spectrometer; synthetic spectra; nanosatellite

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1. Introduction

The planet's fossil fuel resources are estimated to be around 4000 and 6000 gigatons of carbon (Gt-C) [1]. This material was slowly deposited over millions of years in underground formations by emissions from different sources, including carbon dioxide (CO_2) concentrations of approximately 1500 ppm.

Over the last 300 years, 5% of fossil fuels have been used, which has significantly boosted economic growth. However, only 15% of today's energy comes from non-fuel sources. The burning of 280 gigatons of fossil fuels since the 18th century has raised CO_2 levels from 280 ppm (in the 1700s) to 421 ppm, as reported in May 2022 by the International Panel on Climate Change (IPCC) [2–4]. This is the highest level in 650,000 years, impacting global temperature through the greenhouse effect. This anthropogenic climate change is evidenced by the temperature increase of 0.08 °C per decade since 1880, with 2022 being the sixth-warmest year on record.

To assess the significance of these changes, it is necessary to understand the physical and chemical processes that control the global atmosphere. Accurate assessment of the impacts of current and future anthropogenic activity or natural phenomena on the behavior of the system, which comprises the atmosphere and the Earth's surface, requires quantitative knowledge of the temporal and spatial behavior of various atmospheric constituents (gases, aerosols, and clouds), from the local to the global scale, in the troposphere, stratosphere, and mesosphere. These datasets are also needed to test the predictive ability of the theories currently used to model the atmosphere.

The development of satellite platforms in the past two decades has enhanced the capability to observe the Earth and its atmosphere on a global scale. The possibility of near-simultaneous observations on a global scale has facilitated the emergence of Earth Science. Atmospheric sciences have benefited from satellite observations; this is because remote regions of the atmosphere over land and oceans, where ground stations or land or sea-based measurements are scarce, can now be probed from space [5].

There are two approaches to monitoring the greenhouse gases (GHGs) in the atmosphere: in situ observations and remote sensing. Among the remote sensors, the most widely used in the last 20 years are those that measure atmospheric transparency in different regions of the electromagnetic spectrum, using satellite devices equipped with low-, medium-, and high-resolution spectrometers. Satellite-based GHG measurements are highly accurate and allow gas concentration monitoring at multiple locations on the Earth (greater coverage).

The main satellite systems used to measure GHG concentration launched in the last two decades include the Greenhouse Gases Observing Satellite (GOSAT) [6,7] and the Greenhouse Gases Observing Satellite-2 (GOSAT-2) [6,8,9] from Japan, the Orbiting Carbon Observatory-2 (OCO-2) [10,11] and Orbiting Carbon Observatory-3 (OCO-3) [12,13] from the United States, and the Envisat is equipped with the Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) [14,15] launched by the Europe Space Agency. The GOSAT series is exclusively dedicated to measuring the CO_2 and CH_4 levels and is equipped with a Thermal and Near Infrared Sensor for Carbon Observation–Fourier Transform Spectrometer (TANSO-FTS). GOSAT detects radiation reflected by the Earth and radiation emitted by its atmosphere in the infrared region, specifically, between 0.758–0.775 µm, using an InGaAs detector; in the region between 1.56–1.72 µm and the bands between 1.92–2.08 µm and 5.56–14.3 µm, radiation is detected using a high-sensitivity detector employing HgCdTe (HCT).

The OCO series (2 and 3) were designed for their mission to record global CO_2 variations. OCO-2 was operational until 2019, and at that point, it was installed on the International Space Station, where it remains to this day. OCO-3 is still fully functional. The OCO series has recorded spectral data in three distinct infrared regions: 0.7576–0.7726 µm, 1.5906–1.6218 µm, and 2.0431–2.0834 µm. Each spectral band is measured with a different spectrometer, and each one is equipped with an HCT detector.

The SCIAMACHY instrument (operating on the ENVISAT satellite) is capable of measuring both incident and reflected solar radiation from the Earth over a broad spectral range of 240–2380 nm, encompassing ultraviolet (UV) visible and near-infrared (VIS-NIR) wavelengths, as well as shortwave infrared (SWIR) wavelengths. The absorption of various atmospheric gases, including CO_2, can be recorded in this spectral region. The system comprises an optical assembly that enables the measurement of eight spectral bands using silicon and InGaAs photodetectors.

Finally, certain ground-based or in situ systems utilize high-precision Fourier transform spectrometers (FTIR) situated at various points of interest on Earth (the poles, the ocean, etc.). The three most significant networks of this kind are the Total Carbon Column Observing Network (TCCON), the Network for the Detection of Atmospheric Composition Change (NDACC), and the Collaborative Carbon Column Observing Network (COCCON). The aim of these systems is to provide highly accurate and precise measurements of gas concentrations, including CO_2, CH_4, CO, N_2O, and other species in the near-infrared (NIR) and mid-infrared (MIR) regions. In addition, data from ground-based systems, such as TCCON, are used to calibrate satellite-based measurements [16]. In the Colombian context, bottom-up measurements conducted by ECOPETROL in certain operational regions provide high-precision data that enhance the calibration of the FACSAT-2 integrated sensor, thereby supporting research on climate change. These data are also used as reference points.

On the other hand, the determination of GHG concentration using ground or satellite-based devices requires mathematical and statistical (computational) algorithms based on the physical principles that describe the behavior of these gases when interacting with electromagnetic radiation, especially absorption, scattering, and emission of radiation at specific wavelengths. If we consider absorption as the most significant process, the behavior of the gas's interaction with radiation can be explained by the Beer–Lambert law:

$$I(\lambda) = I_0(\lambda)e^{-\sigma(\lambda)cz}, \tag{1}$$

where $I_0(\lambda)$ is the initial intensity of electromagnetic radiation and $I(\lambda)$ is the intensity of radiation after traveling an optical path of length z through a medium with a molar absorptivity $\sigma(\lambda)$. From this equation, the concentration of the gaseous medium can be easily derived if the intensities before and after passing through the medium are measured and its molar absorptivity is known. However, in gas concentration measurements in open systems, such as the atmosphere, it is difficult to determine the true value of $I_0(\lambda)$. To overcome this problem, a technique called Differential Optical Absorption Spectroscopy (DOAS) is used, in which the intensities surrounding the absorption band of the atmospheric gas to be measured are used as $I_0(\lambda)$.

This type of methodology cannot be used in the infrared spectral region because the molar absorptivity is pressure–temperature-dependent. To overcome this problem, several alternative methods and algorithms have been implemented; they are all based on retrieval methods; these consist of the development of a wavelength-dependent radiation model, the concentration of the gaseous species in question, and environmental conditions such as temperature and pressure [16–19].

This paper presents the generalities of the integration process of the SWIR spectrometer, ARGUS 2000 [20] with the Colombian FACSAT-2 mission satellite bus, and the in-orbit spectral calibration process. After the launch, the acquisition parameters and the resulting data were characterized, allowing the start of the development of algorithms to obtain synthetic spectra from atmospheric and instrumental parameters of greenhouse gases as a first step in the development of the recovery process to monitor the emissions and atmospheric distribution of GHG in Colombia's atmosphere.

2. Materials and Methods

2.1. FACSAT-2 Mission

On 15 April 2023, the Colombian Air Force marked its second historic space milestone. After three years of arduous work, technical and administrative efforts were consolidated with the successful launch and placement into orbit of FACSAT-2 "Chiribiquete".

FACSAT-2 is a Colombian nanosatellite based on the 6U CubeSat standard, launched in 2023 in a 97° SSO Low Earth Orbit (LEO). This nanosatellite features an eight-band multispectral (spectral range 450–900 nm) camera with spatial resolutions ranging between 4.75 and 5 m as its primary payload and an ARGUS 2000 spectrometer contributed by ECOPETROL operating in the shortwave infrared spectral range of 1000–1650 nm for greenhouse gas monitoring as its scientific secondary payload. This last sensor is the only one of its kind to be integrated in a satellite developed in South America. Its mission entails observing Colombian territory for environmental protection purposes [21].

Colombian staff participated in the design of the FACSAT-2 mission through the planning and co-development of different phases of the life cycle, including the definition of objectives and requirements, mission characterization, critical design, and payload integration. After launch, the satellite is currently operated by the Colombian Air Force

(COLAF) from the Space Operation Center (SPOC), located in the city of Cali, Colombia. From there, the tasks of the launch and early orbit phase and the in-orbit calibration of the payloads were carried out.

With the launch of FACSAT-2, the possibility of acquiring specific data through two Earth observation sensors has been opened. These data are crucial for understanding the distribution and emission sources of GHG in Colombia and for exploring potential alternative uses through the mission development. To facilitate the processing and analysis of these data, the development of algorithms to quantify gases efficiently and accurately is required, particularly for Colombia, due to its meteorology and topography characteristics. Additionally, further studies will be conducted to explore the feasibility of other applications using the satellite-acquired data.

2.2. SWIR Spectrometer

FACSAT-2 is equipped with the ARGUS 2000 (Thoth Technology, Pembroke, ON, Canada), a miniature SWIR spectrometer with integrated optics that operates in a spectral range between 1000 and 1650 nm and uses an InGaAs detector array of 256 elements. Table 1 shows detailed characteristics of the ARGUS 2000 SWIR [20].

Table 1. Technical specifications of the ARGUS 2000 spectrometer.

ARGUS 2000	Specification
Type	Grating spectrometer
Configuration	Single-aperture spectrometer
Field of View	0.15° viewing angle around centered camera boresight with 15 mm fore-optics
Mass	~280 g
Accommodation	46 mm × 80 mm × 80 mm
Operating Temp.	−20 °C to +40 °C operating temperature
Survival Temp.	−25 °C to +50 °C survival temperature
Detector	InGaAs diode arrays with Peltier cooler
Grating	300 g/mm
Electronics	Microprocessor-controlled 10-bit ADC (co-adding feature to enhance precision to 13-bit, models 01–03), 3.6–4.2 V input rail 250 mA–1500 mA (375 mA typical)
Operational Modes	Continuous cycle, constant integration time with co-adding feature Adaptive exposure mode
Data Delivery	Fixed-length parity-striped packets of single or co-added spectra with sequence number, temperature, array temperature, and operating parameters
Interface	Serial interface RS232
Spectral Range	1000–1650 nm
Resolution	~6 nm
Integration Time	From 500 µs to 4.096 s
Spatial Resolution	1.5 km at 500 km orbit

2.3. Integration of the Spectrometer to the Satellite

The selection of the secondary payload for the satellite mission was a work carried out by the researchers of the project in an alliance between COLAF and ECOPETROL. After a market study and technological surveillance on sensors for the analysis of GHG that were compatible with a 6U structure (due to the half-U size restriction) and had space inheritance (ARGUS was first launched aboard a CanX-2 microsatellite in 2008 as part of a technology demonstration mission), it was determined that the ARGUS 2000 spectrometer was the only one that met the requirements and restrictions of the proposed mission.

In addition, the integration of the secondary payload required a new system design to enable communication, data control, and power supply between the satellite bus and the ARGUS 2000 sensor. For this, a Printed Circuit Board (PCB) was developed to allow the interface and consists of a six-layer PCB with 26 SMD components. The PCB has dimensions of 42.3 mm × 26 mm × 4.77 mm, an operating voltage of 3.3 V, and the entire design is based on the ECSS-Q-ST-70-12C standard [21]. The PCB has an optimized mechanical design to be included inside the spacecraft structure with a System-on-Chip (SoC) module and transceiver modules. The Payload PCB is a customized space product designed by the COLAF that underwent environmental validation tests at the technology partner's facilities [21].

These challenges enable the deployment of a space-based sensor for data acquisition aimed at quantifying GHG, particularly CO_2, through different processes such as geolocation, in-orbit calibration, synthetic spectra simulation, and data conversion, among others. The following sections describe these processes in more detail.

2.4. Acquisition Conditions

After the launch and within the in-orbit payload's calibration tasks, the first step was the identification of the optimal acquisition parameters, as well as the development of scripts for the reading of the acquired information and the interpretation of the spectral signatures, in the case of the information acquired by the ARGUS 2000 sensor.

In this work it was necessary to synchronize the information acquired by the Attitude Determination and Control System (ADCS), which provides satellite attitude and ephemeris information, with the acquisition times of the spectral signatures, to estimate the geolocation of the different scans; in each session, the acquisition of at least 10 scans has been established; these scans cover approximately an area of 1.25 km × 20.5 km.

Figure 1 shows 88 points that were defined worldwide, characteristically of large GHG emissions, such as cities, carbon calibration columns, islands with sequences of water → land → water, refineries, and other places that allow the calibration of the data.

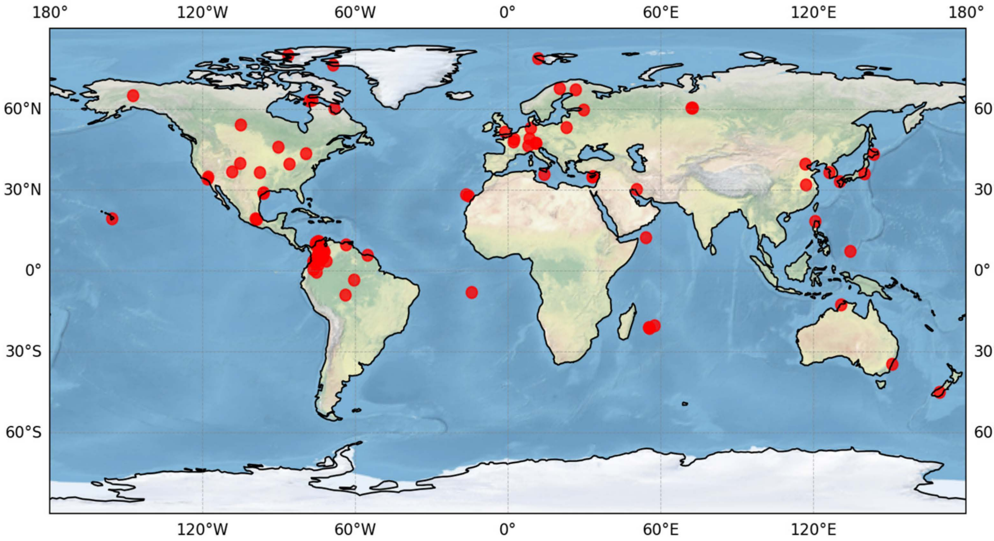


Figure 1. Points defined for sensor calibration.

2.5. Spectra Geolocation

FACSAT-2 has an integrated ADCS to determine its attitude during spectrometer acquisition sessions. The ADCS generates a quaternion vector, representing the satellite's orientation and rotation during the acquisition of spectra, allowing the determination of the ARGUS 2000 footprint coordinates for each of the scans acquired in a session. The quaternions obtained from the satellite are used in a simulation in the STK 12.8.2 (System Tool Kit) software to yield approximate latitude and longitude coordinates corresponding to the point over which the spectrum was captured with an uncertainty of 6.3 km.

Table 2 presents the quaternions used to simulate the satellite's attitude in STK for each scan, corresponding to the timestamps obtained from the metadata of session 328 of the spectrometer. This approach replicates the satellite's orientation at the time each of the spectra was acquired, as illustrated in Figure 2 using the STK software.

Table 2. Quaternion for every ten scans.

Scan	Julian Time	Quaternion (w, x, y, z)	Latitude (°)	Longitude (°)
1	1,709,638,169.748	0.81408318, 0.266145815, 0.452224919, −0.248852724	28.185955640	−16.362316437
2	1,709,638,170.066	0.814152046, 0.266183116, 0.452107415, −0.248801007	28.205980290	−16.367118404
3	1,709,638,170.383	0.814220701, 0.266220013, 0.451990415, −0.248749405	28.226886890	−16.371764579
4	1,709,638,170.701	0.814287598, 0.266279465, 0.451861428, −0.248701098	28.247119771	−16.376342816
5	1,709,638,171.019	0.814350929, 0.266379523, 0.451711421, −0.248659053	28.267147226	−16.380449143
6	1,709,638,171.337	0.814411662, 0.266508912, 0.451546216, −0.248621524	28.287117203	−16.384509888
7	1,709,638,171.655	0.814471783, 0.266644829, 0.451377603, −0.248584993	28.306280802	−16.387407952
8	1,709,638,171.972	0.814532562, 0.266770165, 0.451214747, −0.248546999	28.327094352	−16.392585544
9	1,709,638,172.290	0.814593614, 0.266894521, 0.45105206, −0.248508665	28.347157058	−16.396679694
10	1,709,638,172.608	0.814654628, 0.267018864, 0.450889353, −0.248470318	28.367102193	−16.400683271

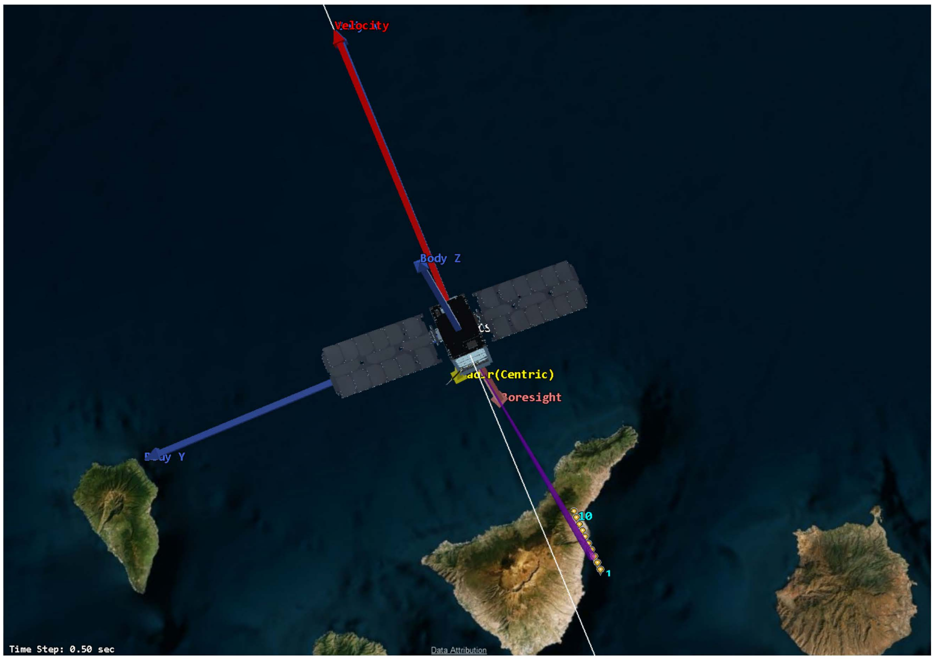


Figure 2. Simulation of satellite attitude using the STK software.

2.6. In-Orbit Spectral Calibration

The ARGUS 2000 spectrometer was calibrated in orbit to consider possible optical variations due to mechanical stresses caused by the launch, a process essential to improve data quality and maintain consistency in data processing. The calibration was developed using the most prominent bands of H_2O, O_2, and CO_2 observed in the spectrum measured by the ARGUS 2000 in orbit, as shown in Figure 3 (in each selected point, the label shows the pixel value and its equivalent that correlated wavelength value with synthetic convolved spectrum.). The bands considered for calibration show their maximum absorption at 1124.89 nm and 1364.94 nm for H_2O; 1267.26 nm for O_2; and 1571.90 nm and 1605.109 nm for CO_2 [22].

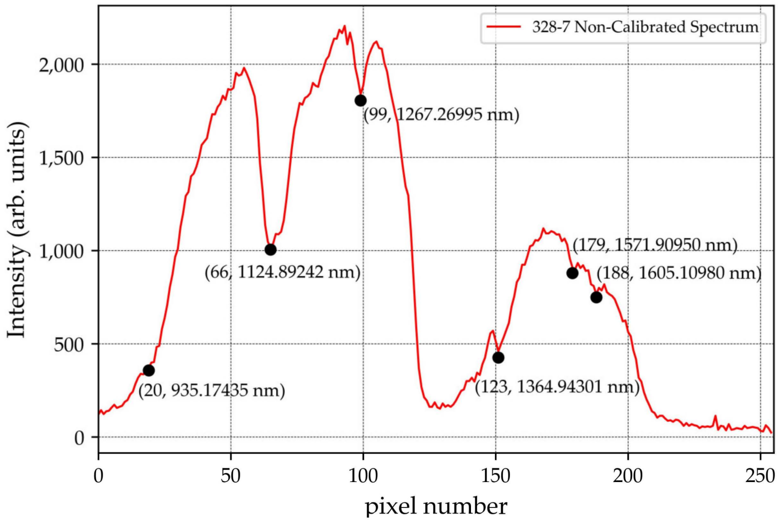


Figure 3. In-orbit calibration points used to establish the pixel–wavelength correspondence.

The following is a description of the generalities of the process:

1. The most prominent wavelengths (control points) in the synthetic spectrum are preselected.
2. The pixel values corresponding to the control points in the ARGUS raw spectrum are selected.
3. The wavelength–pixel scatter is plotted.
4. A polynomial fit is applied to the quasi-linear trend of the wavelength–pixel scatter.
5. The wavelength pixel calibration is applied to both the raw and simulated spectra.
6. The correlation between the ARGUS and simulated spectra is measured.
7. If the correlation is unacceptable, the control point selected on the raw spectrum is repeated (step 2).

2.7. Simulated Spectrum Algorithms

The first stage of the retrieval process consists of obtaining synthetic spectra that simulate the measured spectra from input parameters such as: types of gases, considered gases concentrations, radiation sources, emissive or reflective surfaces, optical path, and state conditions such as temperature and pressure. These input parameters must be optimized to obtain a synthetic spectral model that fits the measured spectra. Then, the simulation procedure can be represented as follows:

$$Y = F(X, b) + \varepsilon, \tag{2}$$

where Y is the measured spectrum; F is the model; X is the concentration profile of the considered gases; b is a set of input parameters, such as the molar absorptivity (or absorption coefficient of the gas) of the molecular gases, the observation geometry, reflectivity, and emitting surface, pressure, temperature, instrumental parameters, etc.; and ε represents the errors associated with the measurement system [16–19].

In Equation (2), F is also called the forward model of the retrieval, and its good fit will allow to reduce the error ε. The forward model is an approximation that describes radiative transfer, atmosphere, surface reflection, solar radiation, and instrument effects on incident radiation to generate a spectrum. The radiative transfer modeling tool (Genspect) was used to implement the forward model. Genspect is a line-by-line radiative transfer software, written in MATLAB, for the absorption, emission, and transmission of a wide range of atmospheric gases [23]. Despite Genspect not including scattering effects, aerosols, clouds, and other non-linear behavior, this code allows computing the line spectra from information such as gas type and amount, pressure, path length, temperature, and frequency range.

Genspect is used in this study to simulate the atmosphere by dividing it into plane-parallel layers, thus generating synthetic spectra models. Additionally, in this algorithm, each atmosphere layer is divided into sublayers for the calculation of radiative transfer and for the calculation of the absorption cross-section, which is highly dependent on temperature and pressure.

The absorption lines of CO_2, H_2O, O_2, etc. are modeled according to the HITRAN 2000 spectroscopic database, and natural, thermal Doppler, and pressure line broadening are modeled using the Voigt function [22]. Although the latest HITRAN databases are available, the Genspect forward modeling code only works with the HITRAN 1996 and HITRAN 2000 spectral databases; the most recent was chosen. In addition, obtaining the forward model (synthetic model spectrum) depends on parameters related to the circumstances of the measurement, such as the solar zenith angle, the viewing angle of the satellite, the relative azimuth, the reflective surface, and the characteristics of the measuring instrument, like the field of view (solid angle), spectral resolution, optical parameters, the response function of the detector, and the slit function of the spectrometer. Genspect generates the synthetic spectrum in the selected spectral range in terms of radiance; however, to be compared with the measured spectrum, it must be converted into detector counts. For that conversion, it is necessary to know the instrument characteristics mentioned above and the integration time of the spectral acquisition [18,19,24–26]. Figure 4 presents the scheme of flow for the retrieval process used in this study.

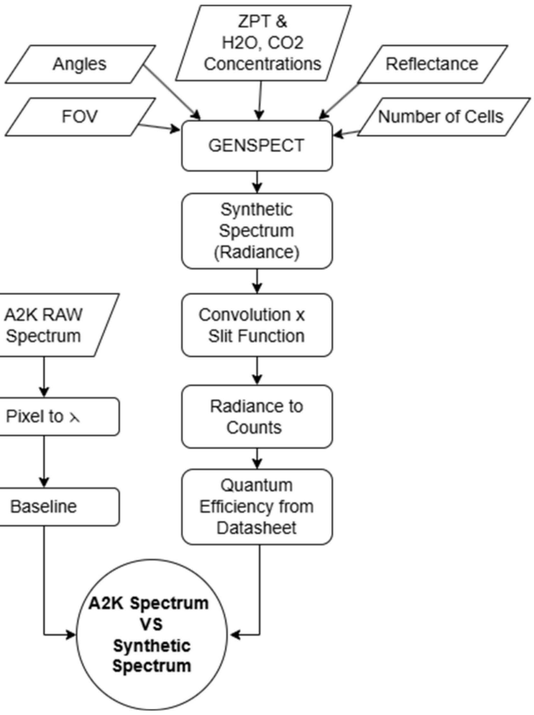


Figure 4. Flow scheme of the retrieval process.

Spectral Radiance to Detector Counts

Acquired ARGUS 2000 spectra are saved as instrumental counts vs. pixel number, while Genspect software generates synthetic spectra in radiance [W sr^{-1} m^{-2}] vs. wavenumber. To facilitate a comparison between acquired and synthetic spectra, it is essential to convert the pixel number to the wavelength range of the ARGUS raw data and to transform the radiance of the synthetic spectra into detector counts. To carry out the latter process, the procedure reported by Jagpal was used [26,27]. Radiance synthetic spectra are convolved with the slit function of the ARGUS 2000. The convolution procedure is explained as follows:

The resolution of acquired spectra by any spectrometer is dependent on its geometric characteristics (finite slit or diffraction mirror grating size). To simulate the instrument's finite resolution, the high-resolved simulated Genspect output spectrum is convolved with the slit function $B(\nu)$ as follows:

$$\mathrm{C}(\nu) = (S\mathrm{x}\, B)(\nu) = \int_{-\infty}^{\infty} S(\nu')B(\nu' - \nu)d\nu'$$

where ν is the wavenumber. The slit function must satisfy $(1\mathrm{x}\ B) = 1$. Ideal and commonly used slit functions have different shapes, such as Gaussian, Lorentian, and Voight. Slit functions are dependent on the wavenumber ν as shown:

$$B(\nu) = \frac{1}{\gamma}\left(sinc\frac{\nu}{\gamma}\right)^2$$

where γ is a parameter that controls the Full Widh at Half Maximum (FWHM) and γ is regularly related to the spectral resolution. As wavenumber spectral resolution varies in the ARGUS 2000 wavelength range (1000–1650 nm), the resolution control of convolved spectrum is possible by assigning $\gamma = \alpha h_\nu$, with $\alpha \geq 1$ and h_ν being the wavenumber spacings. As h_ν can take several maximum, minimum, and average wavenumber spacing values, the h_ν is assigned to be the varying wavenumber spacing. This implies a dynamic generalization of convolution, where the slit function is shifted along the wavenumber axis.

Then, the convolved synthetic spectra are multiplied by the spectral pixel width (dependent on ν) and the solid angle FOV measured in stereo radians, where θ = 0.15°:

$$FOV = 2\,\pi\left(1 - \cos\frac{\theta}{2}\right)$$

Accordingly, instrumental count spectra are obtained by multiplying intensity synthetic spectra [W m^{-2}] by the lens area [m^2] and exposure time, from which the energy spectra can be obtained. Then, these spectra are divided by the instrument joules/counts rate polynomial function:

$$JC(\lambda) = A\lambda^3 + B\lambda^3 + C\lambda + D$$

In addition to the transformation workflow proposed by Jagpal [26,27], the limited detectability will be incorporated due to the quantum efficiency of the linear InGaAs array reported by the sensor manufacturer [28]. For this purpose, the synthetic count spectra were multiplied by the quantum efficiency of the detector function.

2.8. Total Carbon Column Observing Network TCCON

To validate the measurements obtained with ARGUS 2000 on FACSAT-2, this project was carried out by using TCCON, which has been the most widely used database for this purpose in the last 20 years. The use of this ground-based network to measure GHG is due to the high resolution and precision with which TCCON makes GHG measurements. TCCON instruments are Fourier transform spectrometers with a direct view to the sun, and therefore their measurements are not affected by surface properties and are minimally affected by aerosols. However, TCCON is limited to measuring through optically dense clouds. To use this network, it is necessary to make measurements with the system in orbit, at locations on Earth where TCCON measurements are available. Figure 5 shows some locations where TCCON is located, and spectra have been taken with FACSAT-2.

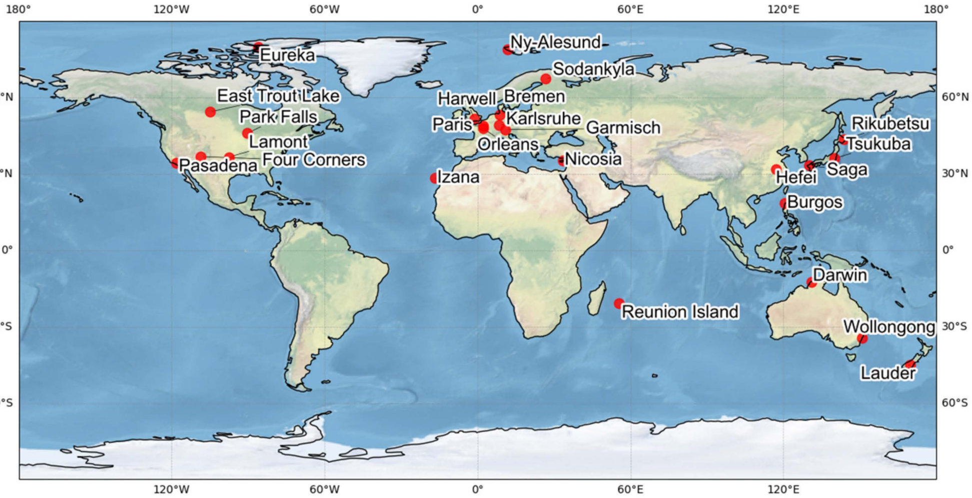


Figure 5. Total Carbon Column Observing Network location.

3. Results

3.1. Spectra Acquisition

Figure 6 shows spectra obtained over Tenerife, Spain. In this acquisition, 10 spectra were observed in the spectral region between 1000 and 1650 nm. The acquisition time of a spectrum (one scan) is approximately 0.256 s; at this time, the FACSAT-2 was displaced 1.95 km. Earth surface reflectivity can vary significantly in the distance between two successive scans, producing variations in the intensity of the acquired spectra. In this acquisition (Figure 7), the observation area covers both land and sea surfaces. The spectra acquired over the land surface exhibit a higher intensity than those acquired over the sea surface. In all the spectra, it is possible to observe the CO_2 bands corresponding to the absorption at 1571.909 and 1605.109 nm.

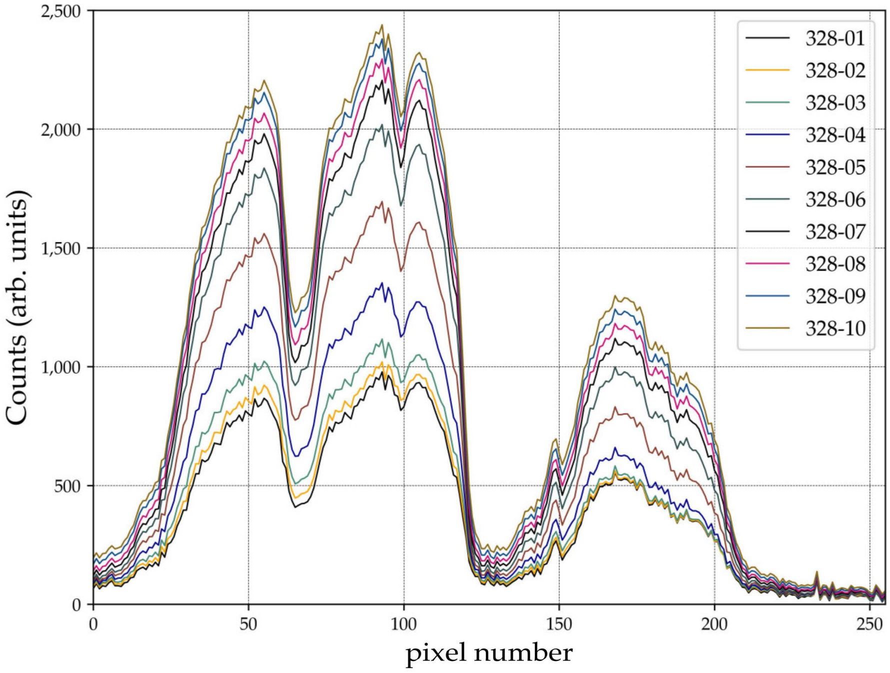


Figure 6. Measured spectrum by ARGUS 2000 SWIR spectrometer onboard of FACSAT-2.

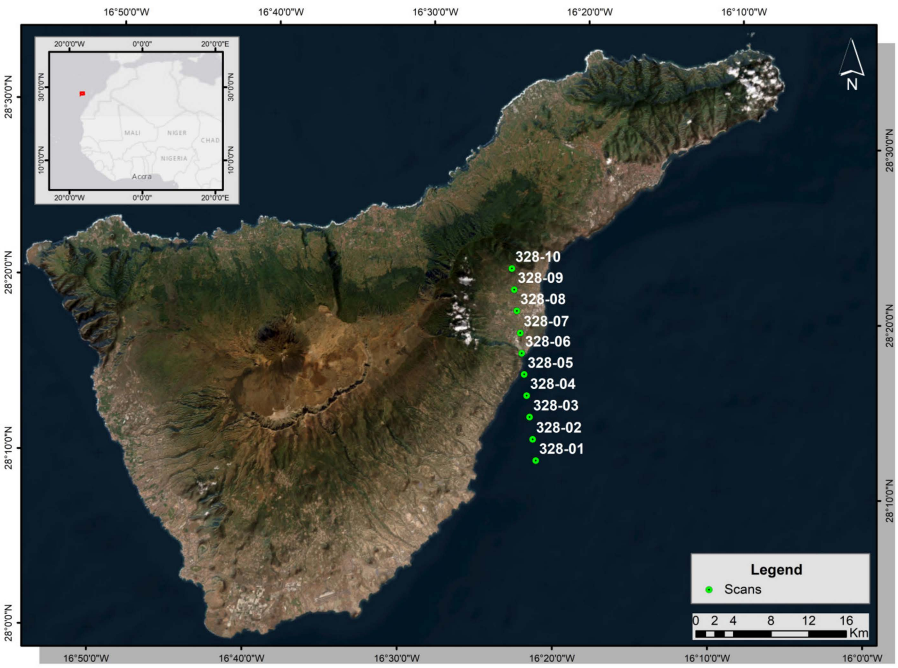
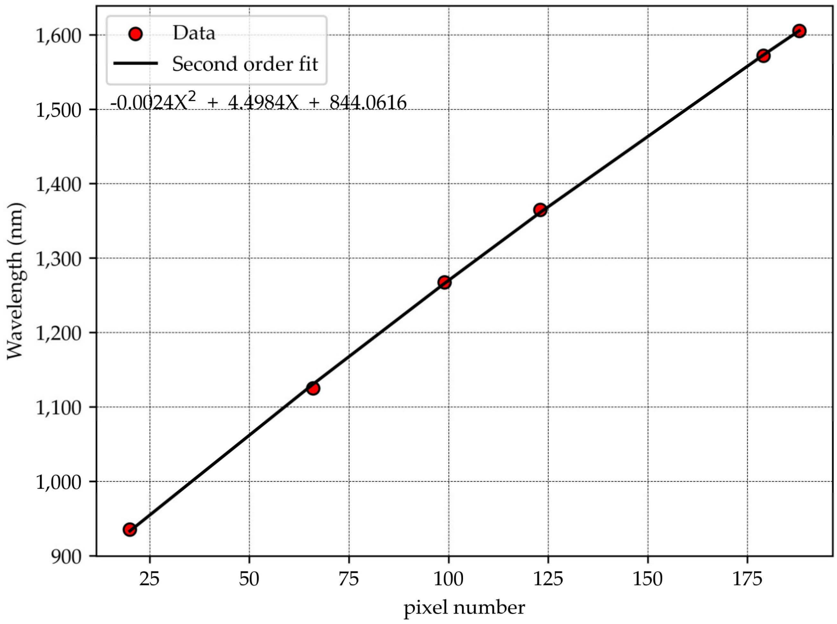


Figure 7. Geolocation of 10 scans from session 328 over Tenerife.

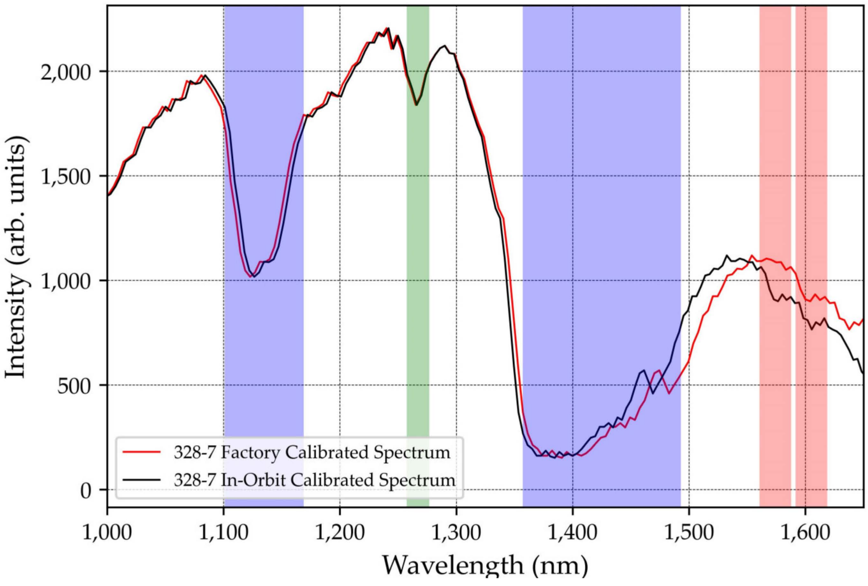
3.2. In-Orbit Spectral Calibration Results

Figure 8a shows the wavelength calibration curve of the spectral response of the spectrometer. The wavelength calibration fits slightly with a second-order polynomial. Figure 8b presents the calibrated measured spectrum. Bands in red, blue, and green correspond to CO_2, H_2O, and O_2, respectively. In contrast to factory calibration, in-orbit calibration more accurately aligns with the CO_2 absorption bands.



(**a**)

Figure 8. *Cont.*



(**b**)

Figure 8. (**a**) Wavelength vs. number of pixel calibration curve. (**b**) Comparison between in–orbit and factory calibrations relative to absorption bands of H_2O (purple), O_2 (green), and CO_2 (red).

3.3. Simulated Spectrum Algorithms Results

Figure 9 shows a synthetic spectrum generated with the Genspect code. The simulation was performed in the spectral range between 900 and 1700 nm for an altitude of 70 km above the ground and a gas mixture of CO_2, CO, O_2, and H_2O. As reported by Thompson et al. [29], these gases have widely characterized absorption bands in the ARGUS 2000 spectral range. The TCCON platform provides concentration profiles and atmospheric reference data (pressure and temperature profiles) for the location where the gas profile measurement was performed [30]. The atmospheric model is divided into 51 atmospheric sub-layers, one concentration per sub-layer. The construction of the synthetic spectrum requires other parameters such as the nadir angle of observation, the zenith angle of the sun, the radiation model, and the reflectivity of the observation surface. The satellite and solar zenith angles computed for this simulation were ~4.094° and 43.94°, respectively, according to the acquisition performed by FACSAT-2 on this point of the Earth presented in Figure 6. For the construction of the blackbody radiation model of the Sun and the Earth, temperature values for the Sun and the Earth of 6000 and 278 K [31], respectively, have been introduced. Finally, an earth reflectivity factor of 0.35 has been selected. Nevertheless, the reflectivity value, in addition to the Sun and Earth temperature values and the concentration profile, can be modified to achieve an optimal alignment between the synthetic and measured spectra.

Instrumental parameters such as resolution, the FOV angle (solid angle), the geometry of the focusing lens, and the ARGUS 2000 slit function are included in the synthetic spectrum. Figure 10 shows the six slit functions that have been evaluated.

Figure 11 shows convolved spectra with each of the slit functions used here. Figure 12 shows the results of the conversion of the radiance convolved spectra to Figure 12, energy spectra (Figure 12a), and count detector spectra (Figure 12b). A Full Width at Half Maximum (FWHM) of approximately 1.5 times the average wavenumber, spacing around 1600 nm, has been used. The Michelson and rectangular slit functions have considerable noise along the spectrum for the chosen resolution. For each slit function, the mean square error was computed in the 1570–1620 nm wavelength range, obtaining 0.0072 for Michelson, 0.0037 for Gaussian, 0.0038 for triangular, 0.005 for dispersion, 0.0045 for rectangular, and 0.0035 for diffraction slit functions. The findings indicate that, for the case of CO_2 absorption, the diffraction function and the Gaussian function are observed to exhibit the most optimal performance.

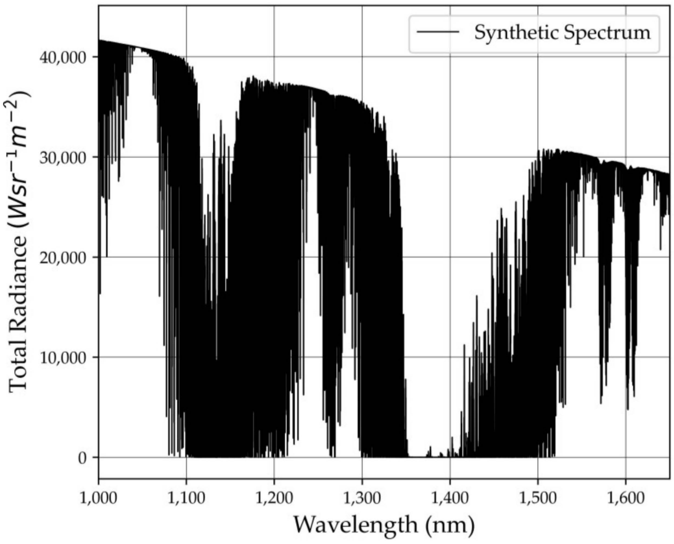


Figure 9. Synthetic spectrum generated with Genspect Toolbox.

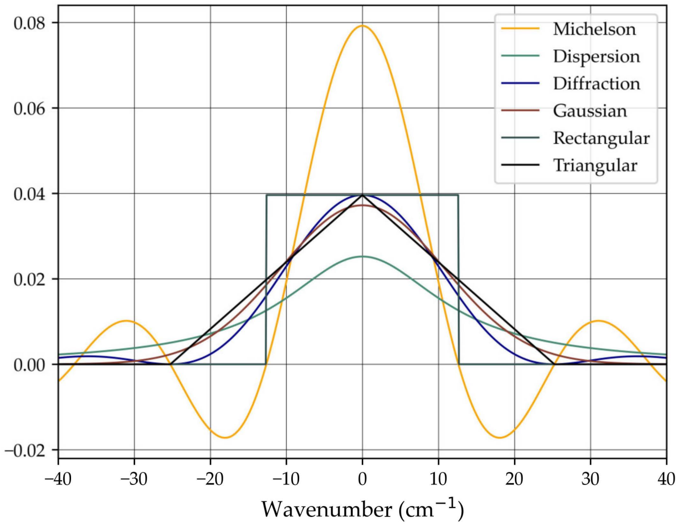


Figure 10. Slit functions.

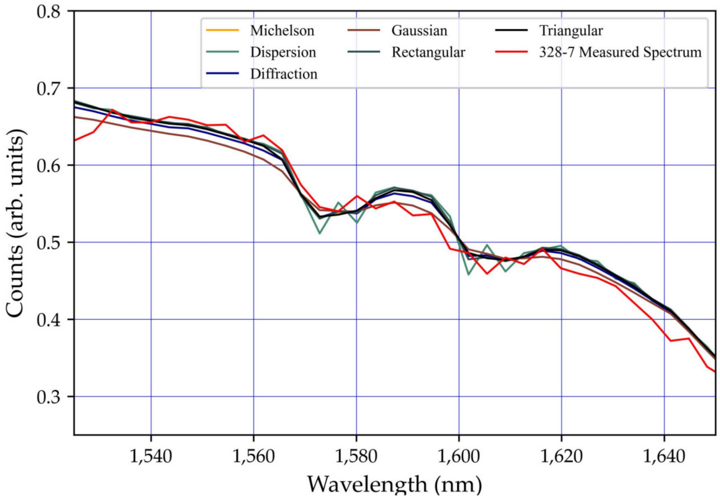
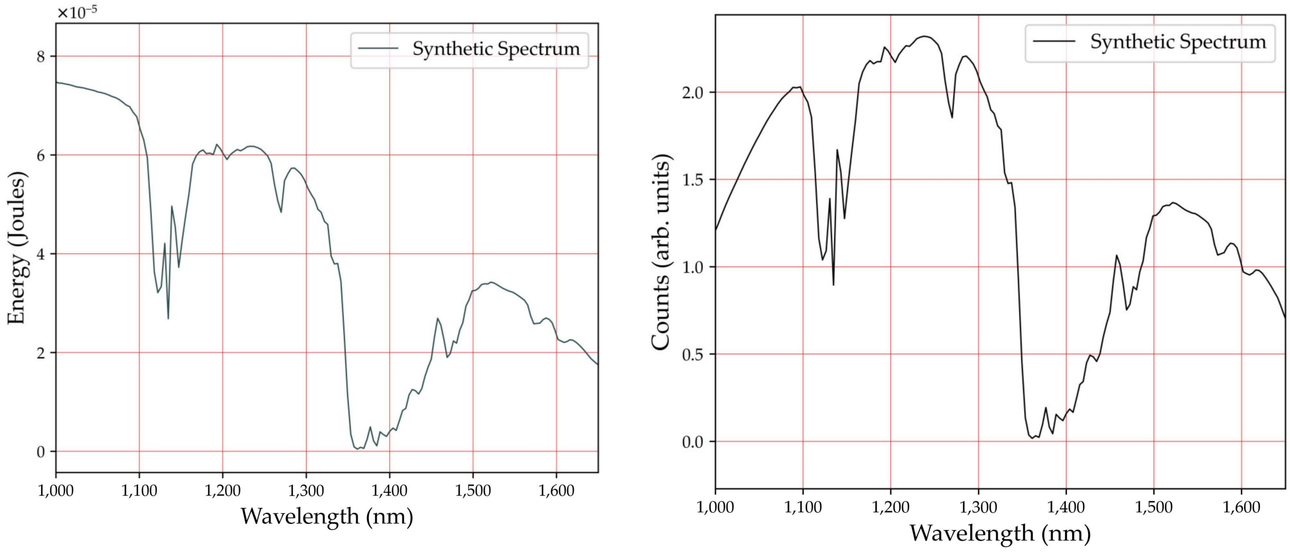


Figure 11. Match between the convolved synthetic spectrum with several slit functions and the real spectrum acquired by ARGUS 2000.



(**a**) (**b**)

Figure 12. (**a**) Conversion of synthetic spectrum from radiance to energy units and (**b**) conversion from energy to instrumental counts.

Figure 13 presents the first spectrum measured over the sea in session 328 (as depicted in Figure 6). That is compared to a synthetic spectrum generated using a concentration profile aligned with the TCCON results for that location. The two spectra show high concordance, especially in the spectral region where the CO_2 absorption bands appear. The O_2 absorption band also shows a high relation in the experimental spectrum (measured spectrum) and the synthetic spectrum. However, the H_2O absorption bands differ in their relative intensity because the concentration of water in the atmospheric column depends on seasonal processes and meteorological conditions.

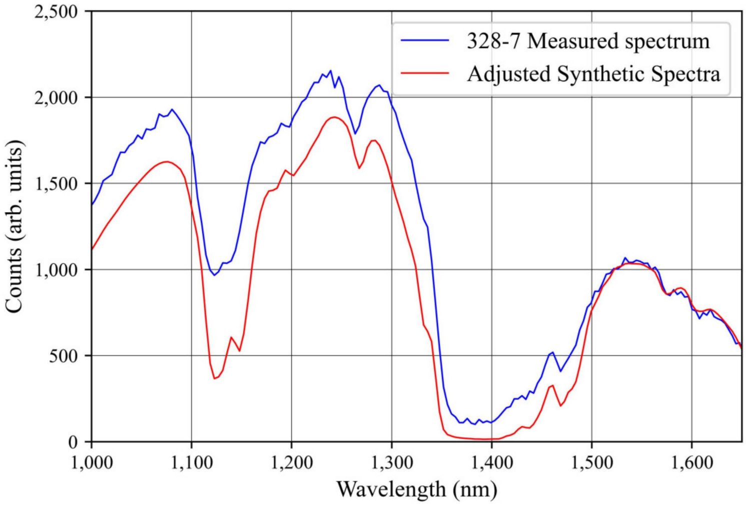


Figure 13. Comparison between synthetic and measured spectra.

4. Discussion

The successful integration, commissioning, and in-orbit calibration of the ARGUS 2000 SWIR spectrometer onboard the FACSAT-2 satellite represent a significant milestone in Colombia's space exploration efforts, particularly in the remote sensing of GHG. The ability of the satellite to acquire consistent spectral signatures over a year in orbit demonstrates the reliability of the instrument.

One of the key aspects of this study involved the development of retrieval algorithms using the Genspect commercial software to generate synthetic spectra. By incorporating instrumental parameters such as FOV angle, quantum efficiency, slit function, and spectral resolution, the synthetic spectra were fine-tuned to align closely with the real spectra acquired from the satellite. The effectiveness of the Gaussian and diffraction slit functions in accurately simulating the experimental spectra is particularly noteworthy, as it highlights the importance of choosing appropriate slit functions in spectral analysis.

The comparison of the synthetic spectra with real data using TCCON concentrations as a benchmark provides a strong validation of the calibration and retrieval processes employed. The match between the synthetic spectra and the spectral signatures acquired by FACSAT-2 over Tenerife indicates that the methodologies used in this study are effective for accurate remote sensing of atmospheric gases; however, it also raises questions about the limitations and potential sources of error in the current approach.

One area that guarantees further exploration is the treatment of nonlinearities in the spectrometer's response. While the current approach has been successful without explicitly considering these phenomena, future work needs to investigate their impact on the accuracy of the retrieved spectra. In addition, global optimization processes could be explored to better tune the parameters that influence the simulated spectrum to check if they offer further improvements in the spectral match.

The outcomes of this work validate the operational capabilities of the spectrometer and provide valuable insights into the challenges and opportunities associated with the remote sensing of GHG from space. This study lays the groundwork for further advancements in this field, particularly in refining the retrieval algorithms, expanding the analysis to other atmospheric gases, and exploring new methods for spectral calibration and validation.

5. Conclusions

Over approximately one year in orbit, the satellite has consistently acquired spectral signatures, which have been used in characterizing the data and performing the calibration processes. The spectral calibration presents a behavior following a second-order adjustment model, ensuring accuracy and reliability in the spectral data obtained.

To analyze the spectral data, retrieval algorithms were developed to generate synthetic spectra using the Genspect commercial software. These synthetic spectra, derived from the spectroscopic data of atmospheric gases (H_2O, O_2, CO, and CO_2) in the HITRAN database, were enhanced by incorporating key instrument parameters such as spectrometer resolution, the field of view angle, the quantum efficiency of detection, and the instrument slit function. Among the six slit functions tested, the Gaussian and diffraction functions prove to be the most effective in simulating the experimental spectra.

To compare the synthetic spectra with real data, a profile of Total Carbon Column Observing Network (TCCON) concentrations was used as a benchmark, resulting in a good match between the synthetic spectra and the spectral signatures acquired by FACSAT-2 over Tenerife. This validation demonstrates the accuracy and efficacy of the retrieval algorithms and the overall calibration methodology employed.

The outcomes of this work not only validate the operational capabilities of the FACSAT-2 ARGUS 2000 SWIR spectrometer but also contribute valuable insights into the remote sensing of GHG from space. Future work will focus on refining the retrieval algorithms, exploring the potential of additional slit functions, and expanding the analysis to other atmospheric gases.

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project administration, L.P.C.E., J.P.M. and A.C. All authors have read and agreed to the published version of the manuscript.

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