

# Measuring atmospheric CO<sub>2</sub> from Space using Full Spectral Initiation (FSI) WFM-DOAS: Initial Results and Validation

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## Abstract

Atmospheric CO<sub>2</sub> concentrations, retrieved from spectral measurements made in the near infrared (NIR) by the SCIAMACHY instrument, using a new retrieval algorithm called Full Spectral Initiation Weighting Function Modified Differential Optical Absorption Spectroscopy (FSI WFM-DOAS), are compared to ground based Fourier Transform Infrared (FTIR) data and to the output from a global chemistry-transport model. Comparisons to CO<sub>2</sub> measurements made by the ground based FTIR spectrometer at Egbert, Canada, reveal a negative bias in the FSI WFM-DOAS columns of approximately -4.0%, though this offset appears to be decreasing with time. Similar comparisons to the TM3 chemistry transport model show that the temporal behaviour of the seasonal cycle is captured well but that its amplitude is over estimated. From these comparisons, the overall precision and bias of the CO<sub>2</sub> columns retrieved by the FSI algorithm are estimated to be close to 1.0% and <4.0% respectively.

## 1. Introduction

Over the last 200 years there has been a dramatic 30% increase in the concentration of atmospheric CO<sub>2</sub>. This is expected to lead to significant future climate change [1]. To accurately predict the response of our climate requires a full understanding of the transport and storage of carbon within the carbon cycle. Current understanding of the global carbon cycle, provided by inverse modelling techniques, estimate the carbon fluxes by means of chemistry transport models constrained with accurate measurements of the atmospheric CO<sub>2</sub> concentration. Whilst there have been significant advances using this approach [2] it is still only possible to estimate the carbon cycle fluxes at continental or ocean basin scales, as the present inversion system is data limited [3]. Satellite observations of atmospheric CO<sub>2</sub> concentrations can help reduce the flux uncertainties and locate unidentified carbon sources and sinks, as they offer greater temporal and spatial coverage than the current observing network [4]. To improve over the existing ground network monthly averaged column data, at a precision of 1% (2.5 ppmv) or better, for an 8° by 10° footprint are needed [5], although regionally this threshold can be relaxed [4].

In this work, atmospheric CO<sub>2</sub> vertical columns are retrieved from SCIAMACHY NIR measurements using a new algorithm called Full Spectral Initiation (FSI) WFM-DOAS are compared both to FTIR measurements and to a global chemistry-transport model to ascertain the quality and accuracy of the retrieval method.

## 2. SCIAMACHY

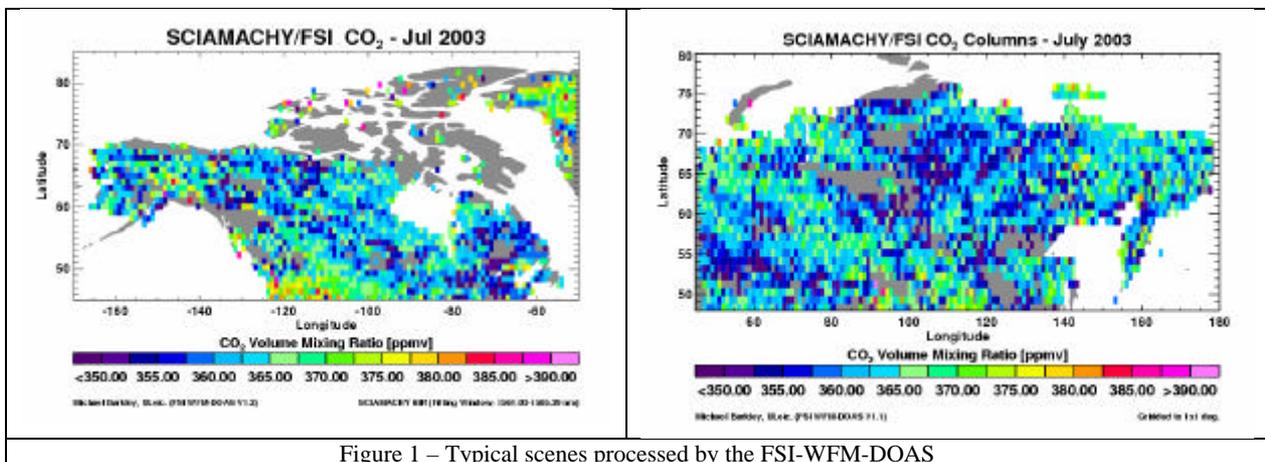
Launched onboard the ENVISAT satellite, in March 2002, the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) instrument is a passive UV-VIS-NIR hyper-spectral spectrometer designed to investigate tropospheric and stratospheric composition and processes [6]. The instrument measures sunlight that is reflected from or scattered by the atmosphere, covering the spectral range 240-2380 nm (non-continuously) using eight separate grating spectrometers (or channels). For the majority of its near polar sun-synchronous orbit SCIAMACHY makes measurements of the atmosphere in an alternating limb-nadir sequence. In addition the solar irradiance and lunar radiance are measured using solar/lunar occultation. The vertical column densities (VCDs), (units of molecules cm<sup>-2</sup>), of various trace gases, whose absorption features lie within SCIAMACHY's spectral range, can then be determined through the inversion of the logarithmic ratio of the earthshine radiance and solar irradiance via differential absorption spectroscopy (DOAS) [7]. In this analysis, atmospheric CO<sub>2</sub> distributions are determined by retrieving CO<sub>2</sub> VCDs from nadir observations made in the NIR, focussing on a small micro window within channel six, centred on the CO<sub>2</sub> band at 1.57 μm. For channel 6, the nominal size of each pixel within the swath is 60 by 30 km<sup>2</sup>, corresponding to an integration time of 0.25 s. Global coverage is achieved at the Equator within 6 days.

### 3. Full Spectral Initiation (FSI) WFM-DOAS

Since the launch of the SCIAMACHY instrument on-board ENVISAT there is the ability to measure total vertical columns of CO<sub>2</sub> in the near infrared (NIR) using a new retrieval technique called *Weighting Function Modified Differential Optical Absorption Spectroscopy* (WFM-DOAS) [8]. The WFM-DOAS method is based on fitting the logarithm of a linearised radiative transfer model plus a low-order polynomial to the logarithm of the ratio of a measured nadir radiance and solar irradiance spectrum as measured by the SCIAMACHY instrument.

An initial assessment of this algorithm's sensitivity, described in [9], discovered it is necessary to include suitable *a priori* information within the retrieval in order to constrain the errors on the retrieved CO<sub>2</sub> columns. Using this premise, a new CO<sub>2</sub> retrieval algorithm called **Full Spectral Initiation (FSI) WFM-DOAS** [9], has been developed which generates a reference spectrum for each individual SCIAMACHY observation, based on the known properties of the atmosphere and surface at the time of the measurement. As the calculation of radiances is computationally expensive, FSI is not implemented as an iterative scheme rather each reference spectrum only serves as the best possible linearization point for the retrieval. Each spectrum is generated using the radiative transfer model SCIATRAN [10], using several different sources of atmospheric and surface data that serve as input, the details of which are described in full in [9].

The FSI algorithm is only applied to cloud free pixels, determined using a cloud detection method outlined in [11], with the retrieved CO<sub>2</sub> VCD normalized using the input *a priori* surface pressure to produce a column volume mixing ratio (VMR). Only CO<sub>2</sub> VMRs where the retrieval (statistical) fitting error is less than 5% and which lie in a range 340-400 ppmv are used. To avoid various instrumental issues that have hampered retrievals in the NIR channels [12] the raw SCIAMACHY spectra have been calibrated in-house with corrections applied for non-linearity effects, associated with analogue-to-digital converter, and also the orbit specific dark current. To improve the quality of the FSI spectral fits, the latest version of the HITRAN molecular spectroscopic database [13] has been implemented in SCIATRAN. Unlike other studies [14], adjustment of the absolute columns values *via* scaling factors, has not been necessary. The advantage of the NIR over the thermal infrared is the sensitivity to changes in the CO<sub>2</sub> concentration in the lowermost part of the troposphere. This is demonstrated by the FSI averaging kernels (not shown) which peak in the planetary boundary layer indicating that the FSI algorithm is sensitive to changes in the CO<sub>2</sub> near the surface, i.e. where the carbon sources and sinks occur. An example set of FSI retrievals is shown in Fig 1.



### 4 Comparisons to FTIR CO<sub>2</sub> measurements over Egbert, Canada

A comparison between the columns retrieved by the FSI algorithm to CO<sub>2</sub> columns measured by a ground based (g-b) FTIR spectrometer has been undertaken to assess possible biases in the retrieval. This FTIR instrument, run by Environment Canada, is located at the Centre of Atmospheric Research Experiments (CARE), Egbert, Canada (44.23°N -79.78°E). It is situated within a large rural area, away from background pollutants, thus rendering it ideal for making atmospheric measurements. Solar absorption spectra are recorded, in cloud-free conditions, approximately twice each

month using an ABB Bomen DA8 FTIR spectrometer that has an apodized resolution of  $0.004 \text{ cm}^{-1}$ . Measurements of the  $\text{CO}_2$  total columns are derived from the recorded spectra, using two wavelength intervals  $2625.35 - 2627.06 \text{ cm}^{-1}$  and  $936.44 - 937.18 \text{ cm}^{-1}$ , to an accuracy of 8.9% (error estimate based on the discussion in [15]). The detailed methodology of the comparison is dealt with in [16] with the results only summarized here.

During 2003 there were a total number of 5150 successful cloud-free  $\text{CO}_2$  FSI retrievals over the Egbert site. These are illustrated in Fig. 2, together with the corresponding 74 g-b FTIR measurements, shown both as VCDs and VMRs. The mean yearly bias of the FSI  $\text{CO}_2$  columns with respect to the g-b data is  $-4.1\%$ , with a standard deviation of 3.0% and scatter of 0.8%. These results are consistent with the WFM-DOAS results presented in Dils *et al.* (2005) [17] who also reported a significant negative bias, though in this analysis the mean bias is approximately half their reported value. The spread of the FSI retrievals is quite small (0.8%) when compared to the scatter of the FTIR data (1.3%). Normalizing the  $\text{CO}_2$  vertical columns, using the ECMWF surface pressure, does not have a dramatic effect only slightly increasing the bias on both grids by about 0.2%, though the scatter does become almost twice as great. Irrespective of whether the  $\text{CO}_2$  columns are expressed as VCDs or VMRs a perceptible seasonal trend (not shown) of the bias is apparent. The origin of this bias and its seasonal variation has not been identified. Differences between the SCIAMACHY and FTIR averaging kernels may account for some of the negative bias whilst the limited number of the g-b measurements may partly explain its temporal evolution. Nevertheless, this bias does decrease rapidly in the latter months of 2003, thus a more comprehensive set of FTIR observations for 2004 is required to see if this seasonal pattern is repeated.

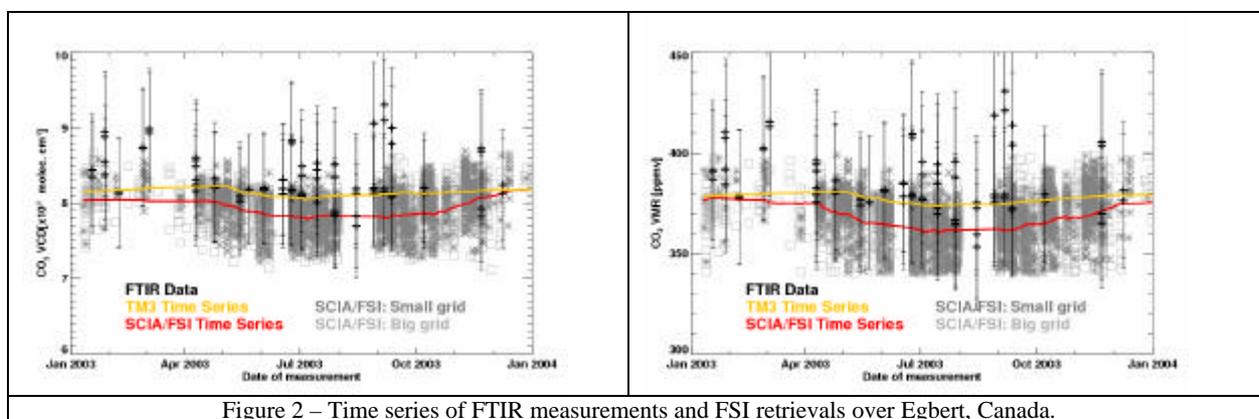


Figure 2 – Time series of FTIR measurements and FSI retrievals over Egbert, Canada.

## 5. Comparisons to the TM3 chemistry transport model

The TM3 is a global atmospheric tracer model [18], developed by the Max Planck Institute for Biogeochemistry (MPI-BGC), which solves the continuity equation for an arbitrary number of atmospheric tracers. The atmospheric transport is driven by National Center for Environmental Prediction (NCEP) meteorological fields using a model grid of  $1.8^\circ$  by  $1.8^\circ$  with 29 layers. The ocean air-sea fluxes are based on a monthly  $p\text{CO}_2$  climatology [19] whilst the natural terrestrial biospheric fluxes were modelled using the BIOME-BGC model driven with daily NCEP data, using a simple diurnal cycle algorithm [20]. Anthropogenic fossil fuel  $\text{CO}_2$  emissions are derived from the EDGAR 3.2 database [21]. The TM3  $\text{CO}_2$  columns have been calibrated to for an optimal match with in-situ observations made at the South Pole station and with a mean FSI averaging kernel applied to the model data to account for the increased sensitivity of SCIAMACHY to the lower part of the troposphere. The model itself, has been sampled at the exact location and time (using the model's closest 3 hourly time step) for each FSI retrieved  $\text{CO}_2$  column that has passed the quality filter. Both data sets have then been averaged onto a  $1^\circ$  by  $1^\circ$  grid with the temporal and spatial behaviour of the  $\text{CO}_2$  distributions then examined. In this paper comparisons have been made for two specific regions: Siberia and the Gobi desert.

The temporal behaviour of  $\text{CO}_2$  concentration over the Siberian region is illustrated in Fig. 3, with the time series plot of the monthly averages demonstrating that there is quite good agreement between the model and the FSI algorithm. The correlation coefficient between the two time series is 0.75 and the TM3 monthly means lie within the FSI error limits for all but the summer months. The most noticeable difference is that whilst during the winter months there is excellent agreement between the model and observations, during the rest of the year SCIAMACHY detects lower  $\text{CO}_2$  concentrations. The yearly average of the absolute difference is 7.3 ppmv (2%) with the mean of the standard deviations (of the monthly differences) being 7.6 ppmv.

The mean CO<sub>2</sub> concentration for the whole year detected by SCIAMACHY is 371.2 ppmv whereas the model average is 377.5 ppmv. This suggests a negative bias between the model and FSI retrievals of about ~2.0% (relative to the FSI scene mean). The amplitude of the seasonal cycle (peak to peak) is 20.7 ppmv detected by SCIAMACHY is just under three times that of the model (7.9 ppmv) with both time series agreeing on the timing of the minimum CO<sub>2</sub> concentration in July, though disagreeing on the occurrence of the maximum (April for the TM3 and January for SCIAMACHY). Similar results were presented by [14] who reported a factor of four greater amplitude. Inspecting the time series of the CO<sub>2</sub> anomaly shows that the transition from positive to negative, as biospheric photosynthesis exceeds respiration, begins slightly earlier for the FSI data (late April) than the model (early May). Both data sets agree on the return crossover in mid-October. Over the Gobi Desert the match between the TM3 model data and the retrieved CO<sub>2</sub> concentrations is excellent with the correlation between the time series now being 0.95 and with both agreeing on the timing of the maximum (April) and minimum (July) CO<sub>2</sub> concentrations. The CO<sub>2</sub> anomalies are thus in phase and the small difference between yearly means, 374.0 ppmv (FSI) and 377.3 ppmv (TM3) (about 1%), is most likely due to the increased signal to noise ratio produced by the high albedo of the desert surface. In spite of the better agreement, SCIAMACHY still detects a seasonal signal, transported from other regions, which is just over twice that of the TM3 data (10.1 ppmv to 4.9 ppmv).

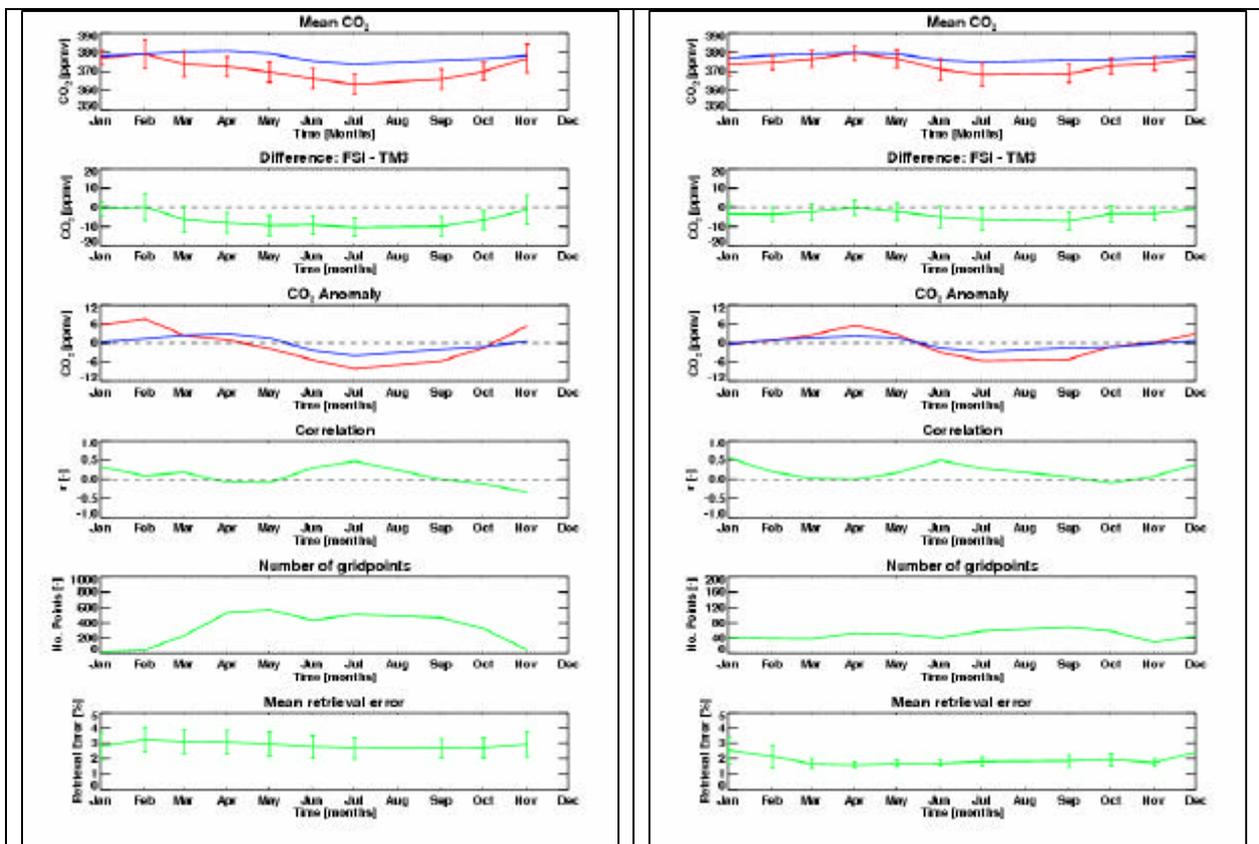


Figure 3 - Comparisons between the TM3 model data (blue lines) and the FSI retrieved CO<sub>2</sub> columns (red lines) for the (a) Siberian (left) and (b) Gobi desert (right) regions for the year 2003. Top Panels: The mean CO<sub>2</sub> concentration of each scene. The error bars on the FSI data represent the 1 $\sigma$  standard deviation of the mean. Second panels: The mean difference between the FSI columns and the TM3 data (equivalent to the difference between the monthly averages). The error bars represent the 1 $\sigma$  standard deviation of this difference. Third Panels: The CO<sub>2</sub> anomaly (i.e monthly averages minus the yearly mean). Fourth Panels: The correlation coefficient between the two data sets. Fifth Panels: The number of TM3 grid points used in the calculation of the scene means. Bottom Panels: The mean FSI retrieval error of the observed CO<sub>2</sub> columns with the 1 $\sigma$  standard deviation, which is consistently less than 1%. Note, at the time of processing, SCIAMACHY data for August was not available and that for December there was not enough valid FSI retrievals to perform a sensible comparison.

## 6. Precision and Errors

It is important to give some assessment of the accuracy (bias) and precision of the CO<sub>2</sub> VMRs retrieved by the FSI algorithm. The mean retrieval (spectral fitting) errors over the selected scenes is <3%. These fit errors are predominantly affected by the signal to noise ratio of the spectra and thus are strongly influenced by the surface albedo. The standard deviation of the 'raw' (un-gridded) FSI CO<sub>2</sub> columns is ~3.0% which seems consistent with the mean retrieval errors. The mean of the standard deviations, of the retrieval errors over each scene, is consistently below 1% implying that FSI spectral fitting procedure is itself quite precise. The mean root mean square (RMS) error of the spectral fits is also extremely stable at 0.1-0.3%. It is difficult to estimate the bias of the retrieval using FTIR data from only a single ground station. The normalized CO<sub>2</sub> columns retrieved over the Egbert instrument have a negative average monthly bias of approximately -4.0%, although this does vary seasonally and decreases dramatically towards the end of 2003. Without comparisons to other column measurements made at other locations it is impossible to determine whether this bias is consistent globally or intrinsic only to the Egbert station. However, comparisons of the FSI retrievals to the TM3 data suggest a negative bias of about -2% with respect to the model, which when coupled with the -2% bias of the TM3 data to the FTIR measurements themselves, implies that a bias of -4% to the true CO<sub>2</sub> concentration is probably realistic (assuming both the FTIR and model data are correct).

## 7. Summary

Atmospheric CO<sub>2</sub> VMRs have been successfully retrieved from SCIAMACHY measurements in the NIR using the FSI retrieval algorithm with comparisons to both ground based FTIR data and to the TM3 global chemistry transport model also performed.

With respect to the measurements made by the Egbert FTIR station, the yearly bias and its standard deviation of the FSI CO<sub>2</sub> VCDs are found to be approximately -4.1% and 3.0% respectively, with the relative scatter comparable to the scatter of ground-based measurements themselves. Inspection of the average monthly biases reveals an apparent seasonal trend, the cause of which has not been established. Normalizing the FTIR VCDs with the surface pressure does not remove this bias or its seasonal variation. Intermittent observations by the FTIR instrument and differences between its averaging kernel and that of SCIAMACHY may partly be responsible for these dissimilarities.

Comparisons to a global chemistry-transport model, performed over Siberia and the Gobi desert show good agreement, with the correlation, between the time series of the SCIAMACHY and model monthly scene averages, being greater than 0.7. The yearly means are detected by SCIAMACHY are to within 2% of those of the model with the mean difference between the CO<sub>2</sub> distributions being also approximately 2%. The amplitude of the seasonal cycle, peak to peak, however, is overestimated by a factor 2-3, which as yet cannot be explained.

From these comparisons, the overall precision and bias of the CO<sub>2</sub> columns retrieved by the FSI algorithm are estimated to be close to 1.0% and <4.0% respectively.

It also must be re-stressed that at no stage whatsoever have scaling factors been applied to the FSI retrieved CO<sub>2</sub> VMRs as they have been in other studies. Whilst these results are encouraging they are still not of the desired quality for inverse modelling. It is hoped that further improvements to the retrieval algorithm, through better calibration of the SCIAMACHY data and by improving the quality of the input *a priori* data used in the creation of the reference spectra, will overcome this issue in the future.

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