An evaluation of CO₂ observations with Solar Occultation FTS for Inclined-Orbit Satellite sensor for surface source inversion

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[1] An assessment of the utility of CO₂ vertical profile measurements by a solar occultation based satellite sensor is made. We have compared the impacts of these possible vertical profile observations and optimal extensions of the present surface measurement network on the estimation of CO₂ regional sources by inverse model. Time-independent inverse models at two spatial resolutions (22 and 53 regions) and a global transport model are employed in this study. A realistic satellite measurement frequency distribution, obstruction of observation due to clouds, an observation error model for natural CO₂ variability have been used. The satellite measurements are valuable to constrain the source uncertainties for the tropical lands with no existing observations. The optimal extension of the surface network appears to be the more effective way to reduce average inverse model uncertainty under both low and high inverse model resolutions; however, in high-resolution inversion the relative merit of the satellite data is higher than that in the low-resolution case. Our study suggests that the CO₂ observation at greater data density can constrain the inverse model fluxes better. We show that the systematic errors in satellite observations can lead to significant shifts in the inverse model-estimated fluxes. INDEX TERMS: 0322 Atmospheric Composition and Structure: Constituent sources and sinks; 0368 Atmospheric Composition and Structure: Troposphere—constituent transport and chemistry; 0394 Atmospheric Composition and Structure: Instruments and techniques; 1640 Global Change: Remote sensing; KEYWORDS: CO₂, measurements, network optimization, source inversion


1. Introduction

[2] Inversion of atmospheric data for the estimation of carbon dioxide (CO₂) surface sources relies vastly upon the quality and quantity of atmospheric measurements, and the ground based measurements have been supporting this effort till now [Tans et al., 1990; Fan et al., 1998; Bousquet et al., 2000; Gurney et al., 2002]. The utility of satellite observations in estimating the surface sources of CO₂ is evaluated very recently under certain assumptions [Rayner and O’Brien, 2001; Pak and Prather, 2001; Rayner et al., 2002]. Most of the assumptions arise due to the unknown parameters such as effect of clouds and aerosols on observation statistics, data variability at different layers of the troposphere, error in the retrieval algorithm and instrumental precision. Only now attempts are being made to retrieve interannual and seasonal variation of CO₂ and other radiatively active gases from the past records of satellite instruments [Chédin et al., 2002]. Feasibility studies are also conducted on recent and forthcoming remote sensors, such as the Interferometric Monitor for Greenhouse Gases (IMG) on board the Advanced Earth Observing satellite (ADEOS), Infrared Atmospheric Sounding Interferometer (IASI) on the European METOP, Atmospheric InfraRed Sounder (AIRS) launched on NASA Aqua platform [Chédin et al., 2003]. Probably, more sophisticated retrieval algorithm and higher spectral resolution are needed to fulfill the goal of utilizing satellite derived products in estimating the global source/sink distribution of atmospheric trace gases. Such measurements are expected to play positive role in quantification of the terrestrial carbon sources and sinks at a sub-continental
scale (~10^7 km^2), while an uncertainty ‘less than the source itself’ is targeted globally [Cihlar et al., 2002]. The present surface monitoring network does not allow assessment of CO₂ sources from each of the inverse model regions with equal confidence. Some studies have indicated that the present surface CO₂ measurement network has to be extended rather uniformly worldwide for better constraining the regional average source uncertainties [Rayner et al., 1996; Gloor et al., 2000; Patra and Maksyutov, 2002]. The upper tropospheric observations of CO₂ on board the aircrafts flying between Tokyo and Sydney are also useful to reduce the uncertainties in flux estimation of Asian regions by a measurable amount [Maksyutov et al., 2003].

It is established for quite sometime now, since the study by Rayner et al. [1996], that observations are needed from tropical/continental locations to constrain the flux estimate uncertainties in atmospheric data inversions. However, the optimal extension of surface observation network has not been realized because of logistical problems. This will probably direct the future measurement strategy of CO₂ toward remote sensing, which should be equally efficient at the sub-continental scale globally. Such observations will also enable us to monitor the progress followed by the international greenhouse gas mitigation policies such as Kyoto-protocol on a longer timescale. Recently, the CO₂ measurements from satellites have drawn considerable attention and plans are being materialized by various space agencies; e.g., the SCanning Imaging Absorption Spectrometer for Atmospheric ChartographY (SCIAMACHY) [http://envisat.esa.int/ offers concept, operation, characteristics of this instrument], and the AIRS instrument on board the Aqua-series spacecraft. There are also a few missions undergoing tests for CO₂ observation such as Orbiting Carbon Observatory (OCO) [http://oco.jpl.nasa.gov], Solar Occultation FTS for Inclined-orbit Satellite (SOFIS) [http://eos.nasa.go.jp]. Theoretical and laboratory evaluations for retrieving the vertical profiles of CO₂ in the upper-middle troposphere and stratosphere from the SOFIS radiation spectra are initiated [Uemura et al., 2001; Nakajima et al., 2001; Kuze et al., 2002]. While other studies are focusing on improving the data retrieval mechanisms based on the knowledge of meteorological state of the atmosphere from general circulation models [Engelen et al., 2001].

It has been shown based on 15 transport models and model variants that the distribution of additional atmospheric measurements to constrain the source uncertainties do not differ significantly with models [Patra et al., 2003]. The variations in estimated flux uncertainty with optimally placed additional stations, using the transport model simulations as used in this study, are fairly similar to that can be obtained with the model-ensemble average. That is an important conclusion for this study since we have used the forward model simulations by only one of the TransCom-3 participating models. As inverse models at two different resolutions are worked upon here, simulations from multiple models are not available for the source functions of newly divided inverse model regions. The flux estimate uncertainties using optimal extensions of the present surface observation network and proposed satellite measurements are discussed in connection with the increase in number of inverse model regions and reduction in atmospheric data errors.

Some examples of atmospheric transport model simulations and the details of inverse model frameworks, outline of the proposed satellite technique for CO₂ observations, and assumptions in processing the remote sensing data for inverse modeling purpose are discussed in Section 2. The comparisons of flux uncertainty estimations with several surface measurement networks and various satellite data use scenarios in surface source inversions are given in Results and Discussion section, followed by the Conclusions.

2. Materials and Methods

2.1. Tracer Transport Model

We have used the global transport model developed at the National Institute of Environmental Sciences (NIES) and later improved jointly at FRSGC and Tohoku University. This will be referred to here as NIES/FRSGC transport model. The model has 15 sigma levels in the vertical, 144 longitudes and 72 latitudes in horizontal at a resolution of 2.5 degrees. The advection scheme is semi-Lagrangian and subgrid scale processes are parameterized for vertical diffusion, penetrative mass flux, and turbulent diffusivity in the planetary boundary layer. The model transport is driven by the 12 hourly ECMWF (European Center for Medium-range Weather Forecasts) operational analyses for 1997. Further details of the model configuration and performance analysis can be found in a validation paper [Maksyutov and Inoue, 2000]. Figures 1a, 1b, 1c and 1d show the NIES/FRSGC model simulated CO₂ distributions at different pressure layers in the middle and upper troposphere. The annual average maps are obtained from the simulations of global fluxes from four known sources (also referred to as ‘pre-subtracted’ fields here); namely, the fossil fuel combustions in 1990 [Andres et al., 1996] and 1995 (A. L. Brenkert, Carbon dioxide emission estimates from fossil-fuel burning, hydraulic cement production, and gas flaring for 1995 on a one degree grid cell basis, available at http://cdiac.esd.ornl.gov/ndps/ndp058a.html, 1998), net ecosystem production [Randerson et al., 1997] and the ocean-atmosphere exchange [Takahashi et al., 2002]. Grossly, the CO₂ concentrations are higher in the northern hemisphere (NH) compared to that in the southern hemisphere (SH) at all heights. The interhemispheric gradient decreases from an average value of about 4 ppm at 500 mb to about 2 ppm at 200 mb. The weakening or dilution of the CO₂ source signal with height impose a stricter requirement on measurement.

Figure 1. (opposite) Annual average source signals of CO₂ (Figures 1a, 1b, 1c, and 1d) and the estimated residual standard deviations (RSDs) (Figures 1e, 1f, 1g, and 1h) at various layers of the atmosphere are depicted. The global sources due to fossil fuel emission representing 1990 and 1995, and seasonally varying biospheric and oceanic fluxes are combined for this simulation. The period of the model integration was set to 3 years (e.g., 01 January 1992 to 31 December 1994) and only the second year averages are shown here as the signals. The RSDs are estimated from the daily average time series for two consecutive years. See color version of this figure at back of this issue.
accuracy in the upper-middle troposphere when the data are to be utilized in the study of CO$_2$ seasonal cycle and analysis of longterm trends or in the inverse model estimation of surface sources. On the right panels (Figure 1e, 1f, 1g, and 1h) the residual standard deviations (RSDs) are shown. At each transport model grid, a seasonal cycle is fitted to the daily model CO$_2$ concentrations over a period of two years and RSD is estimated using the deviations of data from the fitted seasonal cycle. The RSDs are commonly used as a measure of deseasonalised variability in atmospheric data or high frequency model outputs, and its derivation procedure is elaborated in an earlier publication [Patra et al., 2003]. The RSDs are assumed to be good proxies for data uncertainties ($C_D$) used in inverse models [Enting et al., 1995] and is a matter of intensive discussion in this work. However, since the source variability on timescales shorter than month is neglected the fluctuations in daily mean CO$_2$ values will be determined by the variations in transport at many places. It is interesting to note that though the CO$_2$ signals were low over the tropics compared to the NH middle and high latitudes, the values of RSDs recorded here are among the highest. The values are reaching up to ~1.2 ppm at 500 mb over tropical part of Africa and South America. The upward vertical velocities and associated standard deviations, estimated from the ECMWF meteorological analysis used in the transport model, are also observed to be the highest over the region of high RSDs due to the prevailing convective activities. The other region of high RSDs is located in the European outflow region over Boreal Asia, which is primarily governed by the larger variability in surface sources itself. However, this high variability does not seem to be reaching up to 200 mb, in contrast to that is observed over the tropics.

### 2.2. Inverse Model Setups

[1] The time-independent Bayesian inversion is adopted for estimation of the annual mean fluxes and associated uncertainty. The limitation of the annual mean source inversion is that the salient features such as the dependency of CO$_2$ flux determination on seasonal variation in satellite data coverage [Rayner et al., 2002] cannot be addressed under this framework. Since the high-latitude regions in the winter hemisphere do not see the Sun, there will be no satellite data based on Sofis measurement principle. This is in contrast to the surface observation. However, since we assign data uncertainty to the observations based on annual total measurement frequency as discussed in section 2.3, the results obtained here would be in some agreement with that from the time-dependent inversion, which derives fluxes on monthly timescale, after aggregation to annual mean timescale. In Bayesian inversion an objective function is minimized to reduce the mismatches between the atmospheric observations and transport model predicted CO$_2$ concentrations based on known source strengths and distribution. Thus the maximum likelihood of regional fluxes ($S$), condition on the a priori flux ($S_0$) and associated error covariances ($C_S$), is expressed as:

$$\langle S \rangle = S_0 + \left(G_T C_D^{-1} G + C_S^{-1}\right) G_T C_D^{-1} (D - GS_0)$$

(1)

Where the diagonal elements of $C_D$ consist error covariances (square of uncertainty, U) of atmospheric CO$_2$ data, and $G$ represents the atmospheric transport (also known as response function) [Tarantola, 1987; Enting et al., 1995]. The predicted annual flux covariance matrix ($C_S$) is calculated by an equation as:

$$C_S = \left(G_T C_D^{-1} + G C_S G^T\right)^{-1}$$

(2)

The pseudo-inverse of the matrix ($G_T C_D^{-1} G + C_S$) is determined by singular value decomposition (SVD) as by Patra et al. [2003, and references therein]. In our analysis, we have hypothesized the systematic component of error introduced by the retrieval algorithm and during instrumental operation, and only in this connection the absolute flux is considered in discussion. The rest of the study deals with estimation of flux uncertainty.

[8] The basic inverse model setup was developed as a part of the international effort called TransCom-3 and is described in detail by Gurney et al. [2002, 2003]; the protocol for transport model simulations is also available on World Wide Web (http://transcom.colostate.edu). In the basic setup, the source/sink estimation of CO$_2$ are made for 22 partitions of the globe, of which 11 are land regions and 11 are ocean regions. Thus for TransCom-3 inversion, forward simulations were performed using the NIES/FRSGC model for four background global fluxes (pre-subtracted fields) and the 22 regional flux maps (also known as basis functions). Figure 2 shows the divided regions in TransCom-3 framework, their names and a priori CO$_2$ flux uncertainties. The inverse model estimated fluxes and associated uncertainties by using the atmospheric data at 115 GlobalView stations [Globalview-CO$_2$, 2000] and NIES/FRSGC model simulations are depicted in Figure 3b (dashed line). The 115 GlobalView stations are selected based upon the criteria that these observation locations have at least 1% real data in the period of 1992–1996. This selection ensures existence of the stations and largest observation network in that time period. The atmospheric CO$_2$ data and uncertainty for each of these 115 stations are assigned by following the procedure described in Gurney et al. [2003] and using the actual Globalview-CO$_2$ [2000] data product. These data uncertainties compares fairly well with the model derived RSDs [see Patra et al., 2003].

[9] Since we are evaluating future measurement scenarios from the space in this work, questions often arise how the requirement of observing the atmosphere will change with the spatial resolution of inverse models and/or the increase in vertical layers in a transport models. For such purpose we have divided the Tropical Asia into 2 regions and each of the remaining 10 land regions of TransCom-3 into 4 regions of near-equal area (eye estimated). We have decided not to split the ocean regions since the oceanic flux exhibits relatively less spatial heterogeneity compared to that of the land regions. Hereinafter this inverse model framework with 53 regions (42 land and 11 ocean) will be referred to as ‘HiRes’ setup. The a priori source uncertainties for the HiRes regions are assumed to be proportional to total flux of that region, and are calculated from the prior flux uncertainty prescribed for the original TransCom-3 region following this relation:

$$U_S(\text{HiRes}) = U_S(\text{TransCom}) \cdot 2 \cdot \frac{S_0(\text{HiRes})}{S_0(\text{TransCom})}$$

(3)
Under such construction the sum of \( C_{S_0} (\text{HiRes}) \) is equivalent to \( C_{S_0} \) for a particular TransCom-3 region. Several other test runs have been conducted with the basic set of observations at different flux uncertainties. The comparison between HiRes and TransCom-3 under this setup is shown here in terms of region-aggregated a posteriori flux and uncertainty estimates (see Figure 3). The region aggregation is done as 
\[
C(i, j) = \frac{\sum U(i, j) \times U(j, i)}{C^2 \times U(j, i)},
\]
where \( j \) varies from 1 to the number of regions to be aggregated. In the HiRes case a total of 57 tracers are transported for a three year period using the ECMWF meteorological data for 1997 in cyclostationary mode. The flux estimations with both inverse models for same regions show fairly good agreement, well within the uncertainty limits, with one another in the test cases using surface data at 115 stations. The estimated fluxes within one better-constrained TransCom-3 region can vary significantly from one HiRes region to another, as seen for the Temperate North America and Europe regions. It is however surprising that the region aggregation error, suggested by Kaminski et al. [2001], does not seem to put a barrier in comparing the results from TransCom-3 and HiRes inverse model version (after aggregation). A good match between HiRes aggregated flux and single TransCom-3 region flux can be explained by the constraints imposed on the flux estimation for any specific region by the observations (and fluxes) of other regions in the inverse model. As a result the aggregated fluxes of several subregions can not vary freely without disturbing the rather well-determined global balance of fluxes and surface CO\(_2\) observations (see Equation (1)).

2.3. Pseudodata Uncertainty

[16] The scaled value of RSD \( (C_{D_{mod}}) \) combined with the recommended instrumental error \( (C_{D_{inst}}) \) is used as the measure of effective pseudodata uncertainty \( (C_{D_{eff}}) \). These are supplied to the inverse models in order to assess the usefulness of the both future observation strategies, the extended surface network or the satellite measurement. The RSDs, as estimated using the daily output from NIES/FRGGC model simulations of pre-subtracted fields (see Figure 1, right panels), are scaled by the frequency of the observations \( (n) \) using following rule:

\[
C_{D_{mod}} = \text{RSD}^2 \times \frac{365}{n}
\]

For the satellite measurements, \( n \) is determined by the number of satellite passes over a location, obstruction in the viewing path due to clouds etc. The clouds, both visible and

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**Figure 2.** The partitions of 11 land (prefix: Lnd) and 11 ocean (prefix: Ocn) regions in TransCom-3 are shown. The region names are given and those will be used in the text frequently. Fluxes are not determined from Greenland and Antarctic land. In HiRes division, the south-west, south-east, north-west and north-east partitions of each TransCom-3 region are post-fixed with labels a (cyan), b (yellow), c (orange) and d (green), respectively. For example, Lnd01 of TransCom-3 is divided into Lnd01a, Lnd01b, Lnd01c and Lnd01d, respectively. A priori flux uncertainties associated with each TransCom-3 regions are: 0.73, 1.49, 1.41, 1.22, 1.33, 1.41, 1.51, 1.73, 0.86, 0.59, 1.42 Gt C per year for 1–11 Land regions, and 0.27, 0.39, 0.37, 0.63, 0.35, 0.27, 0.41, 0.55, 0.72, 0.48, 0.41 Gt C per year for 1–11 Ocean regions of TransCom-3, respectively. See color version of this figure in the HTML.
invisible by the instruments, are the major obstacle in the remote sensing measurements, particularly in the troposphere. In the next sections we incorporate the correction to $n$ due to visible clouds and estimate the number of observations per grid cell per year by the planned SOFIS payload operation. To evaluate the influence of instrumental uncertainty (precision) on estimated flux uncertainty, we have added instrument error covariances ($C_{D_{\text{inst}}}$) to the model estimated data covariances ($C_{D_{\text{mod}}}$). Thus the effective error covariance ($C_{D_{\text{eff}}}$) for the satellite observations are calculated by following relation:

$$C_{D_{\text{eff}}} = C_{D_{\text{mod}}} + C_{D_{\text{inst}}}$$  \hspace{1cm} (5)

The values of $C_{D_{\text{inst}}}$ are varied in the range of 0 to 25 ppm$^2$, equivalent to the instrumental precision of 0 to 5 ppm.

2.4. Cloud Climatology

[11] Since clouds are ubiquitous in the troposphere, the profile measurements of trace constituents by remote sensing techniques are not made at high accuracy in this part of the atmosphere. It is also not straightforward to make corrections due to cloud cover in the retrieval algorithms because the absorption of radiation depends on thickness, height of occurrence, the microphysical properties of the clouds, and horizontal viewing path of the satellite. Even though, a few satellite sensors can take measurements if some type of clouds exists, the algorithm

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**Figure 3.** A posteriori fluxes and associated uncertainties (in Gt C per year) for each of the inverse model regions, estimated using the CO$_2$ observations near the surface. We have used observations at 115 GlobalView stations and inverse models at two spatial resolutions; one with 42 land and 11 ocean regions (Figure 3a), and the other with TransCom-3 regions (Figure 3b, dashed line). Figure 3b also shows the HiRes inverse model results after aggregating to the TransCom-3 land regions and the ocean regions for a better comparison (solid line). An aggregation to larger regions of hemispheric scale from both the inverse model results show fairly good matches and is seen in Figure 3c. The consistency in derived fluxes using the inverse models at two spatial resolutions is important since both will be used in this study. See color version of this figure in the HTML.
for atmospheric data retrieval becomes much more complex than in the case of clear sky condition. These algorithms are not very advanced at present to derive the concentrations of atmospheric trace species at good accuracy in the presence of clouds. We have corrected the measurement frequency for annual mean cloud cover fraction. We assume that no observation could be made if cloud cover frequency is 100% and the measurement frequency to be same as the number of times the satellite scans through the Earth’s atmosphere under cloud free conditions. Presently, we know of no estimate of obstruction due to clouds along the long horizontal viewing path of an occultation type sensor. Thus the annual average cloud cover frequency, integrated from top of the atmosphere to the lower layers of the atmosphere (i.e., 500, 400, 300 and 200 mb), are taken from the University of Wisconsin HIRS 6.5 year average cloud climatology [Wylie et al., 1994]. Typically the cloud occurrence frequency is higher (over 60% at 500 mb) in the tropical convective zones, e.g., eastern Pacific Ocean, Indian Ocean and Atlantic Ocean. The cloud covered area decreases as the altitude increases to 200 mb and a maximum of about 15% cloud cover frequency is observed. It should be pointed out here that the Wisconsin HIRS cloud climatology reports more clouds in upper troposphere than that produced by the ISCCP (International Satellite Cloud Climatology Program) [Jin et al., 1996].

2.5. Processing of Vertical Profiles

[12] The occultation based techniques have been successfully employed for the vertical profile measurements of trace gases, but are restricted to the upper layers of the atmosphere (e.g., stratosphere and mesosphere). For instance, HALogen Occultation Experiment on the Upper Atmosphere Research Satellite [Russell et al., 1993] and the Improved Limb Atmospheric Spectrometer (ILAS) on ADEOS [Sasano et al., 1999] have already demonstrated multispecies data retrieval capability of this technology for trace gases mainly in the stratosphere and mesosphere. Here we focus on how the observation from SOFIS sensor, an advanced version of new generation ILAS instrument (ILAS-II) that was launched in December 2002 on ADEOS II [Sasano et al., 2001], would influence surface source inversion of CO₂. This instrument is designed for measuring vertical profiles in the middle and upper troposphere region. The launch of SOFIS payload is planned around 2007 on a NASDA Global Change Observation Mission satellite. Since the limb viewing satellite instruments are designed to have similar data frequency and spatial coverage, the results from this study are believed to be general to a certain extent. The proposed SOFIS measurement statistics have been reduced to observation frequency per horizontal grid per year. Figure 4 shows the spatial distribution of the measurement frequencies by the SOFIS instrument under cloud free condition. We have set a horizontal grid resolution of 10° longitude × 5° latitude for accumulating enough number of observations to reduce the noise from seasonal and short-term variation of CO₂. In the control case studies, we assume the SOFIS measurements are possible only at 4 layers in the upper-middle troposphere at 500 mb, 400 mb, 300 mb, and 200 mb heights. This is consistent with vertical resolution of cloud climatology data and transport model outputs. Such restriction does not allow us to evaluate SOFIS observations to the fullest extent, which is presently targeting retrieval of CO₂ concentration on six layers in the troposphere [Kuze et al., 2002]. The actual number of measurements per grid cell per year varies from only a few in the 30°S to 30°N latitude belt to a few tens of the measurements around 60° of each hemisphere. Thus the ‘effective’ RSDs used in the inverse model calculation become extremely high, sometimes up to 10 ppm in the equatorial latitudes, compared to the estimates from model derived daily CO₂ values that are commonly < 1.2 ppm (see Figure 1). As discussed later in this article, significant improvement in surface source inversions can be
achieved by keeping the RSDs associated with SOFIS measurement at lower values.

3. Results and Discussion

[13] Time-independent inverse model calculation were performed with the NIES/FRSGC model simulated signals of 11 land and 11 ocean region fluxes in one inverse model (TransCom-3), and 42 land and 11 ocean regions in the other (HiRes), in addition to the 4 common background fluxes (fossil fuel emission maps representing 1990 and 1995, net ecosystem production, and oceanic emission). The data covariances (\(C_D\)) are supplied by the cloud-cover corrected measurement frequency and model estimated RSD values as described above. To evaluate the advantages and disadvantages of vertical profile measurements over the surface observations in source inversion of CO\(_2\), we have compared the flux uncertainties estimated using satellite measurements with the surface observations from present and future (optimally extended) measurement networks, and also in combination of both satellite and surface observations.

[14] Case 1: The basic surface network used in this study is obtained out of the full set of GlobalView stations [Globalview-CO\(_2\), 2000]; sites that consist 1% real data in 1992–1996 period are included. This network has 115 stations, representing a ‘present-day’ scenario. It is important however to mention here that most of these stations are operated by the developed nations and primarily aimed at recording the background CO\(_2\) concentrations.

[15] Case 2: Thus a second surface network is used based on the optimally extended network of surface observations, which proposes expansion of CO\(_2\) measurements that would make the global coverage spatially uniform [Patra et al., 2003]. Their results suggested that an optimal increase of the CO\(_2\) observation network from 115 stations (case 1) to 130 stations can result in a 58% decrease of flux uncertainty under TransCom-3 framework (a ‘future’ scenario of ground based observation).

[16] Case 3: This case pertains to the results obtained with the increased horizontal resolution of the inverse model. A 53 region inverse model setup is employed and the test cases 1 and 2 are repeated under this framework.

[17] Case 4: Lastly, we have examined the impact of using 75, 50 or 25% RSDs, on the inverse model results with varying instrumental precision. This test explores a possibility of improved CO\(_2\) transport modeling in the future to follow the observed synoptic scale variability more accurately and an overall increase in measurement frequency for reducing the estimated data uncertainty as seen from Equation (4).

3.1. Optimal Extensions of Surface Network

[18] The optimal extension of present surface observation network have been studied in details by using incremental optimization under the inverse model framework of the TransCom-3 [Patra et al., 2003], a technique that was introduced in an earlier study [Patra and Maksyutov, 2002]. In Figure 5 we have compared two optimal networks, one using the TransCom-3 basic inverse model
(22 regions) and the other using the HiRes setup with 53 regions (42 land and 11 ocean), to show the impact of horizontal resolution of the inverse models on optimal network design. It is evident from the diagram that preference of atmospheric sampling location changes significantly with the variation in inverse model setup. We have learnt from the previous studies that an observational data has maximum influence on the reduction of flux uncertainty of a region where the station is located and affects the flux estimation of other regions marginally, if connected through atmospheric transport [Gloor et al., 2000; Patra et al., 2003].

In HiRes inversion setup most of the optimal stations are placed in the continental regions since the TransCom-3 land regions are divided into 4 smaller regions. In addition, one could notice that the station locations spread much more widely in space within the land regions in HiRes inversion than in the case of TransCom-3. For instance, four stations in the Boreal Asia are placed far apart from each other in HiRes setup. While most stations in Boreal North America were located in the central region under TransCom-3 framework, in HiRes inversion they are distributed over a relatively greater area of space in the central and eastern Canada.

[19] Figure 6 shows the changes in average flux uncertainties \( \sqrt{\sum \sigma_{i,j}^2} \) per region for the HiRes case, which is fairly comparable to that estimated in TransCom-3 (~0.50 Gt C/yr per region). However, the sum of regional uncertainties of CO\(_2\) sources \( \sum \sigma_{i,j} \) is about 2.35 Gt C per year and 3.44 Gt C per year, respectively, for the TransCom-3 and HiRes (before aggregation to TransCom-3 regions) inversion cases. With an addition of 20 or 40 optimal stations to the basic set, the global flux uncertainty is reduced to about 1.30 or 1.15 in TransCom-3, and 2.30 or 1.69 in HiRes inversion, respectively. This is because more inverse model regions become flux under-determined in the HiRes case due to smaller number of regions to observation stations ratio. The under-constrained TransCom-3 and HiRes regions are located primarily in the Tropical and South America, Tropical and South Africa, and some parts of Asia, which are covered with little or no CO\(_2\) measurement. Further the changes in slope of average flux uncertainty reduction with new stations differ remarkably with respect to the optimal network size. At the beginning the slope of TransCom-3 case is much sharper compared to the HiRes case till about 5 additional stations, and beyond that the average flux uncertainty change per new station tends to saturate for TransCom-3 case. That slope continues to be large till about 12 new stations in HiRes inversion. We believe such situation is arising in TransCom-3 case because the contribution of single optimally placed station to the average source uncertainty reduction is large at the beginning and the flux under-determined regions become rather well constrained after about 5 additional stations. On the other hand, the average flux uncertainty reduction due to one additional station in HiRes is relatively small from the starting and remains similar even after the addition of 5 optimal stations. Also the average of regional flux uncertainties in HiRes after aggregation (~0.37 Gt C/yr) is higher compared to the TransCom-3 (~0.29 Gt C/yr) after adding 15 optimal stations. The change in slope with new stations is similar before and after the region aggregation in HiRes case.

3.2. Regional Flux Estimations Using Solar Occultation FTS for Inclined-Orbit Satellite and Surface Data

[26] Figure 7 shows the comparison between the regional flux estimate uncertainties by using the 115 stations surface network (Case 1) and vertical profile measurements from satellites with several data uncertainties. It may be worth recalling that we have used measurements of CO\(_2\) at four layers in the middle-upper troposphere, on 500, 400, 300, 200 mb pressure surfaces. The random component of data uncertainties are considered in the inverse calculations by adding different error (instrumental and retrieval) values of 0.0, 1.41, 2.24, 3.16, 4.0 and 5.0 ppm to the measurement frequency corrected RSD values. The RSDs are included in our data error estimation in order to incorporate a realistic data error model in the satellite data inversion, which is also consistent with the optimal extension of surface network. This condition also avoids the singularity problem of Equation (2) at zero instrumental precision. If the atmospheric data errors are considered close to zero, the ‘perfect model’ condition pushes the average flux estimate uncertainties toward zero. Under this assumption the inverse model calculation forces a match between the atmospheric data and model simulated CO\(_2\) concentrations artificially.

![Figure 6](image-url)

**Figure 6.** Change in the regional average flux uncertainties with the optimal increase in basic set network of 115 stations at two inverse model resolutions. The filled circles and fitted line \( y = 10^{-0.5} \cdot (59225 - 2619.8x + 104.64x^2 - 2.0859x^3 + 0.015844x^4) \) are the average flux uncertainties after aggregating the HiRes results to the TransCom-3 regions. It should be noted here that the flux estimate uncertainties on per area basis (e.g., Gt C km\(^{-2}\) per year) would shift the dashed line upward. See color version of this figure in the HTML.
although it is well-known that the model transport is still far from being perfect. Figures 7 (a and e) illustrate that if zero measurement errors can be achieved, the satellite observations produce better surface source inversion results for quite a few regions (green to red colour). However, as the satellite measurement error grows, more and more regions become loosely constrained compared to that is obtained by using the surface observations at 115 locations. The clear advantages of satellite observations are seen in the regions that are not covered by surface observations, such as the continental Africa and South America (left panels). It is also interesting to note that when the satellite observations are utilized in addition to the existing surface measurement (panels on the right), the scope for improvement enhances. At all measurement errors, apparently there are notable benefits to four TransCom-3 land regions in Africa and South America. Some improvements in flux uncertainties of North America, Temperate Asia and South Atlantic can also be seen at 0 ppm instrumental precision.

Figure 7. (opposite) Panels show net gain (green to red) and loss (blue to cyan) in estimated flux uncertainty (in Gt C/yr per region) of CO2, by using the SOFIS sensor at several measurement errors (0.0, 1.41, 2.34, and 3.16 ppm, starting from bottom to top panels, respectively) compared to the existing surface measurements at 115-stations network. The net gain/loss is calculated by subtracting \( a \ posteriori \) flux uncertainty of each region using SOFIS only (left panels) or SOFIS and surface measurements (right panels) from that is obtained using the surface observations at 115 stations. See color version of this figure at back of this issue.

[21] Similar comparison is also made for 130 stations surface network consisting 115 GlobalView stations and 15 optimally located stations (Case 2). Only selected results at instrumental precision of 0.0 and 1.414 ppm are displayed in Figure 8. No remarkable improvement could be seen in regional flux uncertainty reductions due to the use of CO2 vertical profile measurements from satellite while compared with the use of atmospheric data from an optimally extended surface network. The impact of each surface CO2 station is large when they are placed and operated optimally (mainly from the data void region), primarily because of greater signal strength near the ground. The RSDs estimated from the GlobalView surface CO2 data range from 0.3 ppm in the high-latitude SH (\( \geq 45^\circ S \)) to typically about 2 ppm in the midlatitude NH (30–60\(^\circ\)N). On the other hand, the CO2 signals in upper-middle troposphere are weak and the CDmod for satellite pseudodata are relatively high due to smaller measurement frequency and larger RSDs. Since the optimal surface station are placed in the tropics where the satellite
measurements. The average uncertainty reduces from about 

0.000 0.757 0.397 0.307 0.720 0.444 0.300 0.793 0.344 0.315
1.414 1.020 0.464 0.332 1.009 0.542 0.328 1.030 0.371 0.335
2.236 1.191 0.511 0.342 1.225 0.610 0.340 1.156 0.386 0.344
3.162 1.362 0.559 0.349 1.457 0.682 0.347 1.259 0.400 0.351
4.000 1.499 0.599 0.353 1.652 0.741 0.351 1.328 0.411 0.355
5.000 1.646 0.642 0.357 1.866 0.804 0.355 1.390 0.422 0.359
No Satellite 3.885 0.999 0.366 5.175 1.309 0.363 1.845 0.533 0.369

The poor performance of satellite data over the ocean regions compared to the land regions can be thought to be caused by the lower values of oceanic prior flux uncertainties in the TransCom-3 setup. Table 1(b, c) show the a posteriori flux uncertainties, while the prior flux uncertainties are chosen to be 4 and 8 times higher than those in the TransCom-3 setup. The estimated flux uncertainties deteriorate significantly if 4 times larger prior flux uncertainties are used, and that does not grows proportionally with further relaxing the prior uncertainties up to 8 times. For example, the estimated flux uncertainties of the ocean regions increased by 2.25 or 2.67 times for changes in the prior flux uncertainties by 4 or 8 times, respectively, for SOFIS only data at zero instrumental precision. However, since the land regions are relatively less constrained in TransCom-3, the changes in estimated fluxes are only about 1.54 or 1.71 times, respectively, under the above loosely constrained inversion setups. The crossover point of flux uncertainties due to SOFIS and present surface network data inversion also shifts to 1.34 and 1.07 ppm for 4 and 8 times higher prior flux uncertainties, respectively, which was at 1.35 ppm with TransCom-3 basic inversion. This is because the surface CO2 data are effectively more precise than the SOFIS data used in this study. The SOFIS only observations in loose prior inversions produce relatively higher flux uncertainties for the ocean regions compared to the land regions at any data precision due to lesser contrast in the atmospheric data and basis function distributions of the ocean regions. The use of surface data and a priori information appear essential in this context.

The only previous study that dealt with the utility of vertical profile measurements in CO2 surface source inver-

measurement frequencies are low, our results tend to prefer the surface observation over the measurements using SOFIS. This is partly also a consequence of how the signal and noise from the natural data variability is considered in a time-independent inversion. Apparently, in time-dependent inversion some part of this noise consists of usable information to locate the origin and estimate the strength of CO2 sources, provided that noise is simulated successfully by the transport models [Law et al., 2002]. However, the comparison between utilities of extended surface network and satellite measurements is expected to be valid as the same data error model is utilised in both the scenarios.

3.3. Change in Average Flux Uncertainty With Data Error

A summary of the effects of measurement error and prior flux uncertainties on the average flux estimate uncertainty per inverse model region is given in Table 1. Since the RSDs associated with CO2 concentrations in the upper tropospheric layers are sometimes very large, in the range of 2–6 ppm, the flux uncertainties tend to be less sensitive to the measurement error if it is of the same order (i.e., ≥2 ppm). This sensitivity is still smaller when the inverse calculation is made by using the surface and satellite observations in combination. More discussion on this issue is given toward the end of this section. Detailed comparisons of several data use scenarios and varying instrumental precision are given in Table 1 (a) for the TransCom-3 setup. The satellite only measurements reduce the average a priori uncertainty (∼1.29 Gt C/yr per region) of the land regions by 53% to about 0.612 Gt C/yr per region at 1.414 ppm instrumental error. However, the flux uncertainties of the ocean regions are not very well constrained by the satellite measurements. The average uncertainty reduces from about 0.461 Gt C/yr per region to 0.382 Gt C/yr per region, only by about 18%.

The only previous study that dealt with the utility of vertical profile measurements in CO2 surface source inver-

Table 1. Summary of Variations of Average Flux Estimate Uncertainties Per Region for Different Combinations of Measurements

<table>
<thead>
<tr>
<th>Precision</th>
<th>SOFIS</th>
<th>S+N1</th>
<th>S+N2</th>
<th>SOFIS</th>
<th>S+N1</th>
<th>S+N2</th>
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<td>Land Average</td>
<td></td>
<td></td>
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<td>Ocean Average</td>
<td></td>
</tr>
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</tr>
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<td>1.280</td>
<td>0.479</td>
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<td>3.691</td>
<td>0.605</td>
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</tbody>
</table>
The inclusion of model derived RSDs in previous studies derived monthly mean fluxes etc. The differences in transport and inverse model setups - cloud coverage (aside from the respective, (ii) only this study has explicit treatment of the CO2 data by remote sensing is fairly consistent across work of Rayner and O'Brien, Pak and Prather, and this work) are in fairly good agreement. All suggest that the profile and column measurement accuracies to be in the range of 1.35–1.7 ppm and 2.2–2.5 ppm, respectively, for keeping the average flux uncertainty at similar level as that with the presently operating surface network. This agreement is obtained despite the facts that (i) surface CO2 networks with 56, 76 and 115 stations used in Rayner and O'Brien, Pak and Prather, and this work, respectively, (ii) only this study has explicit treatment of cloud coverage (aside from the Rayner et al. [2002] study), (iii) differences in transport and inverse model setups - previous studies derived monthly mean fluxes etc. The inclusion of model derived RSDs in C_{24} have made our study instrument precision wise more demanding than the work of Pak and Prather [2001]. The desired accuracy in the CO2 data by remote sensing is fairly consistent across the usage of transport model simulations and inverse modeling frameworks.

3.4. Sensitivity Tests

[25] Following Rayner et al. [2002], we introduce an 1% positive bias to the CO2 pseudodata which could arise from the spectroscopic parameters and/or error in the retrieval algorithm. The biases do not seem to create significant disturbances to the estimated fluxes when only the satellite data are used in the inversion. As depicted in Figure 9a the regional fluxes are perturbed by small amounts (~0.01 Gt C), which are well within the estimated uncertainties for the fluxes itself (~ a few tenths of 1 Gt C). This result is valid under any selection of prior flux uncertainties, and is in good agreement with Rayner et al. [2002]. On the contrary if the surface observations are combined with the satellite data in the inversion, the outcome is radically different. In this case, we have increased the SOFIS pseudodata by only 0.3% (i.e., ~1 ppm). The fluxes are disturbed beyond the acceptable limits for most of the regions, and the South America (Lnd-04) being the most prominent one. This increase in flux from one region pushes the fluxes down from the neighboring ocean regions in SH. Both the North America regions form a dipole with the North Pacific ocean. Thus the biases in the different data sources are as important as the biases in the inter-laboratory calibration error for the surface measurements [Masarie et al., 2001]. While change in fluxes are shown for an addition of 0.3% positive bias to the SOFIS data in Figure 9b, the change is proportional to the percentage bias added to every pseudodatum.

3.5. Effect of Increasing Number of Inverse Model Regions

[26] The comparison between the reductions in inverse model estimated flux uncertainties by using either surface or satellite observations is affected by the size of the source region. The argument against surface measurements is that their actual footprint is smaller than the original TransCom-3 regions and the surface observations at about 100 stations are not as representative as several thousands of satellite data. Therefore the surface measurements may get unfair advantage over the satellite observations when the sources are determined for large regions. To investigate the sensitivity of flux uncertainty to the size of source regions, we formulated a high-resolution inverse model with about 4 times more land regions than in the TransCom-3. The detailed description of this inverse model is given in Section 2.2. This is also in concurrence with the targets for quantifying carbon sources and sinks at the sub-continental spatial resolution [Cihlar et al., 2002]. We have carried out Cases 1 and 2 tests in the high-resolution inverse model configuration with 42 land and 11 ocean regions (Case 3). Figure 10 shows the summary of flux uncertainty reductions after aggregation to the TransCom-3 regions with varying instrumental precision. A few points can be highlighted here, e.g., the region aggregated average flux uncertainty is higher (~0.54 Gt C/yr per region) in HiRes compared to that in TransCom-3 (0.51 Gt C/yr per region) at
instrumental error of 1.414 ppm with SOFIS data alone, as more number of regions remained loosely constrained in the high-resolution inversion. The optimal surface network with HiRes requires 2–3 times more number of stations compared to that with the TransCom-3 inverse model to achieve similar level of average flux estimate uncertainty, say about 0.29 Gt C/yr per region (ref. Figure 6). It suggests that the TransCom-3 inverse model regions are larger than the footprint of surface observations, and division of these regions in HiRes inversion increases the degrees of freedom for the regional fluxes of CO₂ to vary. Thus each HiRes land regions need about a couple of stations to constrain the regional \textit{a posteriori} flux uncertainty.

Overall, the regions in the high-resolution inversion are also less well constrained, compared with the TransCom-3 regions, when using the satellite observations. The explanation for this could be that the signal strength of smaller source regions is weak in the middle and upper troposphere, while the data errors are remaining the same in our calculation. This is seen as relatively lower slope of flux uncertainty reduction with observation precision, which suggests that more frequent scanning of the earth’s atmosphere is also desired for high-resolution surface source inversion. Nevertheless, the high-accuracy satellite observations do impose better constrains on the fluxes compared to those offered by the surface observation network. The cross-over point of SOFIS-only to surface-only data inversion is found at instrumental precision of about 2.1 ppm in the HiRes, which was at about 1.3 ppm in TransCom-3 (Table 1). Further, the addition of SOFIS data at 1.4 ppm measurement error to surface data at 115-stations network reduces the flux uncertainty from 0.50 and 0.59 Gt C/yr to 0.35 and 0.41 Gt C/yr, respectively, in TransCom-3 and HiRes inversion (ref. Table 1 and Figure 10). To secure the same reduction in flux uncertainty we need to add about 5 and 10 surface stations at optimal locations under TransCom-3 and HiRes framework, respectively. Thus in higher-resolution inverse modeling (HiRes) the satellite CO₂ observations using the occultation based sensors tend to be more useful in comparison to that in a lower resolution inverse model (TransCom-3).

3.6. Impact of Reducing Residual Standard Deviations on Flux Estimate Uncertainty

[28] It is well known that the estimated values of RSDs have large impact on the determination of \textit{a posteriori} flux uncertainties [see for example Patra et al., 2003]. It was suggested that the model-RSDs may underestimate the actual data variability by a factor of 2 or 3 at some optimal stations when those are established on the ground or below the planetary boundary layer. Because the simulated fluxes due to net ecosystem production do not include diurnal variation, this could be a problem particularly for the land sites. Patra et al. [2003] have shown that doubling RSD values of the additional stations increases the flux estimate uncertainty from 0.29 Gt C/yr per region to 0.37 Gt C/yr per region after adding 15 optimal stations under the TransCom-3 framework. However, it is unlikely that the diurnal-scale variabilities in CO₂ surface sources will reach the middle-upper troposphere without the presence of convective clouds. Here we have studied the variations in average flux uncertainty with reduced RSDs values and the results are depicted in Figure 11 (Case 4). The estimated RSDs based on actual measurement frequency are scaled down by 75, 50 and

**Figure 10.** The changes in average flux uncertainties with instrumental precision when the high-resolution inversion is employed (see legends for detail). For a better comparison with the data in Table 1, first we have aggregated the HiRes results to TransCom-3 regions and calculated the average flux estimate uncertainties. See color version of this figure in the HTML.

**Figure 11.** The diagram shows the impact of reducing \( C_{Dmod} \) on the estimated flux uncertainty in the high-resolution inversion case. The estimated \( C_{Dmod} \) based on SOFIS measurement frequency and cloud cover fraction, is decreased by 75, 50, or 25% in the three test cases. See color version of this figure in the HTML.
25%. We found that at lower RSDs, the flux uncertainty gradient with the change in precision increases sharply, indicating that the estimated flux uncertainties become more sensitive to the measurement error at lower RSDs. The estimation of RSDs depends on actual measurement frequency by the satellite instrument and matching of observed CO₂ variability with the transport model simulation. The flux average uncertainties at 2.5 ppm precision are estimated to be 0.59, 0.58 or 0.57 Gt C/yr per region by factoring RSDs with 0.75, 0.50 or 0.25%, respectively. These values are comparable to 0.59 Gt C/yr per region due to the present surface network of 115 stations. At 0 ppm instrumental error and 50 or 25% RSD the average flux uncertainties are better estimated than by the expanded surface network (present + 15 optimally located stations). While instrumental precision can be improved for the atmospheric trace gas measurements, it is also likely that the tracer transport dynamics would become more accurate in the future so that the model-data mismatch can be reduced by a few times. Finally, the satellite measurement techniques can be altered for increasing the actual frequency of observations; for example a factor of 4 larger observation frequencies would result a decrease in RSDs by half.

4. Conclusions

[29] In conclusion, it can be stated that the satellite measurements by the SOFIS instrument are promising source of atmospheric CO₂ data in terms of global coverage. The vertical profiles measurements of CO₂ offer greater benefit to a posteriori flux estimates of the tropical land regions in Africa, South America and Asia compared to those in the high-latitude regions. Our results also suggest that combined use of surface and satellite observations provide maximum constraint on the estimation of CO₂ fluxes from the ground. Average of TransCom-3 and HiRes flux estimate uncertainties are estimated to be about 0.51 and 0.54 Gt C/yr per region, respectively, by using the SOFIS data product at 4 vertical layers in the middle-upper troposphere at the 1.41 ppm instrumental precision. These values are about 102% and 93%, respectively, of that is estimated using a present-day surface network (115 stations) of CO₂ measurement in the respective inverse models. As the inverse model resolution is increased the regions with-out surface observations becomes more loosely constrained and the average source uncertainty appears to be less sensitive to the measurement error in space-borne data. An attempt to achieve low model derived data uncertainties to the satellite observations appear to be very useful, while keeping the instrumental error as low as possible. These findings are valid to a great extent for any occultation-type satellite sensor and also to the choices of a priori flux uncertainties. However, it should be cautioned that although the homogeneously distributed biases in the satellite measurements do not disturb the inverse model estimations significantly, but a small bias will lead to radically different results when these are used in combination with the surface CO₂ observations.

Acknowledgments. Thanks are due to Don Wylie for generously supplying the Wisconsin HIRS 6.5 Year Cloud Climatologies. PKP appreciates discussion with Rachel Law on high resolution inversion. Comments from Makoto Suzuki and Shoichi Taguchi on an initial draft have helped us to improve the quality of the manuscript. Comments and suggestions from all the anonymous reviewers have greatly helped to improve the quality and clarity of the article. We appreciate the support of Hajime Akinoto for this research. The transport model runs and most inverse model calculations could not have been feasible without the support of NEC SX-5 computer system at FRSGC.

References


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T. Nakazawa, Center for Atmospheric Oceanic Studies, Tohoku University, Sendai 980-8578, Japan. (nakazawa@mail.tains.tohoku.ac.jp)
Figure 1. (opposite) Annual average source signals of CO₂ (Figures 1a, 1b, 1c, and 1d) and the estimated residual standard deviations (RSDs) (Figures 1e, 1f, 1g, and 1h) at various layers of the atmosphere are depicted. The global sources due to fossil fuel emission representing 1990 and 1995, and seasonally varying biospheric and oceanic fluxes are combined for this simulation. The period of the model integration was set to 3 years (e.g., 01 January 1992 to 31 December 1994) and only the second year averages are shown here as the signals. The RSDs are estimated from the daily average time series for two consecutive years.
Figure 7. (opposite) Panels show net gain (green to red) and loss (blue to cyan) in estimated flux uncertainty (in Gt C/yr per region) of CO₂, by using the SOFIS sensor at several measurement errors (0.0, 1.41, 2.34, and 3.16 ppm, starting from bottom to top panels, respectively) compared to the existing surface measurements at 115-stations network. The net gain/loss is calculated by subtracting \textit{a posteriori} flux uncertainty of each region using SOFIS only (left panels) or SOFIS and surface measurements (right panels) from that is obtained using the surface observations at 115 stations.