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Application of a probability density function-based atmospheric light-scattering correction to carbon dioxide retrievals from GOSAT over-sea observations

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ABSTRACT

We present the application of a photon path length probability density function (PPDF) formalism to atmospheric carbon dioxide (CO_2) retrievals from reflected sunlight measured by the Greenhouse Gases Observing Satellite (GOSAT) over the ocean. GOSAT short-wave infrared (SWIR) radiance spectra detected over the ocean surface were shown to be strongly affected by atmospheric light-scattering. In particular, retrievals of column-averaged CO_2 dry-volume mixing ratios (XCO_2) were characterised by steady negative bias and significant scatter when optical path modification due to high variability of clouds and aerosols was neglected. Considering that the ocean surface in SWIR is dark in all directions except that of sun-glint observation, PPDF radiative transfer modelling was simplified by neglecting the contribution of photons that interacted with both aerosols/cloud particles and the ocean surface. This permitted implementation of an atmospheric correction technique based on simultaneous retrievals of CO_2 concentrations and two PPDF parameters: effective altitude of the aerosol layer and relative layer reflectivity. Using this correction, both bias and scatter of carbon dioxide retrievals were significantly reduced. The retrieval results of XCO_2 statistically agreed (both spatially and temporally) with those predicted by the atmospheric transport model.

1. Introduction

Atmospheric carbon dioxide (CO_2) is generally accepted as a dominant anthropogenic greenhouse gas. Because of its high contribution to global radiative forcing ($1.66 \pm 0.17\ Wm^{-2}$), atmospheric CO_2 is an important factor in global climate change (IPCC, 2007). However, current knowledge about carbon dioxide sources and sinks is still insufficient for reliable climate predictions. Ground-based CO_2 observations are too sparse to sufficiently reduce uncertainties in source and sink characterisation. Satellite observations provide global coverage, but their retrieval efficiency for gas can be limited by the high variability of atmospheric light-scattering and ground-surface properties when interpreting reflected sunlight. Retrieval precision and accuracy requirements have been discussed elsewhere (Baker et al., 2010; Chevallier et al., 2007; Rayner & O'Brien, 2001). For column-averaged CO_2 dry-volume mixing ratios (XCO_2), a precision of ~1% (2.5 ppmv) or better for monthly means at the regional scale is required to improve estimates of surface CO_2 fluxes based on in situ measurements (Houweling et al., 2004; Patra et al., 2003; Rayner & O'Brien, 2001). Generally, XCO_2 could be monitored from space using short-wavelength infrared (SWIR) measurements of reflected sunlight, which are sensitive to CO_2 abundances in the atmospheric boundary layer (Crisp et al., 2004).

Atmospheric light-scattering by aerosols and cloud particles remains a major source of XCO_2 retrieval errors that exceed the precision limits (Aben et al., 2007; Dufour & Breon, 2003; Mao & Kawa, 2004; O'Brien & Rayner, 2002; Reuter et al., 2010). Several approaches have been proposed to correct the impact of atmospheric light-scattering when retrieving column-averaged gas values. In so-called full-physics algorithms (Butz et al., 2009; Connor et al., 2008; Yoshida et al., in press), a limited number of effective aerosol and/or cloud characteristics are included in the state vector for their simultaneous retrieval with target gas amounts. Recent studies (Bril et al., 2007; Oshchepkov et al., 2008) have proposed light-scattering corrections based on analyses of photon path length statistics. The measured signal is expressed in terms of a photon path length probability density function (PPDF) with further parameterization of the PPDF. This method is very rapid because it excludes time-consuming radiative transfer computations from the retrieval procedure. In this study, we present a methodology and initial results of simultaneous XCO_2 and PPDF retrievals from Greenhouse Gases Observing Satellite (GOSAT) over-sea observations.

GOSAT was launched on 23 January 2009 to monitor the global distributions of atmospheric carbon dioxide and methane. The satellite has a sun-synchronous orbit at an altitude of 666 km and a 3-day recurrence with the descending node around 12:48 local time. The GOSAT mission instruments are the Thermal and Near infrared Sensor for carbon Observation-Fourier Transform Spectrometer (TANSO-FTS) and -Cloud and Aerosol Imager (TANSO-CAI) (Kuze et al., 2009).

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The TANSO-FTS has three narrow bands in the SWIR region (0.76, 1.6, and 2.0 μm) which are used for XCO_2 and PPDF retrievals. For SWIR bands, incident light is divided by a polarization beam splitter and then simultaneously recorded as two orthogonal polarization components (hereafter called P and S components). The TANSO-FTS instantaneous field of view is 15.8 mrad, which corresponds to a nadir footprint diameter of about 10.5 km. The pointing mechanism of the TANSO-FTS enables off-nadir observations, e.g., sun-glint over-sea observations. Because of the limited driving angles of the pointing mirror (±35° in the cross-track direction and ±20° in the along-track direction), GOSAT performs sun-glint measurements within narrow (~30°) near-equator latitude ranges. More details on the TANSO-FTS have been provided by Kuze et al. (2009).

2. Retrieval algorithm

The retrieval procedure was based on the constrained minimization of the residual between the predicted R and observed R^* spectral radiance. According to the Gauss–Newton method, the estimate can be found iteratively by the maximum *a posteriori* approach (Rodgers, 2004) as

$$\mathbf{X}_{k+1} = \mathbf{X}_k + \left(\mathbf{K}_k^T \mathbf{S}_Y^{-1} \mathbf{K}_k + \mathbf{S}_a^{-1}\right)^{-1} \left[\mathbf{K}_k^T \mathbf{S}_Y^{-1} \left(\mathbf{Y}^* - \mathbf{Y}(\mathbf{X}_k)\right) + \mathbf{S}_a^{-1} \left(\mathbf{X}_a - \mathbf{X}_k\right)\right], \quad (1)$$

where $\mathbf{X}_k$ is a state vector at the k^{th} iteration, $\mathbf{X}_a$ is an *a priori* state vector, $\mathbf{S}_Y$ is the covariance matrix of measurements $\mathbf{Y}^*$, $\mathbf{S}_a$ is a covariance matrix of *a priori* data $\mathbf{X}_a$, and $\mathbf{K}_k$ is the Jacobian of the forward model at $\mathbf{X}_k$. Components of the vector $\mathbf{Y}^*$ were constructed using the measured radiance values R^*

$$Y_\nu^* = -\ln\left(R^*\right). \quad (2)$$

The modelled spectrum Y was approximated using a differential optical absorption spectroscopy (DOAS) approach:

$$Y = -\ln R = -\ln\left(\left\langle S_\nu^0 \cdot T_{eff}(\mathbf{x}) \right\rangle\right) + \Pi^{(2)}, \quad (3)$$

where S_ν^0 is solar irradiance, and $\Pi^{(2)}$ is the second-order polynomial on a wavelength scale that accounts for the low-frequency part of the Y^* spectrum. The angular brackets in Eq. (3) denote convolution with instrument line shape. To allow for the effects of atmospheric light-scattering, effective gaseous transmittance T_{eff} was expressed in terms of the PPDF. According to the equivalence theorem, the PPDF is applicable to certain spectral ranges over which optical properties of scattering media are similar. For arbitrary plane-parallel atmospheres that consist of J layers, the effective transmittance can be expressed as

$$T_{eff}\left(k_1, k_2, \ldots, k_j\right) = \int_0^\infty \ldots \int_0^\infty dL_1 dL_2 \ldots dL_J \exp\left(-k_1 L_1 - k_2 L_2 \ldots - k_J L_J\right) P\left(L_1, L_2, \ldots, L_J\right), \quad (4)$$

where k_j and L_j are the gaseous absorption coefficient and photon path length in the j^{th} layer, respectively. To account for optical path modification by cloud and near-surface aerosol layers, Oshchepkov et al. (2009) proposed the following parameterization of a three-dimensional PPDF:

$$T_{eff} = \alpha_c T_3 + (1-\alpha_c) T_{12}^c \cdot T_a T_3, \quad (5)$$

$$T_3 = \exp\left[-C_\mu \tau_3\right], \quad (6)$$

$$T_{12}^c = \exp\left[-C_\mu \cdot (1+\delta_c) \cdot \tau_{12}\right], \quad (7)$$

$$T_a = (1-\alpha_a) \exp\left[-C_\mu \tau_a \delta_a\right] + \alpha \exp\left[+C_\mu \tau_a\right], \quad (8)$$

where $C_\mu = \frac{1}{\cos(\theta)} + \frac{1}{\cos(\theta_0)}$, θ and θ_0 are Solar and satellite zenith angles, respectively, and $\tau_a = \int_0^{h_a} k(h)\ dh$, $\tau_{12} = \int_0^{h_c} k(h)\ dh$ and $\tau_3 = \int_{h_c}^{H_{TOA}} k(h)\ dh$ are the gaseous optical thickness of the layers,

$$\delta_a = \rho_a \cdot \exp\{-\gamma_a \cdot \tau_a\}, \quad (9)$$

$$\delta_c = \rho_c \cdot \exp\{-\gamma_c \cdot \tau_{12}\}, \quad (10)$$

where α, ρ, γ, h are PPDF parameters, and subscripts c and a denote cloud and aerosol layers, respectively. These parameters can be interpreted as follows (Oshchepkov et al., 2009): α is the relative cloud/aerosol layer reflectivity, i.e., the ratio of photons scattered by the cloud/aerosol to the total number of photons coming into the view of the detector; ρ is the scaled first moment of the PPDF under the cloud or within an aerosol layer; γ is an adjustment parameter used to account for the second and higher moments of the PPDF; h_c and h_a are altitudes of the cloud and the top of the aerosol layer, respectively; and H_{TOA} is the altitude at the top of the atmosphere. Assumption of plane-parallel atmosphere in Eqs. (4)-(10) was justified for the present study by the limited solar zenith angles in the used GOSAT observations (e.g., in sun-glint mode, these are due to the limited driving angles of the pointing mirror (Kuze et al., 2009)).

The retrieval procedure was implemented for a combination of several subsets of available observation data. Basically, the equivalence theorem and PPDF-formalism are applicable to the individual polarizations and their combinations (e.g. scalar radiance). Test XCO_2 retrievals obtained by using P and S polarizations (both separately and in combination) were in close agreement. In the present study, we estimated XCO_2 by combining P components of observed radiance from two spectral regions: 6185–6272 cm^{-1} from the 1.6-μm "weak" CO_2 band and 4815–4885 cm^{-1} from the 2.0-μm "strong" CO_2 band.

Generally, the state vector of retrieved parameters included CO_2 mixing ratios at different pressure levels. In the present study we retrieved XCO_2 under the assumption of fixed CO_2 vertical profile. This procedure was implemented using an empirical expression for off-diagonal terms of the covariance matrix S_a which provided unrealistically strong vertical correlation of CO_2 concentration:

$$S_a^{i,j} = \left(S_a^{i,i} \cdot S_a^{j,j}\right)^{1/2} \cdot \exp\left[-0.01 \cdot \left|\ln\left(p_i/p_j\right)\right|\right], \quad (11)$$

where p_i is atmospheric pressure at the i^{th} level. Altitude-independent diagonal terms $S_a^{i,i}$ were set to provide XCO_2 *a priori* uncertainty of 5 ppmv. Unless otherwise specified, an altitude-independent CO_2 dry-volume mixing ratio of 385 ppmv was chosen as the *a priori* distribution.

The state vector of retrieved parameters included also a correction factor to scale *a priori* the water vapour profile (provided by the Japan Meteorological Agency), and effective altitudes of cloud or the top of an aerosol layer. In addition, for each spectral region in the 1.6-μm and 2.0-μm bands, the retrievals permitted three polynomial coefficients, a stretch factor to allow for wavenumber grid distortion, and the remaining PPDF parameters. Aerosol and surface properties for selected spectral regions were expected to be rather similar; we accounted for this by expressing each individual PPDF parameter $\beta^{(j)}$ in the spectral region j as $\beta^{(j)} = y^{(j)}\beta^{(0)}$, where $\beta^{(0)}$ is a "basic" parameter value (common for all spectral regions and signal polarization) and $y^{(j)}$ is a region (component)-specific factor that was constrained to unity with a prior variance of 0.05^2.