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Space- and ground-based CO₂ measurements: A review

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Abstract The climate warming is mainly due to the increase in concentrations of anthropogenic greenhouse gases, of which CO_2 is the most important one responsible for radiative forcing of the climate. In order to reduce the great estimation uncertainty of atmospheric CO_2 concentrations, several CO_2 -related satellites have been successfully launched and many future greenhouse gas monitoring missions are planned. In this paper, we review the development of CO_2 retrieval algorithms, spatial interpolation methods and ground observations. The main findings include: 1) current CO_2 retrieval algorithms only partially account for atmospheric scattering effects; 2) the accurate estimation of the vertical profile of greenhouse gas concentrations is a long-term challenge for remote sensing techniques; 3) ground-based observations are too sparse to accurately infer CO_2 concentrations on regional scales; and 4) accuracy is the primary challenge of satellite estimation of CO_2 concentrations. These findings, taken as a whole, point to the need to develop a high accuracy method for simulation of carbon sources and sinks on the basis of the fundamental theorem of Earth's surface modelling, which is able to efficiently fuse space- and ground-based measurements on the one hand and work with atmospheric transport models on the other hand.

Keywords Accuracy, Carbon satellites, Retrieval algorithms, Space- and ground-based measurements, HASM

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1. Introduction

The rising atmospheric CO₂ concentration is believed to be the primary cause of global climate change (Meehl and Washington, 1996; West and Marland, 2002; Buchwitz et al., 2006). For CO₂ stabilization at 450, 550, or 650 ppm, corresponding ranges of global warming over the next 100 years are about 1.2–2.3, 1.5–2.9, and 1.7–3.2°C, respectively (O'Neill and Oppenheimer, 2002). To keep the increase of global mean temperature at the 2°C level and to minimize the risk of extensive negative impacts of climate change, CO₂-concentrations in the Earth's atmosphere should be stabilized at the 400–450 ppm level (Wigley et al., 1996; Moss et al., 2008; Oberheitmann, 2010, 2013). Unfortunately, the average CO₂-concentration has increased from 344 ppm in 1984 to 396 ppm in 2013, while the average CO₂-concentration was 281 ppm during the 17th and 18th centuries (Pearman et al., 1986). CO₂-emissions are still growing at a rate of 1.75 ppm per year.

The emission estimates of CO_2 have large uncertainties. For instance, there was a 16.9% average absolute difference for emission estimates of power plants from the U.S. Department of Energy's Energy Information Administration (EIA) and the U.S. Environmental Protection Agency's GRID database (Ackerman and Sundquist, 2008). For the EU-25 nations, emission uncertainty was 7% when comparing four in-

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ventory methods (Ciais et al., 2010). For China, the uncertainty was between 15% and 20% when including both fossil fuel consumption and cement production (Gregg et al., 2008). Insufficient knowledge of CO_2 leads to large uncertainties in future climate predictions because CO_2 observations are spatially and temporally limited around the globe (Yoshida et al., 2011). The climatological, ecological, and social impacts associated with any given level of atmospheric CO_2 concentrations are still uncertain; and the equilibrium impact on global temperature of a doubling of the CO_2 concentration alone is estimated by the Intergovernmental Panel on Climate Change (IPCC) to at least have an uncertainty of 3°C (IPCC, 2013).

Three approaches, which are space-based observations, ground observations, and simulations, have been used to characterize the spatio-temporal variability of CO_2 concentrations. This paper describes the typical workflows along with the strengths and weaknesses of the various approaches and what would be needed to use all three approaches together.

2. Space-based observations

2.1 Carbon related satellites

Satellite measurement is one of the most effective approaches to monitoring the global distributions of greenhouse gases at high spatiotemporal resolution and is expected to improve the accuracy of source and sink estimates of these gases (Rayner and O'Brien, 2001). Two satellites, Japan's Greenhouse Gases Observing Satellite (GOSAT) and NASA's Orbiting Carbon Observatory (OCO), have been designed specifically to measure the column-averaged dry air mole fraction of CO₂ (XCO₂).

The Japanese Aerospace Exploration Agency (JAXA) successfully launched GOSAT in January 2009. Although NASA's OCO-1 satellite was lost due to launch failure in February 2009, OCO-2 was successfully launched in July 2014 with an instrument that is almost an exact copy of the OCO-1 instrument. Immediately after the loss of OCO-1, the GOSAT Project Team in Japan invited the NASA's OCO team to contribute to the GOSAT's TANSO-FTS data analysis and NASA has reconstituted the OCO team as the Atmospheric CO₂ Observations from Space (ACOS) Task Force to support this collaboration.

The scanning imaging absorption spectrometer for atmospheric chartography (SCIAMACHY) on board the European Space Agency's ENVISAT-1 satellite provided the first satellite-based estimates of the global distribution of the CO₂ column abundance from space from March 2002 to April 2012. SCIAMACHY is a passive hyper-spectral spectrometer designed to investigate tropospheric and stratospheric composition and processes (Bovensmann et al., 1999). The nearinfrared nadir spectra of reflected solar radiation measured by SCIAMACHY contains information on the vertical columns of these gases, which was retrieved by using a weighting function combined with a modified differential optical absorption spectroscopy (WFM-DOAS) approach. The horizontal resolution of the nadir measurements depends on both the orbital position and spectral interval but is typically 60 km for CO₂.

In addition to SCIAMACHY, GOSAT and OCO, many other satellite missions, such as the Infrared Atmospheric Sounding Interferometer (IASI), Atmospheric Infrared Sounder (AIRS), and Tropospheric Emission Spectrometer (TES), provide the ability to monitor global carbon dioxide concentrations at coarse spatial resolutions (Dennison et al., 2013). IASI was launched onboard the European MetOp platform in October 2006 and provided the first global maps of CO₂ concentrations in the cloud-free upper troposphere (Crevoisier et al., 2009). AIRS was launched on the Aqua satellite of the Earth Observing System (EOS) in May 2002 (Aumann et al., 2003), and has been used to investigate the variability of mid-tropospheric CO₂ over the entire globe (Jiang et al., 2010). TES was launched on the EOS Aura satellite in 2004 and has been used to provide global maps of tropospheric ozone and its photochemical precursors.

In order to extend the satellite CO₂ global time series after SCIAMACHY, GOSAT and OCO-2, many future greenhouse gas monitoring missions are planned, including TanSat, CarbonSat, MERLIN, Sentinel-5p, MicroCarb and ASCENDS.

The TanSat mission is the first mini-satellite dedicated to carbon dioxide (CO₂) detection and monitoring, and will be launched by China in 2016. This satellite will focus on the CO₂ variation on seasonal time scales. Its scientific goal is to improve the understanding on the global CO₂ distribution and the contribution of CO₂ to climate change.

The Carbon Monitoring Satellite (CarbonSat), which will be launched around 2020, will provide data with a spatial resolution better than 2 km×2 km using a 500 km swath width. There will be no gaps between adjacent (across-track and along-track) ground pixels. The primary goal of the CarbonSat mission is to determine and separate natural and anthropogenic CO₂ and CH₄ sources and sinks (Buchwitz et al., 2013).

The French-German satellite mission MERLIN (Methane Remote Sensing Lidar Mission) will be launched in 2019. This mission will provide spatial and temporal gradients of atmospheric methane (CH₄) columns with high precision and unprecedented accuracy on a global scale.

Sentinel-5P is an approved LEO pre-operational mission within the European GMES (Global Monitoring for Environment and Security) program, a collaborative effort of the ESA and NSO (Netherlands Space Office). The launch of the Sentinel-5 mission is planned for 2020 and will provide measurements of ozone, NO₂, SO₂, formaldehyde, aerosol, carbon monoxide, methane, and clouds. The MicroCarb mission to

be launched by the French Space Agency in 2018 will measure XCO_2 to quantify CO_2 surface fluxes over the globe at regional scales, to identify and monitor global carbon sources and sinks, and to better understand the CO_2 mechanisms operating in oceans and vegetation.

The ASCENDS (Active Sensing of CO_2 Emissions over Nights, Days, and Seasons) platform will provide measurements by day, when photosynthesis occurs, as well as at night, when plant respiration dominates. Simply going from a single daily measurement to two readings, one taken by day and the other at night, can provide a greatly improved picture of CO_2 fluxes. This platform will be launched by NASA sometime between 2023 and 2026.

The current and planned carbon-related satellites referred to above measure the near-infrared (NIR) nadir spectra that contain information about atmospheric trace gases such as CO_2 and CH_4 . To gather a more complete picture of CO_2 fluxes and concentrations, retrieval algorithms must be developed to retrieve the total column amounts of the atmospheric trace gases from the NIR nadir spectra and the various approaches that have been proposed to date are reviewed next.

2.2 Retrieval algorithms

At present, there are nine different retrieval algorithms worldwide: 1) the weighting function modified differential optical absorption spectroscopy approach (WFM-DOAS); 2) the Bremen optimal Estimation DOAS (BESD) approach; 3) the National Institute for Environmental Studies (NIES) algorithm; 4) the photon path-length probability density function (PPDF); 5) the Atmospheric CO₂ Observations from Space (ACOS) approach; 6) the University of Leicester Full Physics (UoL-FP) algorithm; 7) the RemoTeC approach; 8) the simple empirical CO₂ model (SECM); and 9) the ensemble median algorithm (EMMA).

The WFM-DOAS is an unconstrained linear least squares method based on scaling (or shifting) preselected vertical profiles, developed for the scanning imaging absorption spectrometer for atmospheric chartography (SCIAMACHY) on board the European Space Agency Envisat-1 satellite (Buchwitz et al., 2000, 2006). The reference spectra of the linear fit include the trace gas total column weighting functions, a weighting function for a temperature profile shift, and a low-order polynomial. The logarithm of a linearized radiative transfer model plus a low-order polynomial is fitted to the observed sun-normalized radiance. WFM-DOAS was improved by additionally using the SCIAMACHY M-factors that are multiplicative factors linked to the absolute radiometric calibration (Schneising et al., 2008). The application of the M-factors to compensate for detector degradation ensures better XCO₂ results for characterizing long-term behavior. Without the consideration of the M-factors, the XCO₂ growth rate would be biased low by a few tenths of 1 ppm

(Schneising et al., 2011, 2012). WFM-DOAS has been further improved by using both a constant aerosol vertical profile for the radiative transfer simulations and a cloud detection algorithm (Heymann et al., 2012).

The Bremen optimal Estimation DOAS (BESD) algorithm combines optimal estimation (Rodgers, 2000) and WFM-DOAS (Buchwitz et al., 2000) to retrieve CO₂ from SCIAMACHY (Reuter et al., 2010). The BESD/C algorithm to be used for CarbonSat is similar but not exactly identical to the BESD algorithm used for SCIAMACHY XCO₂ retrieval with respect to some of the state vector elements (Bovensmann et al., 2010). BESD/C is also based on optimal estimation and uses a priori information to constrain the retrieval. To improve the computation speed of random and systematic XCO₂ and XCH₄ errors, an error parameterization method was developed as a function of several critical input parameters such as aerosol optical depth, cirrus optical depth and cirrus altitude (Buchwitz et al., 2013). BESD/C has been used to retrieve XCO₂ and XCH₄ as well as the terrestrial vegetation chlorophyll fluorescence (VCF) emissions that need to be considered for accurate XCO2 retrieval (Frankenberg et al., 2012; Joiner et al., 2011).

Japan's National Institute for Environmental Studies (NIES) has developed a retrieval algorithm for column abundances of CO₂ and CH₄ from the short-wavelength infrared spectra obtained using the Thermal And Near infrared Sensor for carbon Observation-Fourier Transform Spectrometer (TANSO-FTS) (Yoshida et al., 2011). The NIES algorithm for GOSAT is also based on this optimal estimation method (Rodgers, 2000). The NIES algorithm includes an unbiased cloud detection algorithm (Ishida and Nakajima, 2009) and the spectral regions of the 1.6 µm CO₂, 1.67 µm CH₄, 0.76 μm O₂ absorption bands are then used for the retrieval. NIES was recently improved by replacing the solar irradiance database, improving the optical properties of aerosols, changing the handling of the aerosol vertical profile and removing the surface pressure bias by scaling the absorption cross section of O_2 (Yoshida et al., 2013).

A parameterization method incorporating the photon pathlength probability density function (PPDF) has also been developed, which accounts for thin clouds in CO₂ retrieval from space-based reflected sunlight observations in near-infrared regions (Oshchepkov et al., 2008). The parameterization of the cloud effects are based on a statistical analysis of photon trajectories simulated using Monte Carlo techniques (Bril et al., 2007). The PPDF-based method mimics DOAS when light path modifications are neglected (Oshchepkov et al., 2012).

The fifth of the aforementioned list of methods, NASA's Atmospheric CO₂ Observations from Space (ACOS) algorithm, was originally developed for the OCO instrument. This algorithm also employs an optimal estimation approach, in which the input parameters of a forward model are optimized to yield simulated spectra that best match the observed spectra, whilst simultaneously being constrained by prior information (Rodgers, 2000; Crisp et al., 2012). The ACOS algorithm, being tested on GOSAT data, will work with OCO-2 data. It only uses information from the narrower OCO-2 windows within the GOSAT spectra, and does not use Cloud and Aerosol Imager (CAI) data except for validation. In other words, OCO-2 does not detect cloudy scenes, but GOSAT does (O'Dell et al., 2012).

The University of Leicester Full Physics (UoL-FP) algorithm includes a forward model and an inverse method (Bösch et al., 2006). The forward model consists of a radiative transfer code, a solar model, and an instrument model, whereas the inverse method is based on the optimal estimation technique (Rodgers, 2000). The UoL-FP algorithm was developed to retrieve XCO₂ from a simultaneous fit of the near-infrared O₂ band spectrum at 0.76 μ m and the CO₂ bands at 1.61 and 2.06 μ m as measured by the OCO-2 instrument. The UOL-FP and ACOS algorithms represent two parallel developments based on the OCO algorithm and thus both algorithms follow a similar retrieval strategy. Both retrieval algorithms differ in their definition of the state vector, a priori values and covariances, and especially in the treatment of aerosols and cirrus clouds (Cogan et al., 2012).

RemoTeC is a retrieval approach that allows for the retrieval of a few effective aerosol parameters simultaneously with the CO₂ total column by parameterizing particle amount, height distribution, and microphysical properties (Butz et al., 2009). Light path modification due to scattering by aerosols and cirrus clouds has been identified as a major source of error when retrieving XCO₂ from solar near-infrared backscatter measurements (O'Brien and Rayner, 2002; Dufour and Bréon, 2003). The key quality of RemoTeC is its ability to simultaneously retrieve gas concentrations and the particle scattering properties of the atmosphere using an efficient radiative transfer model (Hasekamp and Butz, 2008). Particle scattering properties are effectively parameterized by a single spherical particle type characterized through its total column number density, the size distribution parameter, the height distribution parameter (Butz et al., 2011).

SECM was developed to simulate atmospheric CO₂ background concentrations in the form of mixing ratio profiles and XCO₂. SECM is based on a simple equation incorporating 17 empirical parameters, latitude, and date. The empirical parameters were determined by the National Oceanic and Atmospheric Administration's (NOAA) CarbonTracker (Version 2010) least squares fitting to assimilation system (Reuter et al., 2012). SECM, depending only on date and latitude, can explain more than 94% of the variability in current atmospheric CO₂ concentrations. The atmospheric CO₂ profiles simulated by SECM have a linear pressure dependency with different slopes in the troposphere and stratosphere. SECM can be used as a priori knowledge in an optimal estimation framework without additional external information.

Several groups have shown that an ensemble mean, weighted mean, or median can outperform each of the eight aforementioned individual models under appropriate conditions (Kharin and Zwiers, 2002; Vautard et al., 2009). Given this state of affairs, Reuter et al. (2013) developed the ninth and final retrieval method, EMMA, to combine WFM-DOAS, BESD, NIES, NIES-PPDF, ACOS, UoL-FP and RemoTeC results into one new dataset. The basic principles incorporated in these seven algorithms are the same and can be summarized as follows: 1) a satellite instrument measures backscattered solar radiation in the near-infrared O₂ and CO₂ absorption bands; 2) a radiative transfer plus forward model is utilized to simulate the satellite measurement for a known parameter vector and an unknown state vector; 3) an inversion method is employed to find the state vector which results in the best agreement between simulated and measured radiances; and 4) the retrieved state vector is assumed to represent the most likely atmospheric state.

However, the seven methods are based on: 1) different absorption bands; 2) different inversion methods such as optimal estimation, Tikhonov-Phillips and least squares; 3) different physical assumptions on the radiative transfer in scattering atmospheres; and 4) different pre- and post-processing filters (e.g., cloud detection from the O₂-A band or from a cloud and aerosol imager). The EMMA ensemble approach builds a database of individual level-2 retrieval estimates and takes advantage of the variety of different retrieval algorithms and their independent development under an assumption that it is unlikely that the majority of algorithms produce outliers in the same directions.

2.3 Challenges of the retrieval algorithms

The retrievals from different algorithms are not completely comparable because of the lack of international standards for CO_2 retrieval. For instance, the XCO_2 estimated with different retrieval algorithms will vary slightly depending on how the vertical weighting is computed. The OCO retrieval algorithm weights CO_2 concentrations by pressure (Connor et al., 2008), whereas a SCIAMACHY CO_2 retrieval algorithm weights CO_2 concentrations by the total number of air molecules (Reuter et al., 2010) and the dry air component (Wunch et al., 2010).

Similarly, algorithms based on Differential Optical Absorption Spectroscopy (DOAS) in the absence of atmospheric scattering rely on absorption-only techniques (Buchwitz et al., 2000). For the retrieval of SCIAMACHY data, aerosol scenarios and surface albedo are assumed for the DOAS-based algorithms (Buchwitz et al., 2000). It can usually retrieve reasonably accurate values of XCO₂; however, when the actual equivalent optical path length differs from the assumed path length, large errors will appear in the retrieved results. Neglecting scattering can lead to unacceptably large retrieval errors when optically thin clouds or aerosols are present (Butz et al., 2009; Houweling et al., 2005; Aben et al., 2007).

The PPDF-based retrieval (Oshchepkov et al., 2008, 2009), and NIES algorithms (Yoshida et al., 2011) for GOSAT have tried to account for scattering effects in the retrieval of CO₂. However, tests to prove their efficacy in accounting for these scattering effects are sometimes incomplete. This shortcoming might be partly due to light-path modification not only depending on the particle amount but also on particle size and height (Butz et al., 2011).

Three types of vertical structures have been observed: 1) CO_2 concentration changed little with altitude; 2) CO_2 concentrations showed a turning point at certain altitudes and then decreased above that; and 3) CO₂ concentrations showed a clear monotonic decrease with altitude (Li et al., 2014). It was inferred that in the low troposphere, the vertical structure of CO₂ distribution mainly depends on source emission variations at the ground, as well as vertical and horizontal transport of air masses due to meteorological processes. A type of neural network known as a multilayer perceptron with two hidden layers of neurons and a hyperbolic tangent as activation functions was applied to retrieval of CO₂ vertical profiles and its column-averaged concentration by reflected solar radiation from GOSAT. It achieved an accuracy of better than 1 ppm for column-averaged values and better than 4 ppm for the surface CO₂ concentration (Gribanov et al., 2010). Ideally, a vertical profile of the greenhouse gases concentrations would be desirable. Indeed, a full knowledge of the vertical distribution brings additional information on the locations of sources and sinks. However, none of the currently envisioned remote sensing techniques allows the retrieval of such vertical distributions (Bréon and Ciais, 2010).

2.4 Interpolation

Describing the spatial and/or temporal distribution of atmospheric CO₂ through curve fitting or regression has a long tradition in the in situ measurement community (Reuter et al., 2012). For instance, Komhyr et al. (1985) applied the spline fitting technique to surface-based CO₂ measurements of NOAA's flask sampling network in order to analyze the latitudinal distribution and temporal evolution of atmospheric CO2 concentrations. Lancaster and Salkauskas (1986) developed a polynomial spline interpolation for surface fitting and Kobza and Mlčák (1994) constructed a spline surface from known mean values on a rectangular lattice. Masarie and Tans (1995) developed a spatial and temporal interpolation and extrapolation scheme for NOAA's flask sampling network utilizing individual site records as reference time series. A parabolic spline method was developed in order to create regional trace gas maps from satellite observations, in which the spline coefficients are computed using one-dimensional splines, which allow for fast computation for a large number of pixels (Kuhlmann et al., 2014).

Vertical column densities of trace gases, retrieved from the NIR nadir spectra of the satellite measurements, are typically expressed in the instrument's frame of reference using across- and along-track positions. To get a surface of a trace gas, the aforementioned level-2 products have to be projected on a longitude-latitude grid using a suitable gridding method to produce a level-3 product (Kuhlmann et al., 2014). Several approaches have been developed to create full-coverage (i.e., Level-3) maps of column-averaged CO₂ concentrations (XCO₂) from ACOS products. For instance, moving averages were used to generate geographical distribution maps of upper tropospheric CO₂ at spatial resolutions of $5^{\circ} \times 5^{\circ}$ in 2008 retrieved from IASI observations (Crevoisier et al., 2009). The simple average was employed to map CO₂ surfaces at spatial resolutions of $10^{\circ} \times 10^{\circ}$ from the TES (Kulawik et al., 2010). Kriging was applied to generate Level-3 maps of XCO_2 at a spatial resolution of $1^{\circ} \times 1.25^{\circ}$, which are derived directly from the Level-2 observations covering the second half of 2009 (Hammerling et al., 2012a, 2012b). And finally, a method for high accuracy surface modelling (HASM) was used to create full-coverage maps of column-averaged CO₂ concentrations (XCO₂) from ACOS product (Yue et al., 2015).

3. Ground-based observations

The Total Carbon Column Observing Network (TCCON) was established in 2004 with a primary focus on measuring precise and accurate columns of CO2. TCCON is a ground-based network of Fourier transform spectrometers (FTSs) designed to retrieve accurate column abundances of CO₂, CH₄, N₂O and CO from near-infrared (NIR) solar absorption spectra. There are 26 sites currently. The scientific goals of the network are to improve the understanding of the carbon cycle, to provide the primary validation dataset for retrieval of XCO₂ and XCH₄ from space-based instruments, and to provide a transfer standard between the satellite measurements and the ground-based in situ network (Wunch et al., 2011). XCO₂ is insensitive to variations in surface pressure and atmospheric water vapor. It is much less affected by vertical transport than surface in situ measurements because the column vertically integrates the concentration of CO2 above the surface. In contrast to the reflected sun observations of the space-based sensors, the accuracy of the retrieval from the TCCON spectra is minimally influenced by aerosols, uncertainty in air-mass or variations in land surface properties. Therefore, the horizontal gradients in measured XCO₂ are more directly related to the underlying regional-scale fluxes than is the case for the surface *in situ* measurements of CO_2 (Yang et al., 2007).

A reliable in situ CO₂ and CO analysis system has been

developed at eight of the sites in NOAA's Earth System Research Laboratory's (ESRL) Global Greenhouse Gas Reference Network since the early 1990s. The network uses television and radio transmitter towers that are higher than 300 m. The towers are distributed across the US and provide the basis for prototype CO₂ data assimilation systems such as NOAA's CarbonTracker system. Observations from tall towers at several heights along the tower describe the vertical gradient, which reflects the relative influence of remote and local sources (Bakwin et al., 1998). Measurements obtained from sampling levels above 100 m are minimally impacted by nearby vegetation and other local emissions (Andrews et al., 2014).

Eddy covariance (EC) systems are frequently used to quantify exchanges and budgets of carbon dioxide (CO₂), water (H₂O), and energy at ecosystem scales as well. A global network of over 500 EC flux towers called FLUXNET has been established, which continuously measures the aforementioned fluxes at a sampling rate of 5-50 Hz across different ecosystem types (Baldocchi, 2008). FLUXNET data has been used to predict the spatiotemporal dynamics of net CO₂, H₂O, and energy exchanges among the pedosphere, hydrosphere, biosphere, and atmosphere (Stauch et al., 2008). However, EC time-series data obtained from flux towers are noisy due to both stochastic and deterministic atmospheric turbulence processes, and no standard data-denoising protocols exist at present. Evrendilek (2014) recently showed that integration of temporal artificial neural networks (ANNs) and discrete wavelet transform (DWT) denoising provided more accurate and precise estimates of net ecosystem CO₂ exchange.

The Comprehensive Observation Network for Trace gases by Airliner (CONTRAIL) project has been observing vertical CO₂ profiles over 43 airports worldwide (Basu et al., 2014). Automatic Air Sampling Equipment (ASE) and continuous CO₂ measuring equipment (CME) are installed on the racks in the forward cargo compartment of the aircraft. The CME includes a non-dispersive infrared analyzer, a data logger, and two calibration cylinders for *in situ* CO₂ measurements. The ASE is designed for flask sampling; the instrument, connected to a metal bellows pump, is made up of a specially designed control board and can accommodate 12 flasks. The CME platform supports high-frequency measurements of CO₂ and provides detailed spatial observations over large areas, whereas ASE provides useful distributions not only of CO₂ but also various trace gas species, as well as their isotopic ratios. Both sets of sampling equipment are automatically controlled through input of relevant flight parameters from the aircraft data system (Machida et al., 2008).

Next, we turn our attention to a series of simulation models that endeavor to combine satellite- and ground-based measurements to predict spatio-temporal variations in CO₂ and other trace gases.

4 Discussion and conclusions

In terms of the fundamental theorem of Earth surface modelling, a CO₂ surface can be simulated with HASM when its spatial resolution is fine enough, which is uniquely defined by both extrinsic and intrinsic invariants of the surface (Yue et al., 2016). The intrinsic invariant expresses the information observed when we stay on the surface, about the details of the surface. The extrinsic invariant expresses the change of the surface observed from outside the surface (Yue, 2011). In other words, a surface of a trace gas cannot be determined by the satellite-based observations alone, and information from ground-based observations contributes another essential determinant of the surface. When remotely sensed data from satellites are available, ground measurements have to be obtained and incorporated before HASM can be used to generate a more accurate surface. When both remotely sensed data from satellites and ground measurements are available, HASM can be used to generate a surface that is more accurate than the one from either the satellite observations or the ground measurements.

Space-borne observations complement the in situ network by bringing a high density of measurements over most of the Earth, including over regions that are difficult to access. However, generating satisfactory satellite-based estimates of sources and sinks faces a number of challenges. The primary one is accuracy. The concentration gradients that are generated by local sources and sinks are small in comparison to the background concentration. A very high relative accuracy is therefore necessary, and such accuracy is difficult to achieve from space. Space-based measurements of CO2 such as SCIAMACHY, GOSAT and OCO have provided the most realistic opportunity to achieve global coverage at regional scales. However, these space-based measurements have rather high scatter and potentially large-scale artifacts that hinder their use in source-sink estimation; the accuracy of the current estimates is still not sufficient to improve our knowledge on carbon sources and sinks (Crisp et al., 2012).

Ground-based observations, on the other hand, include three ways to estimate the fluxes of CO₂: 1) taking direct measurements from towers above various ecosystems using eddy covariance methods; 2) sampling carbon stocks at various intervals and deducing the flux from the temporal change in stocks; and 3) relying on atmospheric CO₂ concentrations measured at various stations distributed around the globe. Despite the continuous expansion of the in situ monitoring network, it is clear that it will never have the density required for global monitoring of fluxes at a fine scale. Moreover, the in situ monitoring network will not be expandable with adequate density over the oceans, and over large forest areas that are difficult and costly to access (Bréon and Ciais, 2010). In other words, ground-based observations can give an excellent picture of the global atmospheric CO₂ growth rate and even some reasonable information for hemispheric gradients, but the spatial distribution of these observations is too sparse to accurately infer CO₂ concentrations on regional scales (O'Dell et al., 2012).

In short, a surface modelling platform for CO_2 dynamics should be constructed to simulate and visualize CO_2 concentrations. Such a platform would need to incorporate developing international standards for CO_2 retrieval algorithms that completely account for scattering effects and allow the retrieval of CO_2 vertical distributions on the one hand and efficiently fuse space- and ground-based measurements and support coupling with atmospheric transport models on the other hand. A platform with these characteristics offers the best hope for modeling spatio-temporal variability in greenhouse gas concentrations and the relative roles of sources and sinks across various scales across the globe.

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