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Four-dimensional data assimilation of atmospheric CO_2 using AIRS observations

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Abstract

The European GEMS project has built a system that is capable of assimilating various sources of satellite and in-situ observations to monitor the atmospheric concentrations of CO_2 and its surface fluxes. The system consists of an atmospheric 4-dimensional variational data assimilation system that provides atmospheric fields to a variational flux inversion system. In this paper, we describe the atmospheric data assimilation system that currently uses radiance observations from the Atmospheric Infrared Sounder (AIRS) to constrain the CO_2 mixing ratios of the data assimilation model. We present the CO_2 transport model, the bias correction of the observation-model mismatch, and the estimation of the background error covariance matrix. Data assimilation results are compared to independent CO_2 observations from NOAA/ESRL aircraft showing a reduction of the mean difference of up to 50% depending on the altitude of the aircraft observations relative to an unconstrained transport model simulation. First flux inversion results are also positive, showing an improved fit of the forward model simulation to independent NOAA flask observations of up to 40% after the flux inversion. The results show for the first time that there is potential for satellite observations to contribute useful information to CO_2 flux inversions. In the coming years, observations from dedicated CO_2 satellite missions will be added to the system. Together with improved error characterization and bias correction, we hope to show that satellite observations can indeed complement the in-situ observation system to get a better estimate of global carbon fluxes.

1. Introduction

Over the last several years considerable effort has been put in extracting information about atmospheric CO_2 from infrared satellite sounders. The main driving force has been the potential improvement of atmospheric flux inversions, which are still data-limited. Significant progress has been made in expanding the surface based observation networks as well as the airborne CO_2 observations, but most of these observations are still confined to developed countries, which leaves large gaps in for instance the tropics. Satellite data are well-suited to fill these gaps, but the first dedicated CO_2 observing instruments will not be launched before the end of 2008. In the meantime, however, there is already a potential wealth of information through the various infrared sounding instruments. These instruments were mainly designed to observe atmospheric temperature and water vapour, but are also able to detect changes in CO_2. Various efforts have been made to extract this information, so far with mixed results. *Chédin et al.* (2008) showed CO_2 fire emission patterns in the Tropics by looking at the day-night differences of CO_2 estimates from the Television Infrared Observation Satellite (TIROS-N) Operational Vertical Sounder (TOVS), but *Chevallier et al.* (2005b) and *Peylin et al.* (2007) also showed that these TOVS retrievals are not good enough yet for surface flux inversions because of their significant regional biases. *Engelen and McNally* (2005) and *Chahine et al.* (2005) presented CO_2 estimates from the Advanced Infrared Sounder (AIRS) using a one-dimensional variational (1D-Var) data assimilation system and a classic retrieval scheme, respectively, with promising results. However, *Chevallier et al.* (2005a) warned that great care should be taken with these CO_2 estimates when used in flux inversions. Both the quality of the satellite estimates and the quality of the transport models used in flux inversions should be watched very carefully.

As part of the GEMS (Global and regional Earth-system (Atmosphere) Monitoring using Satellite and in-situ data) project (*Hollingsworth et al.* 2008), a data assimilation system to monitor atmospheric concentrations of CO_2 and CH_4 and their fluxes has been built. The system consists of a four-dimensional variational (4D-Var) atmospheric data assimilation system run at the European Centre for Medium-Range Weather Forecasts (ECMWF), a variational CO_2 flux inversion system run at Laboratoire des Sciences du Climat et de l'Environnement (LSCE), a variational CH_4 flux inversion system run at the Joint Research Centre (JRC), an independent CO_2 and CH_4 neural network retrieval system run at Laboratoire de Météorologie Dynamique (LMD), and a validation effort with independent models and in-situ observations run at the Max Planck Institüt - Jena (MPI). This paper describes the atmospheric CO_2 4D-Var system at ECMWF, which is based on the earlier work described by *Engelen and McNally* (2005), but comprises now a full 4D-Var setup for both the meteorology and the tracers. The aim is to assimilate observations from various satellite instruments, such as AIRS, IASI, CrIS, OCO, and GOSAT, to obtain a consistent estimate of the atmospheric CO_2 concentrations, which will then subsequently be used in surface flux inversions. We will show some first results of this flux inversion at the end, although a full description of this work will be given elsewhere.

The outline of the paper is as follows: we will first introduce the CO_2 transport model, the used AIRS observations, and the data assimilation system. Then the bias correction method and the background covariance matrix will be described. Finally, we will show results from the data assimilation with extensive comparisons to independent observations and, as noted above, briefly describe initial results from a flux inversion using the output from the CO_2 data assimilation.

2. CO_2 transport model

A 4D-Var data assimilation system requires a prognostic transport model that will forecast the atmospheric state from specified initial conditions. At ECMWF , tracer transport has been introduced in the Integrated Forecasting System (IFS) using the existing modelling framework for advection, convection and vertical diffusion [ECMWF, 2007, IFS documentation CY31r1. http://www.ecmwf.int/research/ifsdocs/CY31r1/]. For tracers, interpolation is quasi-monotone in the semi-Lagrangian (SL) scheme to avoid negative concentrations and to keep the amplitude of the advected field within the range of values of the initial field (*Hortal* 1994). Although this advection scheme is not fully mass-conserving, the gain of mass is lessened when the surface pressure is constrained by the analyses at the beginning of each forecast. A tracer mass fixer has also been coded now in the IFS (to be used in long forecast integrations) but has not been used here as the gain of mass is not considered significant within the framework of a data assimilation system.

Various climatologies were used to prescribe the CO_2 fluxes at the surface. The terrestrial natural biosphere fluxes are from the CASA process model (*Randerson et al.* 1997) and were provided within the framework of the Transcom continuous experiment (*Law et al.* 2008). They are annually balanced and were used at their 3-hourly resolution to resolve the diurnal cycle of the natural biosphere (*Olsen and Randerson* 2004). A linear interpolation was used to provide the fluxes at the transport model time step. The air-sea CO_2 exchange is described by a monthly mean climatology and is based on the revised version of *Takahashi et al.* (2002). This version uses wind speeds from 10 meter height instead of 0.995 sigma-level. Anthropogenic emissions are based on the EDGAR 3.0 $1°$x $1°$global map for 1990 (*Olivier and Berdowski* 2001) rescaled to the Carbon Dioxide Information Analysis Centre (CDIAC) country level estimates for 1998. These emissions are kept constant throughout the years. Finally, wildfire emissions are from the Global Fire Emission Database version 2 (GFED2) (*van der Werf et al.* 2006) and are provided at a 8-day resolution using MODIS fire hot spots (*Giglio et al.* 2003). These emissions have been injected at the surface given the lack of information on the fire intensity time evolution. All data sets were interpolated to the various horizontal resolutions used in the assimilation system. The IFS transport model has the capability to run at horizontal resolutions ranging from about $2°$ by $2°$ to about $0.2°$ by $0.2°$. For our CO_2 data assimilation runs we use a reduced Gaussian grid with a resolution of $1.125°$ by $1.125°$ at the equator on 60 sigma-hybrid levels (T159L60).

The CO_2 transport model has been extensively compared to in-situ observations both in terms of large-scale and short-scale atmospheric CO_2 variability. The baseline-air seasonal cycle at the surface is very well described by the transport model (left panel of Figure 1), although its amplitude in the northern hemisphere is underestimated

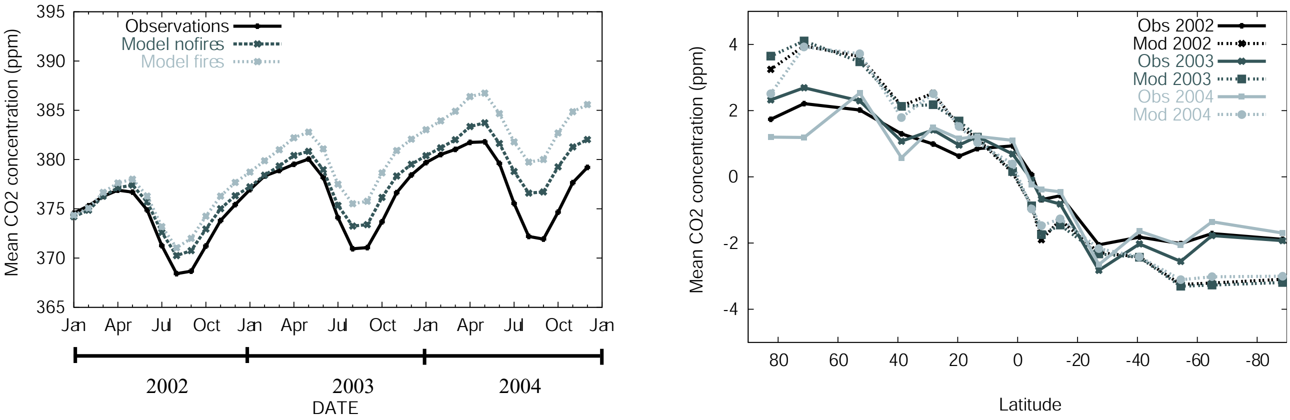

Figure 1: Mean seasonal cycle of atmospheric CO_2 mole fraction as calculated from the average of 8 surface locations in the Northern Hemisphere, observed in solid and modelled in dashed (left panel). The 8 locations correspond to the 8 flask stations Alert (ALT), Barrow (BRW), Shemya Island (SHM), Terceira Island (AZR), Sand Island (MID), Mauna Loa (MLO), Guam (GMI) and Christmas Island (CHR). Mean north-south gradient of atmospheric CO_2 mole fraction constructed from 16 surface locations, observed in solid and modelled in dashed. The model is sampled at the 16 flask stations, from north to south: Alert (ALT), Barrow (BRW), Shemya Island (SHM), Terceira Island (AZR), Sand Island (MID), Mauna Loa (MLO), Guam (GMI) and Christmas Island (CHR), Mahe Island (SEY), Ascension Island (ASC), Tutuila (SMO), Easter Island (EIA), Cape Grim (CGO), Macquarie Island (MQA), Palmer Station (PSA) and South Pole (SPO)

(not shown). The difference to observations is larger during the NH summertime and is due to the enforced annual carbon balance in CASA (respiration is rescaled to balance photosynthesis activity). This generates a larger annual trend in the transport model compared to the observations. Fire emissions were included in the IFS model to better describe the spatio-temporal variation of the atmospheric CO_2 concentration. However, their incorporation in the modelling increases the trend unrealistically. This is because part of fire emissions is reincorporated into the biomass, likely in the tropics during the growth of the vegetation, but is not taken into account in the estimation of the net ecosystem flux.

The modelled north-south (NS) gradient is over-estimated by 3 to 3.5 ppm (right panel of Figure 1). Again, deficiencies in the prescribed fluxes are likely to explain this result, although one cannot exclude a contribution from the transport model. The inter-annual variability shown by the observed NS gradient north of 50°N is not well reproduced by the transport model either. Since most of the CO_2 surface fluxes are prescribed as climatologies, any inter-annual variability in the IFS CO_2 model results can only be explained by the meteorology or fire emissions. These seem insufficient to explain the observed variability.

The difference between the modelled and observed gradients is an indication of the northern hemisphere sink only if we can rule out deficiencies in the transport modelling. Independent simulations with SF_6 have been carried out in a similar way as for CO_2. They show an overestimation of the NS gradient by ca. 0.15 ppt (not shown). Although this could be an indication of too slow inter-hemispheric transport in our transport model, recent studies draw attention to the significant uncertainties in the SF_6 emissions database (*Hurst et al.* 2006). As most of these tracer sources are in the northern hemisphere, uncertainties in the emissions may translate into an incorrect meridional gradient. Therefore, these SF_6 comparisons cannot be conclusive in detecting errors in the transport modelling.

Finally, within the framework of the TransCom continuous data experiment, our transport model has been compared to other transport models and to high frequency observations for the simulation of atmospheric CO_2 short-term variability. It has shown favourable results both for the simulation of the diurnal cycle (Law et al., 2008) and for describing the synoptic CO_2 variability (Patra et al., in revision).The use of ECMWF meteorology at a relatively fine horizontal and vertical resolution is certainly an asset, although the use of erroneous fluxes can locally lead to larger departures from in situ observations. Because of its relatively shallow surface layer, the IFS is more sensitive to erroneous nocturnal fluxes. This partly explains why the amplitude of the diurnal cycle is overestimated at a number of continental stations (*Law et al.* 2008). Deficiencies in the modelling of the nocturnal boundary layer may also have contributed to this result.

3. AIRS data

The Atmospheric Infrared Sounder (AIRS) [Aumann et al., 2003] was launched on board the NASA AQUA satellite in May 2002. After an initial period of testing, data were received operationally at ECMWF from October 2002 onwards. AIRS is a grating spectrometer covering the 650 - 2675 cm^{-1} infrared spectral domain at a resolution of $\lambda/\Delta\lambda = 1200$, giving 2378 channels. Accompanied by an AMSU-A instrument it flies onboard the Aqua satellite with equator crossing times of 1:30 am and 1:30 pm. The AIRS field-of-view (fov) is 13 km at nadir with a 3 x 3 array of AIRS footprints falling into one AMSU-A fov. Due to bandwidth limits in the trans-Atlantic line and other operational constraints ECMWF receives only 324 of the total 2378 channels in near-real time and only 1 out of every 9 AIRS fovs within a AMSU-A fov.

The channel selection is based on an original selection of 281 channels by NOAA/NESDIS appended with 43 extra channels in the two main CO_2 absorption bands based on the work by *Crevoisier et al.* (2003). In our AIRS CO_2 reanalysis the number of channels was further reduced to avoid problems specific to certain spectral bands: i) channels in the short-wave band were excluded from the analysis during local day time, because our radiative transfer model currently does not model solar radiation and the effects of non-local thermodynamic equilibrium; ii) channels in the main water vapour and ozone bands as well as channels sensitive to the surface over land and sea-ice are excluded to minimise the effect of IFS model errors in water vapour, ozone, and the surface skin temperature on the CO_2 analysis; iii) channels sensitive to the upper stratosphere were also excluded from the assimilation, because the IFS model has large temperature biases in the mesosphere of the polar winters. This way we have attempted to remove the known biases as much as possible. However, the cut-offs are somewhat arbitrary, because it is difficult to estimate the exact amplitude of these biases. The largest potentially remaining bias is caused by the mesospheric temperature bias in the IFS model and can reach values as high as 0.5 ppm. However, this bias only applies to the polar winter situation. As will be discussed later, we do not use any of the assimilated fields at latitudes higher than 60°for the use in flux inversions.

4. 4-dimensional variational data assimilation (4D-Var)

Our atmospheric 4D-Var data assimilation system is a practical formulation of Bayesian estimation theory for the particular case of a (near-)linear problem with un-biased Gaussian errors for time-evolving 3-dimensional fields like temperature or CO_2 (*Lorenc* 1986). It seeks an atmospheric model trajectory that is statistically consistent with the information provided by the observations $\mathbf{y}^o$ available for the analysis time window $[t_0, t_n]$ and the information provided by an *a priori* atmospheric model state $\mathbf{x}^b$ called the background state. This background state is usually taken from a short-range forecast valid for time t_0. The atmospheric model trajectory within the assimilation window (the reference state $\mathbf{x}^r$) is then completely defined by the initial state $\mathbf{x}_0$ at time t_0, which is the same as the background state at the start of the minimization, through the use of the dynamical and physical forecast model (i.e., the IFS model).

The analysis correction ($\delta\mathbf{x}(t_0)$) to the atmospheric model initial state is sought as a combination of the information from the observations and from the background using an objective cost function with two terms (e.g., Courtier et al. 1994):

$$J(\delta\mathbf{x}(t_0)) = \frac{1}{2}\delta\mathbf{x}(t_0)^T\mathbf{B}^{-1}\delta\mathbf{x}(t_0) + \frac{1}{2}\sum_{i=0}^{n}[\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i]^T\mathbf{R}^{-1}[\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i] \quad (1)$$

the background term and the observation term. The observation departures ($\mathbf{d}_i$) are the differences between the observed radiances and the atmospheric model simulated equivalent radiances, as in

$$\mathbf{d}_i = \mathbf{y}_i^o - \mathscr{H}_i[\mathbf{x}^r(t_i)] \quad (2)$$

where $\mathscr{H}_i$ is the full non-linear observation operator in the form of the Radiative Transfer for the TIROS Operational Vertical Sounder (RTTOV) radiative transfer model. RTTOV (Matricardi et al. 2004) is a fast radiative transfer model using profile dependent predictors to parameterize the atmospheric optical depths. For the CO_2 assimilation experiments we applied the methods developed for RTIASI (Matricardi 2003) to include CO_2 as a profile variable in RTTOV. $\mathbf{H}_i$, which appears in (1), is the tangent linear observation operator that is part of the RTTOV model. The reference state values at time t_i, needed for the calculation of the observation departures $\mathbf{d}_i$, are evolved according to the full non-linear forecast model $\mathscr{M}$:

$$\mathbf{x}^r(t_i) = \mathscr{M}[\mathbf{x}^r(t_0)] \quad (3)$$

The increments themselves are evolved through time according to the tangent linear model $\mathbf{M}$:

$$\delta\mathbf{x}(t_i) = \mathbf{M}_i\delta\mathbf{x}(t_0) \quad (4)$$

Finally, $\mathbf{B}$ and $\mathbf{R}$ are the background error covariance matrix and the observation error covariance matrix, respectively.

The cost function is then minimized with respect to the increments of the initial state ($\delta\mathbf{x}(t_0)$). These increments are added to the background state to obtain the analysis $\mathbf{x}(t_0)$:

$$\mathbf{x}(t_0) = \mathbf{x}^b + \delta\mathbf{x}(t_0) \quad (5)$$

The advantage of a full data assimilation system is that it seeks to combine all available observations in an (near-) optimal way. At ECMWF ground based and satellite based data are used to constrain the relevant fields in the forecast model. In addition to AIRS, satellite data from various sensors are assimilated, such as the High Resolution Infrared Radiation Sounder (HIRS), the Advanced Microwave Sounding Unit (AMSU-A and AMSU-B), the Special Sensor Microwave / Imager (SSM/I), the Geostationary Operational Environmental Satellites (GOES), and the Meteosat instruments. These data are thinned to reduce spatial correlations of the measurement errors and they also undergo a bias correction. This bias correction seeks to remove biases in the observations and radiative transfer modelling and depends for most instruments on air mass and viewing angle (Harris and Kelly 2001). For most satellite instruments these biases are estimated using the so-called Variational Bias Correction (VarBC) method (Auligne et al. 2007). In this method a bias model is defined consisting of certain predictors with corresponding coefficients. These coefficients are then added to the minimization vector and are optimized at the same time as the meteorological variables, such as temperature, divergence, and humidity. The specific bias correction method chosen for our AIRS CO_2 assimilation will be described in the next section.

The 4D-Var data assimilation system currently only uses radiance data that are not affected by clouds. For this purpose, a cloud detection algorithm was developed specifically for AIRS (McNally and Watts 2003). This scheme detects which AIRS channels are affected by clouds and removes those channels from the assimilation, while retaining the channels that are not affected by clouds. This allows use of AIRS data even where the field-of-view is cloudy. If there is high cloud, only stratospheric information will be assimilated, but, if there are low clouds only, a significant amount of tropospheric information can be used. Finally, some channels were removed from the analysis either because of instrumental problems or because of unaccounted errors in the observation operator. Main example of the latter is the removal during local day time of the short-wave 4.2 μm band, which is affected by solar radiation not modelled in the current version of RTTOV as well as non-local thermodynamic equilibrium effects.

5. Bias correction

An important part of any data assimilation system is the bias correction. Various sources of bias exist, such as systematic errors in the spectroscopy, systematic errors in the IFS model, and systematic instrument errors. Generally, the first guess departures (difference between real observation and the IFS transport model simulated observation) are bias corrected to a certain baseline that can for instance be defined by accurate observations, such as temperature radiosondes. However, this is not always straightforward, either by the lack of sufficient accuracy in the baseline observations or by the lack of enough baseline observations. The former is for instance the case for atmospheric humidity, while the latter is the case for CO_2. When there is no sufficient baseline, it becomes difficult to separate the observation biases (which include biases in the radiative transfer modelling among others) from the IFS model biases. For CO_2 we do not want to correct for the IFS transport model bias, because the main cause for this bias is the inaccuracy of our prescribed surface fluxes. Optimally, we would like to have the observations correct these IFS transport model errors, which will allow us then to estimate more accurate surface fluxes through a surface flux inversion. An extensive description of the various bias correction models that are available is out of scope for this paper, so we will focus on the method used in the CO_2 reanalysis. This so-called gamma-delta method is described by *Watts and McNally* (2004). It is based on the assumption that the main bias comes from systematic errors in the radiative transfer modelling that can be modelled by a multiplier of the total optical depth as illustrated below in the radiative transfer equation for the atmospheric contribution to the observed radiance in channel i of a passive infrared sounding instrument:

$$R_a^i = \int_{p_s}^{0} B^i(T(p))d\mathscr{T}^i(p) \tag{6}$$

where the channel transmission is defined as

$$\mathscr{T}^i(p) = \exp[-\gamma \int_{p}^{0} \kappa^i(p)\rho(p)dp] \tag{7}$$

and $B^i(T(p))$ is the Planck function of temperature T at pressure p, and γ is the constant multiplier of the total optical depth. Both the absorption coefficient κ and the absorber amount ρ are a function of pressure as well. We estimated the γ-values as well as an additional global mean offset δ for each channel by running a VarBC data assimilation experiment in which the bias correction coefficients were part of the mimimization. In this experiment AIRS radiances were only used to calculate increments for the bias coeficients, leaving the initial atmospheric fields entirely defined by the IFS transport model and all other observations. This meant that the CO_2 distribution was fully defined by the IFS transport model, because there were no other CO_2 observations used. We used a northern hemisphere winter month to ensure the IFS model bias was as small as possible. This is based on the comparison of the unconstrained IFS model to in situ observations that shows larger model biases during the Northern hemisphere summer-time (left panel of Figure 1). The reason for these biases is likely to be related to the prescribed natural biosphere fluxes for which an annual carbon balance has been

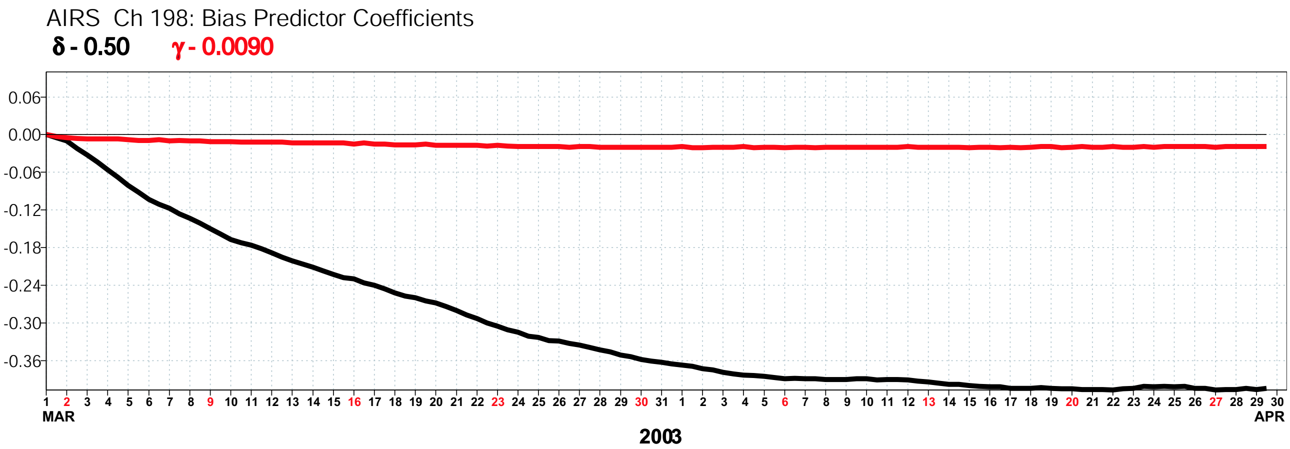

Figure 2: Evolution of bias correction coefficients for AIRS channel 198. The bias model corresponding to the coefficients δ and γ is described in the text.

enforced. The remaining IFS model bias could in principle still be fitted by the γ-δ bias correction model, but we believe that the effect is relatively small. An example of the evolution of the bias correction coefficients is shown in Figure 2. The figure shows the development over time of the coefficients belonging to δ and γ. It can be seen that for this particular AIRS channel (channel 198) the coefficients reach some sort of equilibrium after about 1 1/2 month. Our CO_2 data assimilation runs then use the estimated γ and δ values as fixed values for the AIRS channels we use actively. All the other AIRS channels, although not used to estimate CO_2, are still used for the cloud detection (*McNally and Watts* 2003) and are bias corrected with the operational VarBC bias correction.

6. Background constraint

The background constraint is used to limit the amount of possible solutions of the 4D-Var minimization and by doing so to stabilize the inversion. It also plays an important role in distributing the information from the observations. For the CO_2 problem we use measurements from the AIRS instrument, which observes in the infrared. The weighting functions of these measurements are generally quite broad and therefore contain limited information at high vertical resolution. The vertical error correlations specified in the background covariance matrix are therefore used to distribute the broad information of the observations in the vertical. The assumption is that an error at a specific height is correlated with errors at other heights. If these error correlations are known exactly, it is accurate to use them for the vertical distribution of the satellite corrections. However, in reality the error correlations are only approximations. The same rationale also applies to the horizontal and the background covariance matrix defines how errors in the short-term forecast are correlated between grid boxes. In practice, this works as a smoothing operator on the relatively noisy CO_2 increments from individual observations. To illustrate the combined effect of the broad AIRS weighting functions and the specified background error correlations Figure 3 shows the changes in CO_2 for a single AIRS footprint using 24 of the available CO_2 sensitive channels for two different locations, tropical Africa on the left and mid-latitude Asia on the right. The patterns are broad, both in the horizontal and the vertical. It is nice to see the much deeper vertical structure over Africa, which is caused by the larger temperature lapse rate.

To estimate the CO_2 background covariance matrix we used the method developed by *Parrish and Derber* (1992) (also known as the NMC method). This method consists of taking the differences between forecasts of different length valid at the same time, and assumes that these differences represent a good sample for the

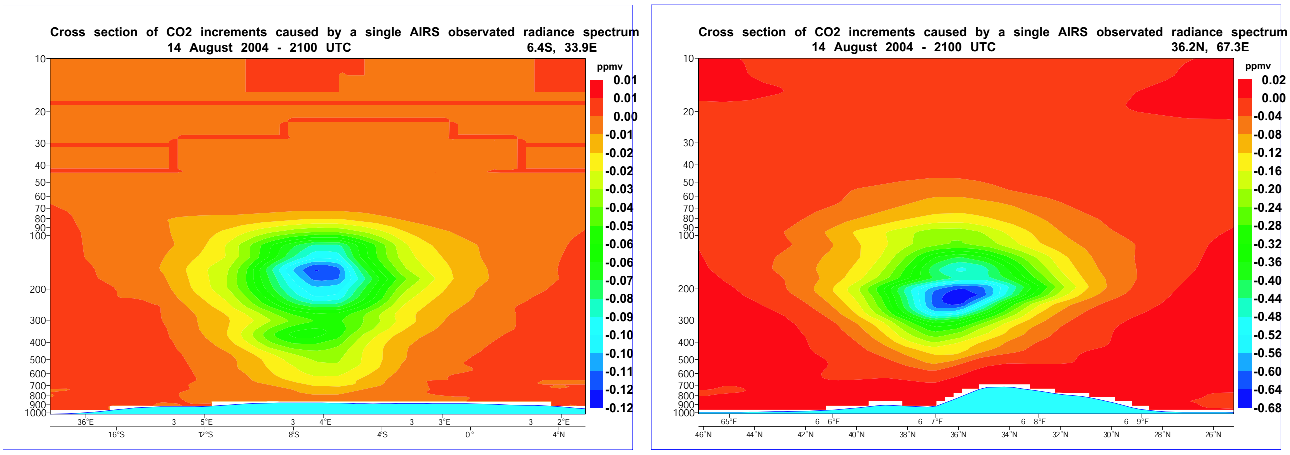

Figure 3: Vertical cross sections of CO_2 increments caused by a single AIRS observation (using 24 CO_2 sensitive channels) over tropical Africa (6.4°S, 33.9°E) and over mid-latitude Asia (36.2°N, 67.3°E).

background error. An extensive description of the application of this method to the new tracer variables in the ECMWF data assimilation system is given by *Benedetti and Fisher* (2007). We used the horizontal and vertical correlations directly from this method, but inflated the standard deviations of the errors to account for the uncertainties in the prescribed surface fluxes.

The mathematical formulation of the background error covariance matrix **B** is based on the work by *Fisher* (2003, 2004), and allows a better representation of the spatial variability of horizontal correlations with respect to the more rigid *Derber and Bouttier* (1999) formulation, thanks to the introduction of the 'wavelet' J_b. In this approach, the properties of the B-matrix are modelled by using the mathematical framework of wavelet-like, non-orthogonal base functions having simultaneous localisation both in space and wave number. For a rigorous mathematical description of the wavelet Jb formulation, the reader is referred to *Fisher* (2003, 2004), while for a less mathematical general introduction the reader is referred to *Fisher* (2006).

7. Reanalysis results and validation

Assessing the quality of a complex system like a 4D-Var is critical. Its various components have to be carefully evaluated. As described in section 2, the transport model has been extensively compared to other CO_2 transport models and surface flask data (e.g., *Law et al.* 2008), which showed favourable results. However, the assimilation of AIRS radiances has the largest impact in the free troposphere. Therefore, other means of validation had to been found. The National Oceanic and Atmospheric Administration/Global Modeling Division (NOAA/ESRL) has compiled a data set of flask samples collected from profiling aircraft at various locations (*Tans* 1996)[C Sweeney, NOAA/ESRL, personal communication, 2008; see also http://www.esrl.noaa.gov/gmd/ccgg/aircraft.h The profiles usually observe the atmosphere between the surface and about 8 km altitude, which is more appropriate to assess the impact of AIRS on the CO_2 fields than the surface flasks. Because the flight profile data have much higher accuracy than the results from our CO_2 transport model and assimiliation system, we assumed them to represent the true atmospheric state. However, care should be taken in the comparisons to properly take the location of the flight profile into account. For example, the profiles observed in Worchester, Massachusetts (NHA) are influenced strongly by both the natural biosphere and anthropogenic emissions from the nearby cities. While we hope to model the natural biosphere fluxes reasonably well, we know that significant errors are introduced in this area by using annual mean anthropogenic emissions. This results sometimes in very different reanalysis profiles compared to the observed profiles as is illustrated in Figure 5b.

In the comparisons shown below, we have tried to reduce the amount of averaging to make the validation tests as demanding as possible. For every measured flight profile in the period January 2003 till December 2004 we have extracted profiles from an unconstrained CO_2 model run and the AIRS reanalysis. The unconstrained model run uses the operational ECMWF analyses to transport CO_2 around starting from the same initial field on 1 January 2003 as the AIRS reanalysis. However, there is no observational constraint on CO_2 during this model run. The AIRS reanalysis uses all available observations to both constrain the meteorology and the CO_2 fields. For the spatial interpolation to the profile location we used the nearest grid box and for the temporal interpolation we used a simple linear interpolation between the closest 6-hour analysis fields. The vertical interpolation from the model pressure levels to the observation altitudes was done using simple hydrostatic equations. Time series were then created at 1000m intervals for each station. For each time series the mean difference (bias) between the unconstrained model run and the observations and between the reanalysis and the observations was calculated as well as the standard deviation of the differences. Figure 4 shows for three altitudes (1000m, 4000m, and 7000m) these bias and standard deviation values for all stations with sufficient data. The figure shows there is no significant change at 1000m (bottom plots) between the unconstrained model and the AIRS reanalysis, both in bias and standard deviation. This is not surprising, because the AIRS sensitivity to CO_2 is very low at this level. Therefore, any information from the observations can only change CO_2 concentrations at this level through the transport or through the information spreading of the background covariance matrix. The latter is most likely not optimal and will therefore spread the information incorrectly. At 4000m there is already a significant improvement in bias visible using the AIRS data and at 7000m this improvement is very clear. The bias in the unconstrained model and the remaining bias in the reanalysis are mainly caused by the incorrectly specified surface fluxes. An insufficiently strong sink is causing a trend in the CO_2 concentrations that is stronger than observed. Although the AIRS observations do partially correct this anomalous trend, they are not able to fully correct it. This is most likely a result of a continuous incorrect forcing at the surface (the incorrect fluxes) that is not significantly corrected by the observations where it matters most (in the boundary layer).

The reduction of the bias by analysing AIRS observations seems to come at a cost, though. While the bias is reduced, the standard deviation of the differences with the profile observations is increased. The exact reason for this increase is difficult to pin down, but several potential causes can be identified. Firstly, the observations have limited capability in adjusting details of a CO_2 profile. The vertical sensitivity functions of the radiance observations are already quite broad and the overlap among the channels is large as well (see for instance Figure 1 in *Engelen and McNally* (2005). Furthermore, this instrument senstitivity function is convolved with the specified model background correlation structures as was shown in the previous section. This broad convoluted increment pattern will often adjust the CO_2 values correctly at the level of the strongest satellite observation sensitivity, but at the same time adjust the CO_2 values above and below this level incorrectly. This will then create more variability which is transported around. Figure 5 shows two examples of this behaviour by comparing observed flight profiles (black) with profiles extracted from the unconstrained model run (blue) and the AIRS reanalysis (red). Figure 5a shows profiles for 17 September 2004 over Briggsdale, Colorado. The reanalysis is clearly able to reduce the bias with the observations compared to the unconstrained model run. But at the same time the profile has more variability than either the model run or the observations. Figure 5b shows profiles for 12 June 2004 over Worcester, Massachusetts. In this case the reanalysis again tries to reduce the bias with the observations, but is only able to do so at higher altitudes. In the lower 2000m it stays close to the unconstrained model profile. The reanalysis profile therefore increases the standard deviation of the difference with the observation.

Another cause of increased variability could be due to inhomogeneous sampling caused by cloud cover. AIRS is able to make relatively large adjustments to the CO_2 field in clear sky areas. All available channels are used in such areas and the model background errors are relatively large, reflecting the errors in the prescribed surface fluxes, leaving sufficient room for increments of up to 10 ppmv. However, in areas with clouds in the upper

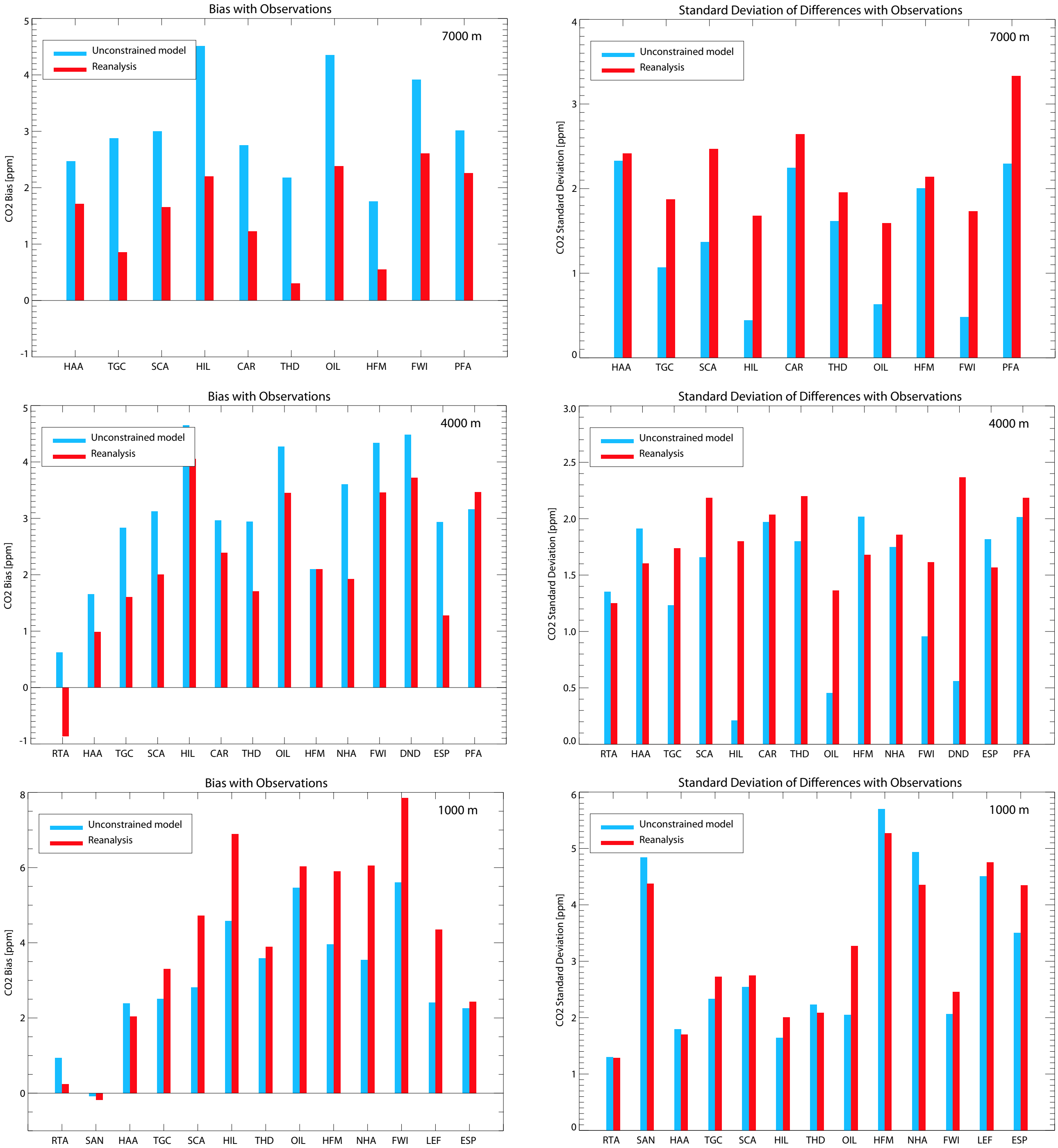

Figure 4: Bias (left) and standard deviation of the difference (right) of the unconstrained model run (blue) and the AIRS reanalysis (red) relative to independent flight observations from the NOAA/ESRL network

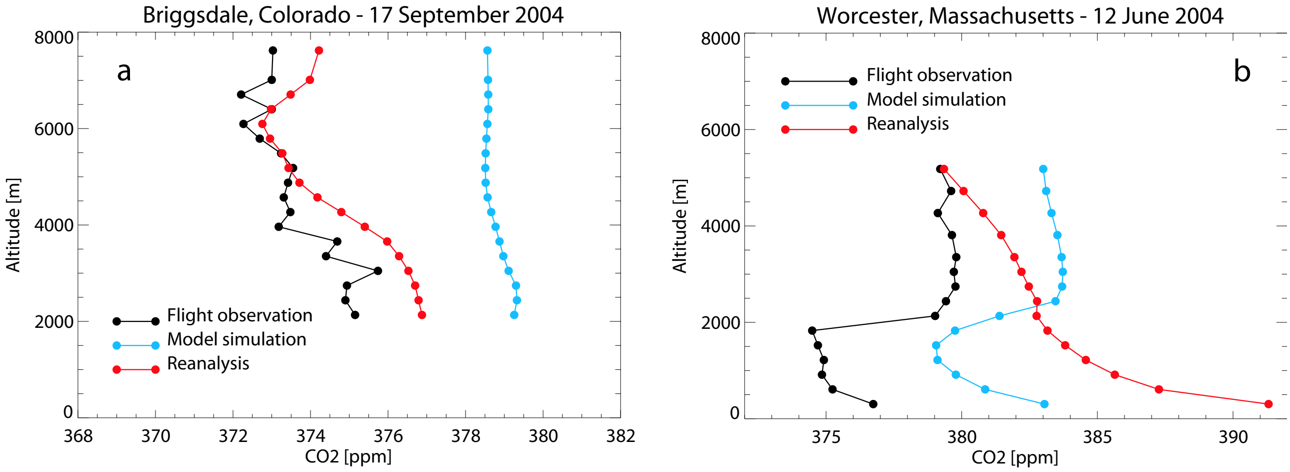

Figure 5: Observed (black), modeled (blue), and reanalysed (red) profiles of CO_2 for 17 September over Briggsdale, Colorado (left), and for 12 June 2004 over Worchester, Massachusetts (right). Flight data were provided by NOAA/ESRL.

troposphere, AIRS is not able to make significant adjustments. This combination of clear and cloudy areas could result in localized adjustments that are then transported down-wind, while in reality a much larger scale adjustment should have been made. This will introduce larger variability, while in the end the mean is much less affected. This effect is probably significant because the CO_2 model is biased (mainly through the deficiencies in the prescribed surface fluxes), which means the observations keep making relatively large adjustments instead of steering the model-observation merge to a certain equilibrium. An illustration is shown in Figure 6. The figure shows on the left the CO_2 increments (change to the model at timestep 0 of the 12 hour assimilation window) over the continental United States for model level 32 (ca. 260 hPa). The AIRS observations that triggered these increments are shown on top in the form of departures (observation value minus model simulated value) for a channel peaking around 260 hPa in its CO_2 sensitivity. Positive departure values mean that the observation brightness temperature is larger than the model simulated brightness temperature, which means that CO_2 should be reduced (assuming the atmospheric temperature stays constant). Negative values initiate the opposite reaction, an increase in CO_2. Because the AIRS observations were made close to the end of the assimilation window, the CO_2 increments had to be made upwind from the observations, which is illustrated by the wind vectors plotted on top. The plot on the right shows the change in the model field closer to the actual AIRS observation time. The incremental patterns have been advected down-wind and resemble very nicely the observation departure patterns as one could expect from a well-working 4D-Var system. However, at the same time, the assimilation system will not make any changes to the initial model forecast in areas that are not covered by observations due to for instance cloud cover as can for instance been seen in the top right of the plots. In principle, this should cause no problems if the specified background error correlations are correct for this geographical area and the weather pattern that is at hand. However, this can never be completely achieved. Therefore, more variability is being created, especially in a system that is not in full equilibrium between the model forecast and the observations.

The ultimate test for any satellite CO_2 retrieval or data assimilation system is the subsequent flux inversion. Our atmospheric CO_2 fields (or anyone's atmospheric CO_2 estimates) should be able to improve our knowledge of the CO_2 surface fluxes. Within the GEMS project flux inversions were carried out using the AIRS reanalysis as 'observational' input and first results are encouraging. The 4D-Var flux inversion (*Chevallier et al.* 2005b) uses a layer average of the CO_2 reanalysis between 200 hPa and 500 hPa as input and also uses exactly the same fluxes that were prescribed in the reanalysis as its a priori flux values to avoid conflicts with the prior information. In contrast to the short atmospheric assimilation windows (12 hours), the flux inversion was performed

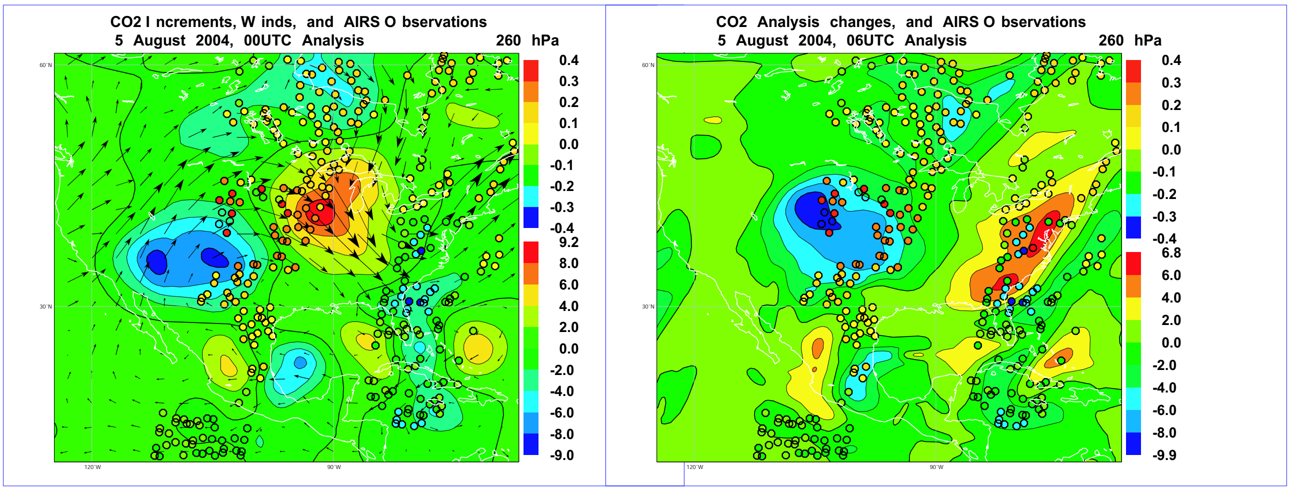

Figure 6: CO_2 increments at 21 UTC (left) and CO_2 analysis changes at 6 UTC (right) at model level 32 for two AIRS overpasses between 7 UTC and 8 UTC (shown as dots using the observation departure value for the color scale). Wind vectors for the same model level are overlaid in the left panel to illustrate the main horizontal advection pattern.

with two 1-year windows. More detailed information about the flux inversion set-up as well as full results will be described elsewhere [Chevallier et al., in preparation], but the results of the flux inversion using the reanalysis fields for 2003 and 2004 were tested by comparing the fit to independent surface flask observations from the NOAA ESRL network in terms of RMS before and after the AIRS flux inversion. Figure 7a shows the relative change in RMS for each station as a function of latitude and Figure 7b the same relative change as function of the prior RMS. For most stations a significant improvement (up to 40%) was obtained, which indicates that the AIRS observations are bringing useful information to the flux inversion. The stations with a negative improvement are mostly located in continental Europe. This area is very hard to model because of the strong heterogeneities in the terrain both in terms of orography and vegetation. This is also reflected in the larger RMS differences of the prior, as shown in Figure 7b. Results from this flux inversion also seem to indicate that AIRS is mostly correcting the trend (global representation of the missing carbon sink), although some geographical information is added as well. Obviously, the global trend correction can be done with very few accurate surface stations; it is the geographical information that we need to extract from the satellite observations. This will be the challenge for the coming years, when more dedicated CO_2 observing satellite instruments will be added to the system. As mentioned above, full details of the flux inversion will be described separately [Chevallier et al., in preparation].

8. Summary

Within the European GEMS project we have built a system that is capable of assimilating various sources of satellite and in-situ data to monitor the atmospheric concentrations of CO_2 and its surface fluxes and to improve our knowledge of these fluxes. The system consists of an atmospheric 4D-Var data assimilation system that provides atmospheric fields to a variational flux inversion system. The atmospheric assimilation system has been described in this paper and results have been compared with independent observations.

Great care has been taken in setting up the transport model, the bias correction, and in defining the background covariance matrix. Although the current system performs well, work will continue to improve the above components of the system. Especially, the estimates of the error correlations needs improvement to make better use of the observations. Also, the specification of the surface fluxes will need to be improved.

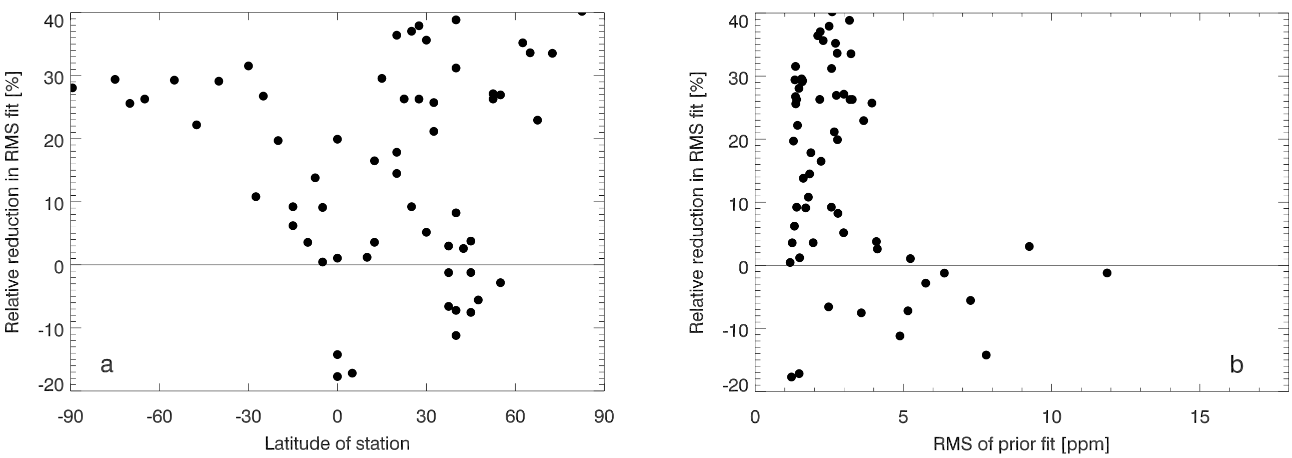

Figure 7: Relative change in RMS difference between the CO_2 model run and surface flask observations before and after the AIRS flux inversion as a function of latitude (left) and as a function of the RMS difference for each station before the flux inversion (right).

We are entering an exciting decade in which the assimilation system will come to its full potential being able to assimilate not only observations from the AIRS instrument, but also from the Infrared Atmospheric Sounding Interferometer (IASI), Orbiting Carbon Observatory (OCO), and Greenhouse gases Observing Satellite (GOSAT) instruments. The system will provide consistent CO_2 fields that match all the observations within the respective errors, which will be a valuable source of information for flux inversions. However, although the first results from the flux inversions using our system are quite promising, it will take time to address all potential sources for systematic errors as carefully as possible. Only when we are able to remove these systematic errors in the satellite-based estimates will flux inversions really provide us with the needed regional information on carbon surface fluxes. This assumes, though, that systematic errors in tracer transport models, which affect flux inversions from the surface-based networks as well, will be addressed at the same time.

It still remains open how the system will use in-situ data. In the current set-up, in-situ data are used for validation of the atmospheric assimilation system and can therefore in principle still be used in the subsequent flux inversion step. This is currently under investigation. However, one could also envisage using the in-situ data directly in the atmospheric assimilation. Especially, continuous surface observations should in principle have a strong enough constraint to be able to steer the data assimilation in the right direction. But in order to get full advantage from this type of observations a denser network is required. Only a few locations will not have the desired impact taking into account the enormous amount of satellite observations. Although the impact of the large amount of satellite data is partially compensated by their larger errors (compared to the very accurate in-situ data), the satellite data are also more likely to suffer from systematic errors. The in-situ data could be an important 'anchor' to the system in case they are able to provide sufficient weight against the satellite observations.

Apart from providing input to flux inversions, the system can also be used as a testbed for new model developments. Both improvements in transport modelling and in surface flux modelling can be tested directly against the various sources of satellite information. It is already envisaged to test prescribed natural biosphere fluxes from the ORCHIDEE model (*Krinner et al.* 2005) as well as in-line modelling of these fluxes using the C-TESSEL model. The improvement or degradation of the fit to the observations will provide crucial information for the improvement of these models.

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