Assimilation of satellite data for atmospheric composition

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ABSTRACT

This overview addresses the state of the art of satellite data assimilation for several types of atmospheric constituents: inert and chemically reactive, or gas phase compounds or aerosols, except water. The diversity of motives and applications are addressed: stratospheric trace gas analyses for improved retrievals and heating rate calculations or monitoring of key constituents like ozone, where space borne sensors include limb, occultation, and nadir viewing techniques. In the middle and lower troposphere only nadir looking sensors are applicable and usable for assimilation. A central application area is air quality forecasting, which typically mix in situ observations with space borne sensors. Close to the ground high spatial resolution is a challenging feature for satellite sensors, and in addition, emission rate estimation is an emerging task, which is extending the objectives of satellite data assimilation. Further topics, which are addressed, include tropospheric aerosol data assimilation, and greenhouse gas inversion and assimilation. Finally, the special case of fire data assimilation is presented.

1 Introduction

The incentive of satellite data assimilation for atmospheric constituent analyse was based on the wealth of earth observation satellites, launched since two decades as a multinational effort in support of the Global Earth Observing System of Systems (GEOSS). For example, many of the assimilation activities make use of data from sensors mounted on the A(fternoon) Train, which is a satellite constellation of six Earth observation satellites in sun-synchronous orbit, and EnviSat (Environmental Satellite). Part of the former A-Train configuration include Aqua with MODIS (Moderate Resolution Imaging Spectroradiometer) detects aerosol properties; land cover and land use change, fires and volcanoes (also on Terra), and AIRS (Atmospheric Infrared Sounder). A further A-train member is Aura with MLS (Microwave Limb Sounder) measures ozone, HNO_3, chlorine and other trace gases, OMI (Ozone Monitoring Instrument) uses ultraviolet and visible radiation to produce daily high-resolution data, mostly assimilated as NO_2, SO_2, CH_2O, and others. TES (Tropospheric Emission Spectrometer) measures tropospheric O_3, CO, CH_4, and NO_2 ozone in infrared wavelengths. EnviSat is the European Space Agency's (ESA) largest, meanwhile inoperative Earth observation satellite, where

data were mostly assimilated from SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY), an image spectrometer with the principal objective of mapping the concentration of multiple trace gases and aerosols in the troposphere and stratosphere with nadir and limb viewing modes. Furthermore, GOMOS (Global Ozone Monitoring by Occultation of Stars) performed star occultation, and MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) is a Fourier transforming infrared spectrometer which provides, among others, pressure and temperature profiles, and stratospheric profiles of key constituents like NO_2, CH_4, HNO_3, and O_3.

While satellite data assimilation of atmospheric trace gas compounds and aerosols, as well as assimilation of any kind of observations of atmospheric composition share a number of features with traditional assimilation for numerical weather prediction (NWP), there is a number of characteristic traits, which render many assimilation applications different, when chemistry is involved. Most similarities with weather forecasting assimilation occur in case of ozone, CO_2 and aerosol data assimilation as auxiliary constituents in forecast models, where better knowledge of field concentrations aims to improve radiative transfer calculations for other retrievals and heating rates (McNally et al., 2006). Other applications serve climate monitoring purposes of key constituents like ozone in the stratosphere, which also resemble reanalysis efforts by state of the art assimilation systems (see Lahoz et al., 2010 for numerous examples). Furthermore, an import climate motivated application is the assimilation of greenhouses gases, which are CO_2, CH_4, and N_2O. In this realm, for most cases it is often not primarily field analyses, which attract interest, but source strengths estimation, which modifies the assimilation task to a source inversion problem (e.g. Chevallier et al., 2014).

A key discipline in compound data assimilation targets the analysis of tropospheric reactive chemistry, including aerosols. Many problems mentioned above are accumulated in case of air quality forecasts. These include: (i) the number of reactive species per grid cell, including aerosol parameters, is one order of magnitude higher than in meteorological models, that is O(100), (ii) chemical kinetics act on a large variety of time scales, μ-seconds to days and longer, generating chemical imbalances, (iii) spatial scales are affected from long range transport to local, and (iv) emission patterns governed point and line source. Most notably, the question, which parameter is to be optimised in the first place, remains to be answered. In numerical weather prediction, data assimilation serves to better control an initial value problem, optimising the prognostic variables, because they critically control the forecast, and, at the same time, are not sufficiently well known. While forecasts with chemistry-transport-models (CTMs) also constitute an initial value problem, emission rates, and partly also deposition velocities as boundary values exert the like influence on the forecast, yet they are insufficiently known as. Consequently, they should be included in the assimilation process, jointly with inverse modelling (Elbern et al., 2010b).

Due to recent rapid developments in compound data assimilation, this overview cannot be complete. The paper continues in the 2nd section with satellite data assimilation in the stratosphere, where retrievals from space borne sensors were used first for compound data assimilation. The 3rd section addresses tropospheric data assimilation, although global models increasingly include both stratospheric and tropospheric height levels (Inness et al., 2013). The topics of tropospheric aerosol assimilation and greenhouse gases are treated in sections 4 and 5, respectively. Finally, the special case of assimilation in case of fires is addressed in section 6.

2 Stratospheric composition assimilation

Presumably the earliest satellite data assimilation study is due to Austin (1992) who assimilated HNO_3 and ozone retrievals from the Limb Infrared Monitor of the Stratosphere (LIMS) satellite data into a 2D isentropic model at the potential temperature values of 600, 850 and 1400 K.

Later motivation for constituent data assimilation was provided by both requirements related to numerical weather prediction, and those related to stratospheric chemistry modelling tasks. In case of the former, for example, the radiance assimilation quality of data from nadir looking sounders for atmospheric temperature analyses, was shown to be affected by the vertical ozone distribution (McNally et al., 2006). The variability of ozone fields and recently also N_2O and water in the stratosphere triggered attempts to infer stratospheric winds (see for example Riishøjgaard, 1996; Semane et al., 2009; Allen et al., 2014). However, while these studies exposed some potential for improved middle atmospheric wind field analyses, these developments are not yet in use operationally.

Due to its radiative properties, better analysed ozone fields have the potential to improve heating rates (de Grandpré et al., 2009). In a three-dimensional variational data assimilation (3D-Var) system it could be demonstrated that the inclusion of ozone assimilation from retrievals of MIPAS improved systematically the performance with respect to a non-interactive assimilation system. Finally, UV-forecasts for skin exposure control are another incentive for stratospheric ozone assimilation (Long et al., 1996, 2003).

Probably most activities of stratospheric chemistry data assimilation include chemistry transport models of various degrees of coupling with dynamical models. At the Global Modelling and Assimilation Office (GMAO) Štajner et al. (2001) implemented a 3D Physical-space Statistical Assimilation System (PSAS) for the stratospheric ozone analyses, assimilating TOMS (Total Ozone Mapping Spectrometer) and SBUV/2 (Solar Backscatter Ultraviolet Instrument) data. Later extensions include POAM-III (Polar Ozone and Aerosol Measurement) retrievals (Štajner and Wargan, 2004) and MIPAS (Wargan et al., 2005). Especially the latter sensor and others like GOMOS and SCIAMACHY offered broad opportunities for constituent assimilation in the stratosphere and uppermost troposphere. Lahoz et al. (2007) presented an assimilation system inter-comparison with respect to MIPAS ozone data. The assimilation techniques that were employed in these studies included three- and four-dimensional variational data assimilation (3D-Var with DARC/Met Office model and 4D-Var by BASCOE, respectively), and suboptimal Kalman Filter (KF) methods (KNMI TEMIS and MIMOSA, Service d'Aeronomie), as well as 3D-FGAT (First Guess at the Appropriate Time), which is a variant of 3D-Var, by MOCAGE-PALM at Météo-France. The 4D-var technique in stratospheric chemistry data assimilation was introduced by Errera and Fonteyn (2001). Errera et al (2008) and Elbern et al. (2010a) are examples of 4D-var assimilation of MIPAS data, the latter with the SACADA (Synoptic Analyses of Compound by Advanced Data Assimilation) system, applying dynamic covariance modelling. An examples is given in Figure 1.

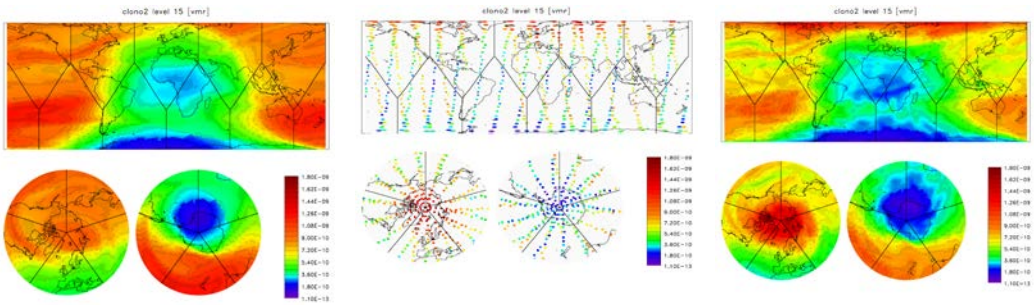

Figure 1: SACADA 4D-var, 24 h assimilation window with results for ClONO2 at 7.6 hPa (~33 km), Nov. 13, 2003 12:00 UTC. Control run (no assimilation, left) MIPAS retrievals (centre), analysis (right).

Recent ozone data assimilation by nadir looking instrumentation was demonstrated in a study by Hao et al. (2014), in which retrievals from two Global Ozone Monitoring Instrument (GOME-2) sensors operated in tandem, flying on board EUMETSAT's (European Organisation for the Exploitation of Meteorological Satellites) MetOp-A and MetOp-B (Meteorological Operational Satellite) are used. Prior to this, GOME-2A total ozone data have been used operationally in the Copernicus atmospheric service projects MACC-II and III (Monitoring Atmospheric Composition and Climate - Interim Implementation, www.copernicus-atmosphere.eu) in near-real-time (NRT) system since October 2013 (Dethof and Hólm, 2004; Dragani, 2011).

Chemistry data assimilation systems are also validated using satellite data -based diagnostics. Ménard and Chang (2000) pioneered this approach by assimilating Upper Atmosphere Research Satellite (UARS) retrievals in a Kalman filter, and conducted χ^2 -diagnostics. By comparing forecast and assimilation results with MIPAS retrievals, Schwinger and Elbern (2010) applied the Desroziers et al. (2005) a posteriori validation of error statistics in observation space to the 4D-var stratospheric chemistry data assimilation system SACADA (Synoptic Analysis of Chemical Constituents by Advanced Data Assimilation). An evaluation of diagnostics results with independent data from the Halogen Observation Experiment (HALOE), the Stratospheric Aerosol and Gas Experiment II (SAGE II), and ozone sondes reveals that the standard deviation of ozone analyses with respect to these instruments is reduced throughout the middle stratosphere.

3 Tropospheric chemistry data assimilation

While in the stratosphere data from both limb and nadir looking instrumentation can be assimilated, middle and lower tropospheric remote sensing from space is only feasible by nadir looking sensors, with microwave limb sounding as exemption. An early example of satellite data assimilation in the troposphere is the estimation of CO mixing ratios and vertical column abundances together with tropospheric NO_2 columns from the GOME satellite by Muller and Stavrakou (2005). NO_2 emission estimates for 1997 were calculated by the global three-dimensional CTM IMAGES and the emissions were optimized using the adjoint modelling technique. Using the same sensor, Elbern et al. (2010b) demonstrated the benefit for improved air quality simulations with the 4D-Var technique applied in EURAD-IM, a full fledged 4D-variational assimilation system with joint initial value-emission rate optimisation. Introducing a daily optimisation with 24-hour assimilation window including grid-resolved emissions provide emission rate estimates in a chemically balanced analysis set-up.

Assimilation of data from more recent sensors based on the similar sensing principles include Chai et al. (2009) for SCIAMACHY, and Wang et al. (2011) for OMI.

Ozone data from the Metop IASI Infrared Atmospheric Sounding Interferometer instrument onboard the European meteorological platforms MetOP and from the AIRS instrument are also available for assimilation. These datasets provide height-resolved observations of the troposphere. An example is given below where the joint assimilation of IASI and surface measurements of ozone in a regional chemical transport model MOCAGE is described. IASI provides global measurements of atmospheric gases twice a day (morning and evening overpasses), with high spatial resolution (12 km at nadir) and a moderate sensitivity to the ozone signature in the free troposphere (Dufour et al., 2012). These measurements represent a good constrain for global (Emili et al., 2014) and regional (Coman et al., 2012; Barré et al., 2013) chemical transport models (CTMs). However, the sensitivity of IASI measurements to the boundary layer ozone concentration is lower and their capability to improve surface air-quality analyses and forecasts has not been yet demonstrated. For this reason, in the framework of the regional assimilation activities of the MACC project (http://www.gmes-atmosphere.eu/), data from both surface stations and IASI were assimilated simultaneously. The synergy of the two datasets through data assimilation provided an accurate ozone profile throughout the troposphere. The MACC system also provides NRT and reanalyses, assimilating O_3, CO, NO_2, and SO_2 for volcanic eruptions (Flemming et al., 2013; Iness et al., 2013).

O_3 tropospheric columns (1000–245 hPa) derived from the SOFRID product (Barret et al., 2011) have been assimilated together with surface O_3 data from the European AIRBASE network in the CTM MOCAGE. The model configuration is the same as used for MACC-III operations (http://www.gmes-atmosphere.eu/documents/maccii/deliverables/ens), where only surface data are routinely assimilated. The background error standard deviation was fixed to 15% of the background ozone values. IASI's observation error was also fixed to 15% of the observations values. Four experiments have been done during an ozone episode in July 2010: i) a model free run without data assimilation, ii) the assimilation of surface data only, iii) the assimilation of satellite data only, and iv) the combined assimilation of surface and satellite data. The obtained ozone fields were compared to the ozone-sondes profiles available in Europe during the episode (14 profiles) for the validation of the four experiments (Figure 2).

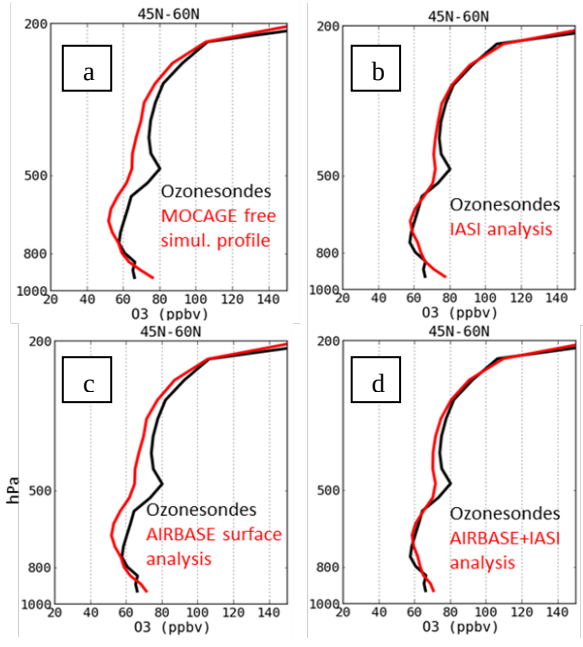

Figure 2: Average ozone profiles during the period 6–12/7/2010; comparison of ozone-sonde profiles (in black) and MOCAGE profiles (in red) a) without data assimilation, b) with assimilation of IASI data, c) with assimilation of surface station data, d) with the combined assimilation of IASI and surface data.

The following conclusions can be drawn:

- The free model simulation shows a positive bias of about 15 ppbv at the surface and a negative bias of 10–20 ppbv in the free troposphere.
- The assimilation of IASI tropospheric columns reduces the ozone bias in the free troposphere whereas the assimilation of surface data reduces the bias in the boundary layer.
- The small sensitivity of IASI column to the boundary layer ozone is taken in account by using the satellite averaging kernels, which results in a correct vertical redistribution of the assimilation increments.
- The best agreement between model and ozone-sondes profiles is obtained by the coupled assimilation of satellite and surface measurements.

This exercise showed that the bias of modelled ozone can change sign throughout the troposphere. Only a combination of measurements that covers the whole troposphere can provide reliable analyses in this case. We have demonstrated that assimilating IASI and surface stations provided good results during the examined pollution episode. The period of analysis will be extended in the future, low-stratosphere measurements from MLS can also be considered to constrain the downward flux of ozone at the tropopause.

4 Tropospheric aerosol assimilation

Most of the current aerosol prediction systems rely on assimilation developments already in place for the meteorological variables: for example ECMWF uses the incremental 4D-Var formulation with augmented control vector to include an aerosol total mixing ratio variable (Benedetti et al., 2009). At the Met Office, 4D-Var assimilation of dust observations follows a similar approach, using total dust concentration as the analysis variable to be optimized (control variable). NRL and NASA GMAO use 2D and 3D-Var approaches. The Barcelona Supercomputing Center (BSC) is currently developing an Ensemble Kalman Filter assimilation system for their global aerosol model. Most of these aerosol analysis systems solve an initial condition problem and the analysis is used to obtain the optimal initial conditions in the aerosol fields in order for the subsequent forecast to match the observations. However, this is not always sufficient as the observed aerosol amounts may be due to sources that are not accounted for. Studies which include direct estimation of emissions have shown promise both for dust (Sekiyama et al., 2011) and other aerosol types (Huneeus et al., 2012), and it is likely that future aerosol analysis systems will include emission parameters in their control variables.

Specific challenges in aerosol assimilation are related also to other factors. Observations do not provide the full picture on all relevant aspects of tropospheric aerosols. For example, information on the individual aerosol species is not obtainable with current satellite sensors. Even just extracting the total aerosol signal from satellite radiances which are affected by other atmospheric quantities, most notably clouds, is challenging. Due to the complex radiative transfer calculations needed to model aerosol-affected radiances from the visible channels of the current generation of imagers, most centres assimilate retrieved products (e.g. Aerosol Optical Depth, AOD) rather than the raw radiance observations. MODIS Dark Target AOD data are assimilated in the ECMWF, NRL and NASA forecasting system, although each centre adopts individual strategies for filtering and bias correcting the MODIS observations. The standard Dark Target MODIS product provides no information on dust over the sources, but it does, for example, over the Atlantic Ocean where dust outflow from the Sahara is the main contributor to the aerosol load. In regions that are not observed, therefore, the model plays

an important role in spreading the information contained in the observations. Recently, enhanced efforts have been made at several centres to assimilate more data, such as the MODIS Deep Blue product, the AOD from the SEVIRI instrument on board of MSG, the AOD from the OMI instrument, a new product from EUMETSAT based on GOME-2 data (PMAP), and aerosol backscatter data from the CALIOP lidar on board the CALIPSO satellite. For reanalysis purposes other datasets such as the AATSR AOD from the ESA Climate Change Initiative are also being utilized. Potential has also been demonstrated for the POLDER instrument on board of PARASOL, which provided reliable retrievals of AOD (Tanré et al., 2011). For dust aerosols, the potential of the AIRS and IASI instruments has been shown by Perydieu et al. (2013). However this has not been applied for operational assimilation systems.

The other aspect peculiar to aerosol assimilation is that the optimisation problem is severely under-constrained due to the fact that several aerosol species have to be constrained with a total column-integrated observation for radiometric measurements or a profile of backscattering for lidar measurements. This implies that there is no one-to-one correspondence between the observations and control variable as it normally happens for meteorological variables and for gaseous components. There are various approaches to get around this problem using reasonable assumptions. For example, ECMWF formulates the aerosol control variable in terms of a total mixing ratio and redistributes the increments from this variable into the single species mixing ratios according to their fractional contribution to the total mass. This avoids having to define error statistics for all species carried in the model as it would be necessary if they were part of the control vector. Other centres, for example MRI/JMA, include the emission parameters in the control vector along with aerosol concentrations and meteorological parameters. In this case, the minimization is better constrained. In the end, it has to be accepted that no matter how complex and sophisticated the aerosol assimilation system, a lot of the information comes from the model rather than the observations.

Even with its limitations, aerosol forecasts from systems with aerosol analysis have been shown to show reduced RMSE and improved correlations with respect to independent observations, when compared to forecasts from the same systems with no aerosol analysis (Benedetti et al., 2009; Zhang et al., 2008). Moreover, aerosol reanalyses, in particular of dust and biomass burning aerosols, are becoming increasingly valued to assess annual and seasonal anomalies and to monitor the state of climate (Benedetti et al., 2013).

A remarkable indirect method to infer aerosol information is presented by Saide et al. (2012), who provide a first steps to overcome the limitation that aerosols cannot be constrained using satellite remote sensing under cloudy conditions. By using MODIS cloud droplet number N_d and those that assimilate GOES10 N_d data assimilation method that uses cloud droplet number retrievals to improve predicted below-cloud aerosol mass and number concentrations.

5 Greenhouse gases

The constraints on trueness and precision for greenhouse gas (GHG) measurements are much more stringent than for species that have not accumulated in the atmosphere because their concentrations are already known beforehand to a large (but insufficient) extent. For instance, ESA's Climate Change Initiative on Greenhouse Gases defined threshold requirements for systematic errors of 0.5 ppm (~0.1%) for CO_2 satellite retrievals and of 10 ppb (~0.5%) for CH_4 satellite retrievals (GHG CCI,

2011), which are very challenging because many significant error sources are involved in the retrieval process. This explains why the remote sensing of the main GHGs of anthropogenic origin (CH_4, CO_2 and N_2O) has been developed only recently, using measurements either in the thermal infrared spectral domain, with a peak sensitivity in the middle troposphere (AIRS, IASI, TES) or in the solar infrared domain (SCIAMACHY, GOSAT-TANSO, OCO-2) with a more uniform sensitivity to GHGs throughout the atmospheric column, including the boundary layer. The usefulness of both measurement types has been demonstrated for NWP-type data assimilation that optimizes the concentration fields only (Engelen et al., 2009), but such developments have been hampered by long delays in the delivery of the GHG retrievals related to the above-mentioned accuracy requirements. However, systematic errors at various space and time scales have hampered the extension of these works to the inversion of global CO_2 surface fluxes up to now. They can be caused by uncertainties in the spectroscopy or by aliasing with other atmospheric signals like aerosols. However, the launch of GOSAT in January 2009 and of OCO-2 in July 2014 has raised expectations for CO_2 flux inversions because those two instruments are the first ones to have been specifically designed for this purpose. Despite the difficult progress of this research (Chevallier et al., 2014), the usefulness of space-borne monitoring of the CO_2 column for global flux inversion has been experimentally confirmed using the calibrated surface measurements of the CO_2 column from the Total Carbon Column Observing Network (TCCON) (Chevallier et al., 2011).

For CH_4, Bergamaschi et al. (2009) showed that the issue of systematic errors in the CH_4 column retrievals can be circumvented by anchoring the inversion with surface measurements. This finding opened the possibility of a decadal monitoring of global CH_4 fluxes from SCIAMACHY, GOSAT and IASI, in orbit since March 2002, January 2009 and October 2006 (for the first IASI instrument), respectively (Bergamaschi et al., 2013; Fraser et al., 2013; Cressot et al., 2014). N_2O satellite retrievals (from IASI) are still in their infancy (e.g., Ricaud et al., 2009) and may not be accurate enough yet to be used to constrain tropospheric concentrations and surface fluxes. In the near future, GHG satellite imagers, like ESA's Carbonsat project (Bovensmann et al., 2010), may provide a substantial step-forward through their capability to monitor GHG plumes and therefore hotspot emissions.

The exceptionally long life time of CH_4, CO_2 and N_2O links any concentration measurement to global surface fluxes of these species in the distant past. This long memory of the measurements imposes very long inversion windows (typically months or years, e.g., Bruhwiler et al., 2005). Combined with the high variability of atmospheric transport at short time-space scales, it hinders the implementation of Bayes' theorem at reasonable computational costs. In practice, compromises have been chosen by various scientific teams. Flux inversion has been traditionally performed based on a closed-form (i.e. analytical) solution to Bayes' theorem (e.g., Gurney et al., 2002) but the computational cost of this analytical solution restricts it to small-size problems (typically less than 104 variables to infer or less than 104 measurements to exploit), while the global inference problem may be intrinsically of much larger size due to the small spatial correlation structures of the prior flux errors and to the long life time of the species. In the context of high-performance parallel computing, ensemble forms of Bayes' theorem (i.e. using a statistical ensemble of simulations) have been increasingly popular (e.g., Feng et al., 2009), but in practice the relatively small sizes that can be currently afforded for the statistical ensembles do not allow tackling problems of higher resolutions than the analytical approach and the aggregation error remains a critical issue. The variational form of Bayes' theorem (i.e., adjoint-based) has been introduced in the mid-00s to lift this restriction (Chevallier et al., 2005). The dimension of the control vector can be artificially reduced by optimizing some internal parameters of flux process

models rather than the fluxes directly (Kaminski et al., 2002). In the case of CO_2, such inversion systems are usually called Carbon Cycle Data Assimilation Systems (CCDASs). Like for the standard inversion approach, CCDASs allow inferring the space-time distribution of surface CO_2 fluxes, but their underlying process model allows them to use a much larger diversity of measurements, e.g., local flux measurements, satellite observations of vegetation activity or biomass inventories. Their model prognostic equations can also spread the observational information well beyond measurement time (Rayner et al., 2011). The downside of this strategy is the interference from the errors of the model equations in the data assimilation process. Indeed these equations are imposed to the inversion as a strong constraint, even though many processes cannot yet be described from first principles at the resolution of global models, in particular for vegetation, and empirical equations have to model them.

For assimilation, it must be considered that the long time-space scales variability of long lived GHG (e.g. CO_2 and CH_4) is small compared to the background values, and detecting this variability requires stringent criteria on the quality of the assimilated observations. However, CO_2 and CH_4 can have also a much larger variability at synoptic and diurnal scales associated to the high variability of the atmospheric transport and surface fluxes (Saeki et al., 2013). This variability needs to be assessed to correctly interpret observations and their variability. The footprint of in situ and satellite observations like those from TANSO or OCO-2 can be small compared to the spatial resolution of the transport models (usually in the order of few hundreds of km). In order to be able to model the short-term variability of the GHG atmospheric fields, there is a need for high resolution models such as the one developed in MACC and based on the ECMWF state-of-the-art NWP system. This model with a horizontal grid cell of 16x16 km^2 has the ability to model the variability of CO_2 on different temporal and spatial scales (Agusti-Panareda et al., 2014).

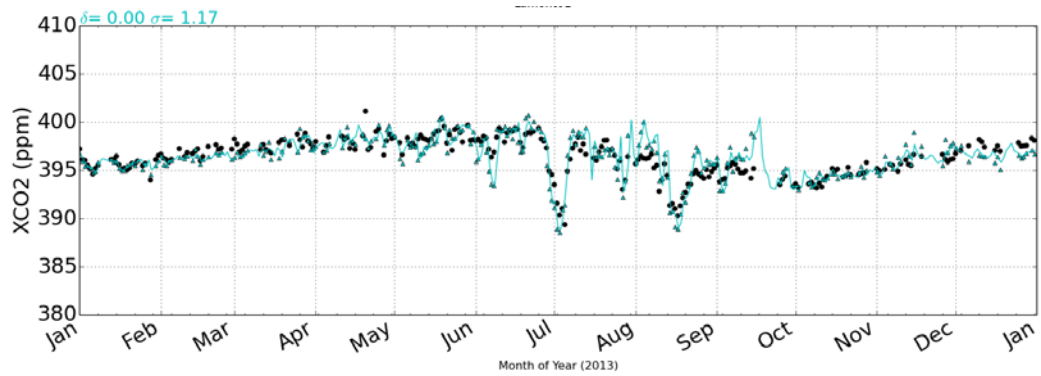

Figure 3: Time series of xCO_2 (in ppm) at Lamont (TCCON station)for 2013: observations (black dots), analysis from TANSO data (cyan line) and analysis in the observation space (cyan dots).The analysis shows a good variability and a low bias compared to the independent observations.

However, errors in the specified or modelled fluxes can lead to accumulating errors in the free running forecast. On the other hand, the NWP-type data assimilation of GHG retrievals from orbiting instruments (TANSO, IASI) that optimizes the atmospheric concentration fields allows to reduce the bias of a free running forecast based on modelled fluxes when compared to measurements from TCCON (Figure 3 and Massart et al., 2014). Compared to flux inversion systems, the assimilation window has to be short (few hours) in order to limit the accumulation of model errors due to the fluxes and transport. Until recently the derived analysis of atmospheric GHG fields was delayed by several months waiting for the GHG retrievals to be available. Due to this delay, the analysis could not be

used to initialise the forecast. The delays in the production of GHG retrievals have been shortened and the some products are now available within a few days. This makes possible near-real time analysis/forecast systems for CO_2 and CH_4 similar to other systems (aerosols, reactive gases, ...).

6 Fire data assimilation

Smoke emissions from open vegetation fires, for example savannah, forest, agricultural or peat fires, have a strong, episodic effect on the atmospheric composition and air quality. Most emissions are released into the boundary layer but pyro-convection may effectively release the smoke in the free troposphere, and occasionally even the lower stratosphere (Damoah et al., 2006). Smoke contains significant amounts of reactive and greenhouse gases, as well as being the largest source of primary particulate organic matter and black carbon on the global scale.

The previous sections have shown that atmospheric composition monitoring with satellite observations is an under-constrained problem, which requires merging with model information in a data assimilation approach. Surface emissions constitute the lower boundary condition and can as such be regarded as part of the required model information. They are particularly important to resolve the ambiguities of atmospheric observations with regard to aerosol speciation, vertical distribution and the wealth of non-observed gases, as well as the insensitivity of thermal infrared observations with regard to the lowest atmospheric levels.

Anthropogenic, biogenic, sea salt and desert dust emissions may be described with inventories and model parameterisations. In contrast, fire and volcanic emissions have such poor predictability that they need to be estimated using satellite observations. Such observations register either the thermal radiation emitted by flames and ambers ("active fire") or the burn scars ("burnt area"). Only the former products are available in near real time. Traditionally, fire emissions have been calculated from burnt area estimates, sometimes indirectly inferred from active fires. With the non-saturating MIR (~4 μm) bands of the BIRD and MODIS satellites, the quantitative active fire product "fire radiative power" (FRP) has become available. It is proportional to the biomass combustion and smoke emission rates, yielding alternative emission estimation (Wooster et al., 2003, 2005; Ichoku and Kaufman; 2005; Heil et al., 2010).

Atmospheric smoke monitoring and forecasting with fire observation was pioneered by Freitas et al. (2005) for South America and expanded to global coverage by Reid et al. (2009). Further global inventories with real time availability have since been implemented by Wiedinmyer et al. (2011), Kaiser et al. (2009), Sofiev et al. (2009), and Darmenov and da Silva (2013). All are based on MODIS observations. The two MODIS instruments in low-earth orbit (LEO) provide global coverage with two daytime observations. Considering that fires generally have a pronounced diurnal cycle with fire durations of a few hours, and that cloud cover prevents observations, observation gaps constitute the dominant error source for fire emission estimation with FRP. Observations from geostationary (GEO) satellites are complementary through frequent sampling, albeit at the cost of large detection thresholds and consequently, a largely, variable and poorly characterised under-estimation of instantaneous FRP.
The Global Fire Assimilation System (GFAS) has been developed in the series of MACC projects for the estimation of open fire emissions (Kaiser et al., 2012). Using MODIS, GFAS has pioneered the global application of the FRP approach. It is unique in that it employs the data assimilation formalism for filling observation gaps and estimating fire duration. The implemented Kalman filter also provides

a suitable framework for improving the temporal resolution from 1 day to 1 hour, which is requested by users and a preparation for merging FRP products from GEOs: This development essentially reduces to a new forecast model for the diurnal cycle, along with its error covariance. Other developments aim at fire model parameter estimation from atmospheric smoke observations.

GFAS is used throughout the Copernicus Atmosphere Monitoring Service (CAMS). It is also used by several non-European meteorological services innear real time, and for scientific and climate analyses (e.g. Blunden & Arndt, 2014). Huijnen et al. (2012) have confirmed the increased accuracy of a combining fire, aerosol and CO assimilation for the aerosol speciation and AOD, and CO concentrations during the 2010 western Russian fire episode, using independent ground-based AOD and CO observations as reference. An example for inter-continental transport of smoke as represented in MACC is shown in Figure 4. In the future, fire data assimilation may provide the most reliable source attribution for regulations like the Singapore Transboundary Haze Pollution Act, which establishes a legal liability for haze pollution from open fires.

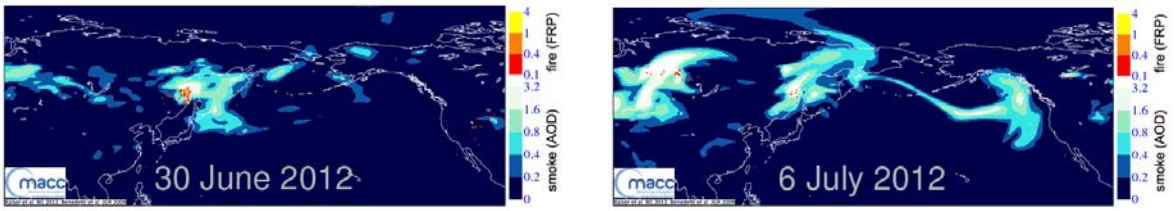

Figure 4: Trans-pacific smoke transport as represented in the CAMS system with combined Fire Radiative Power and Aerosol Optical Depth assimilation.

7 Future directions

Constituent data assimilation systems with reactive chemistry will make use of spatio-temporal data assimilation systems, like Kalman filtering and 4D-var, partly including emission rate optimisation in tropospheric applications. Satellite sensors are expected to support this objective. In case of the recently launched OCO-2, this is in the centre of the application, yet reactive chemistry forecasts will benefit from this approach as well. Novel satellite assimilation studies include the Suomi National Polar-orbiting Partnership satellite (Suomi NPP) with the Ozone Mapping and Profiler Suite (OMPS), an imaging spectrometers to measure ozone levels, and the Visible Infrared Imaging Radiometer Suite (VIIRS) radiometer, collecting infrared and visible light data to observe wildfires, and changes in landforms. Similar, but advanced sensors can be expected from the Joint Polar Satellite System (JPSS), which is the next generation of U.S. polar-orbiting, non-geosynchronous, environmental satellites. European contributions will be provided by Sentinels 3, 4, 5 and 5-precursor. The latter designed to fill the gap between EnviSat and Sentinel 5, which comprises an Ultraviolet Visible Near-infrared Shortwave (UVNS) spectrometer and data from Eumetsat's IRS, the Visible Infrared Imager (VII) and the Multi-viewing Multi-channel Multi-polarization Imager (3MI). Sentinel 4, to be carried on the geostationary Meteosat Third Generation satellites, comprises an Ultraviolet Visible Near-infrared (UVN) spectrometer and data from Eumetsat's thermal InfraRed Sounder (IRS).

NASA's GEO-CAPE (Geostationary Coastal and Air Pollution Events) project will provide information on the identification of human versus natural sources of aerosols and ozone precursors and observation of air pollution transport in the Americas. From ESA's Living Planet Programme

EarthCARE (Earth Clouds, Aerosols and Radiation Explorer) simultaneously measures the vertical and horizontal distribution of clouds and atmospheric aerosols by a backscatter Lidar (ATLID).

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