A GLOBAL SCALE INVERSION OF THE TRANSPORT OF CO_2 BASED ON A MATRIX REPRESENTATION OF AN ATMOSPHERIC TRANSPORT MODEL DERIVED BY ITS ADJOINT

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1. INTRODUCTION

The atmosphere contains a number of radiatively and chemically important trace gases (a.o. carbon dioxide (CO_2), carbon monoxide (CO), nitrous oxide (N_2O) and methane (CH_4)) whose concentrations are changing in the atmosphere, primarily due to human activities. These changing concentrations affect the radiative balance of our atmosphere and may thus lead to climate change. In order to compute reliable projections of the future evolution of the concentrations of these gases their natural and anthropogenic sources and sinks have to be known. Using a direct approach one can extrapolate locally measured fluxes to the entire globe. Because of the many necessary assumptions in the extrapolation, this direct approach, however, is subject to very large uncertainties. In contrast, one can apply an inverse approach, in which ambient observations of the atmospheric trace gas concentrations are used to constrain the surface fluxes. This requires a model of the atmospheric transport which provides the link between the surface fluxes and the concentrations at the monitoring sites.

The trace gases of interest are being monitored at a global network of atmospheric observing stations. However, since this network is spatially sparse, the determination of the surface fluxes constitutes a highly underdetermined inverse problem. Hence, additional information on the fluxes has to be included in the inversion in order to obtain a well-determined problem.

Several inversion studies have been performed on the basis of both, two-dimensional and three-dimensional models of the atmospheric transport [*Enting and Mansbridge*, 1989; *Brown*, 1995; *Hein and Heimann*, 1994; *Hein et al.*, 1996]. In all these studies, the surface flux field is decomposed into prescribed spatio-temporal patterns ("source" or "flux" components) with unknown scaling coefficients. The transport model is run with each of the source components separately and the contributions to the concentration signal at each of the monitoring sites and times are recorded. These contributions can be interpreted as a discretized impulse response or Greens function which quantifies the response of the modeled concentration at the observation sites and dates to unit changes in the magnitude of each source component.

Formally this impulse response or Greens function is the Jacobian matrix representing the first derivative of the modeled concentration at the observational sites and dates with respect to the coefficients of the source components. Computationally, for nf source components, nf model runs have to be performed to compute the nf differential quotients which constitute the columns of the Jacobian matrix. The complexity of the transport model thus essentially limits the number of source components that can be considered.

Here we present an alternative approach employing the adjoint of the three-dimensional transport model TM2 for the efficient determination of the Jacobian in a "reverse mode". The exact Jacobian is computed line by line, for which the cost is proportional to the number of observations and nearly independent of the number of flux components.

This concept is illustrated by a computation of the Jacobian for about 10000 flux components and about 300 observations of the atmospheric CO_2 concentration. Combined to a priori information on the surface fluxes derived from output of high resolution models of both, the terrestrial biosphere and the ocean, and fossil fuel burning statistics we infer the seasonal cycle and mean annual source and sink distribution on the approximately 8 degree by 10 degree horizontal TM2 grid. Thereby we use the observations in the Globalview data set from the NOAA/CMDL program [*Globalview - CO2*, 1996].

The outline is as follows: In Sect. (2) we briefly introduce the transport model followed by the description of the Jacobian matrix in Sect. (3). We sketch the inversion in Sect. (4). Finally, Sect. (5) contains some perspectives.

2. THE TRANSPORT MODEL

TM2 is a three-dimensional atmospheric transport model which solves the continuity equation for an arbitrary number of atmospheric tracers on an Eulerian grid spanning the entire globe [*Heimann*, 1995]. It is driven by stored meteorological fields derived from analyses of a weather forecast model or from output of an atmospheric general circulation model. Tracer advection is calculated using the "slopes scheme" of *Russel and Lerner* [1981]. Vertical transport due to convective clouds is computed using the cloud mass flux scheme of *Tiedtke* [1989]. Turbulent vertical transport is calculated by stability dependent vertical diffusion according to the scheme by *Louis* [1979]. Numerically, in each base time step the model calculates the source and sink processes affecting each tracer, followed by the calculation of the transport processes.

The spatial structure of the model is a regular latitude-longitude grid and a sigma coordinate system in the vertical dimension. The base "coarse grid" version of the model uses a horizontal resolution of approximately 8^o latitude by 10^o longitude (i.e. the horizontal dimension of the grid is $ng = 36 \times 24$) and 9 layers in the vertical dimension. The numerical timestep of this model version is four hours. In the present application the TM2 is forced with the meteorological fields of the year 1987, derived from analyses of the European Center for Medium Range Weather Forecast (ECMWF) which are available to the model every 12 hours.

Prescribing the same monthly surface CO_2 source flux fields every year, and starting from zero initial concentration, TM2 is run for four years. At a particular site S the concentration c_S is computed from the simulated concentration fields of the fourth year by first computing monthly means and then performing a bilinear interpolation in the horizontal from the TM2 grid to the exact location of S. This setup of TM2 in the following will be denoted as standard setup.

In the standard setup TM2 has as input $f \in \mathbb{R}^{nf}$, a vector of $nf = 12 \times ng$ real numbers characterizing the 12 monthly fluxes into each surface grid cell and as output $c \in \mathbb{R}^{nc}$, a vector of $nc = 12 \times ns$ real numbers for the modeled monthly mean concentration at ns observational sites. Since the transport of a passive atmospheric tracer in TM2 is linear, TM2 can be represented by a real $nc \times nf$ matrix T and the application of TM2 can be written as

$$c = Tf \quad . \tag{1}$$

3. JACOBIAN MATRIX

As explained in Sect. (2), for the standard setup, TM2 can be represented by a $nc \times nf$ matrix T. For given surface fluxes f by a model run we are able to compute the resulting concentrations at the station locations $c_{mod} = Tf$. However, the matrix T itself is yet to be determined.

By applying TM2 subsequently to the each of the nf standard basis vectors $e_1 = (1, 0, ..., 0)^T, ..., e_{nf} = (0, ..., 0, 1)^T$ spanning $\mathbb{R}^{nf}$, the matrix T could be computed column by column. This requires nf runs of TM2 and is thus only computationally feasible for a small number of flux components. Instead we apply an alternative, much more efficient approach: Using the model adjoint to TM2 in the standard setup the Jacobian matrix is computed line by line in reverse mode. In this case both, the computational cost and the storage requirements, depend on the number of rows, i.e. on nc, rather than on the number of columns, i.e. on nf.

For the construction of an adjoint model there exist several strategies [*Marchuk*, 1995; *Talagrand and Courtier*, 1987; *Talagrand*, 1991]. The adjoint of TM2 has been derived directly from the model code [*Giering and Kaminski*, 1996] based on the concept of differentiation of algorithms [*Iri*, 1991]. Thereby the Tangent linear and Adjoint Model Compiler [TAMC *Giering*, 1996] has been applied to automatically generate the adjoint code. By means of the adjoint of TM2 in the standard setup the matrix representation T for $ns = 27$ NOAA/CMDL stations (see Fig. (1)) has been computed. The rows of T consist of the sensitivity of the modeled concentration at a particular station and month to the fluxes into each of the $ng = 36 \times 24$ TM2 surface layer grid cells at each month. Conversely the rows of T contain the impact of a particular flux component on the modeled concentration at all stations and months.

We run TM2 and its adjoint on a Cray C916 supercomputer: For our standard setup with $nc = 27 \times 12$ the adjoint model run takes the cost of less than 100 TM2 single tracer runs. The computing time scales with the number of observations nc.

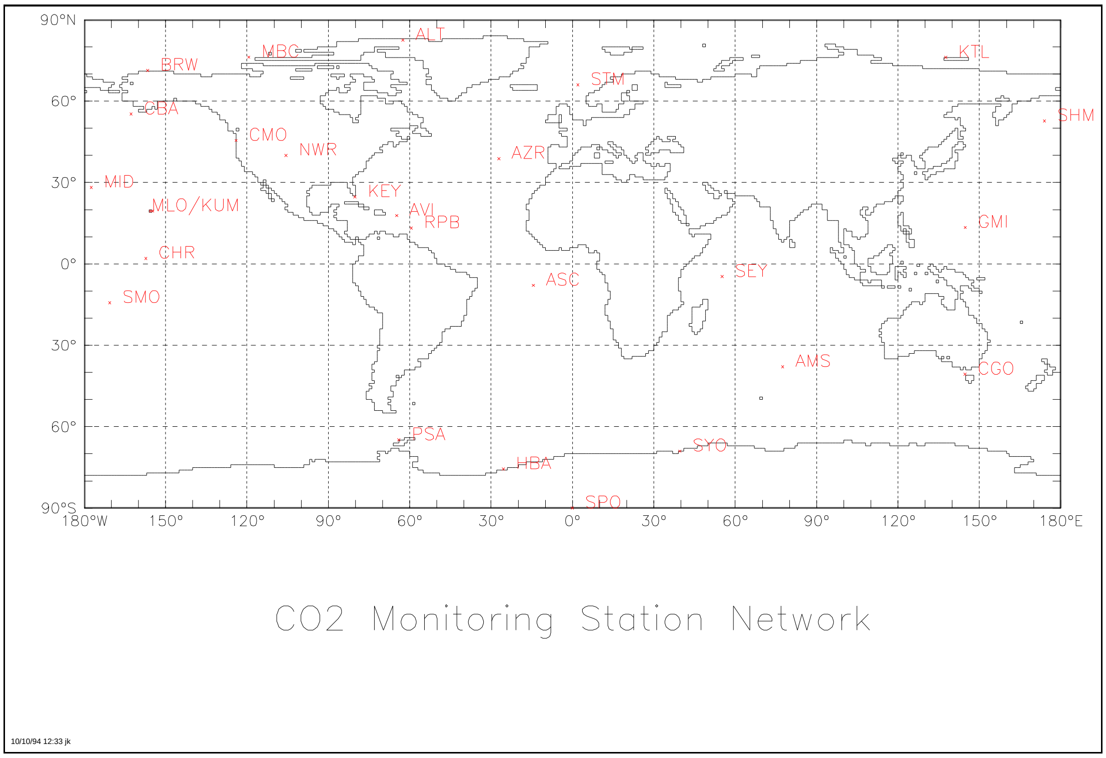

Figure 1. Monitoring Station Network of the NOAA/CMDL

4. INVERSION

The inverse problem associated with Eq. (1) consists in the determination of a flux field f, so that for prescribed concentrations c the equation is satisfied. For our matrix T the problem consists of $nc \approx 300$ equations for $nf \approx 10000$ unknowns, and thus is highly underdetermined, i.e. there will be many flux fields which yield the same modeled concentration.

by using the so-called Bayesian approach we include additional information in the inversion procedure to obtain a unique solution: Both, atmospheric observations and a priori information are described in terms of probability densities. Employing the transport as constraint, consistent probability densities are derived. A detailed introduction to the Bayesian approach is given in the textbooks of *Menke* [1989] and *Tarantola* [1987].

For our inversion, we assume fluxes and concentrations to have a Gaussian distribution with diagonal covariance matrices. Hence, the definition of the probability distributions consists in assigning standard deviations for each component. This special type of inverse problem is known as least squares problem. It results in the minimization of the cost function

$$J(\tilde{f}) = {}^1\!/_2 \left\{ \sum_{i=1}^{nf} \left(\frac{f - \tilde{f}}{\sigma_f} \right)^2 + \sum_{i=1}^{nc} \left(\frac{c_{obs} - T\tilde{f}}{\sigma_c} \right)^2 \right\} \quad , \tag{2}$$

where f is the a priori estimate of the fluxes with uncertainty σ_f and c_{obs} is the observed concentration with uncertainty σ_c.

We compose our a priori estimate of the net fluxes into the atmosphere from three components: the terrestrial biosphere, the ocean, and fossil fuel burning. From fossil fuel burning statistics of *Andres et al.* [1997] on a 1 ^{o} grid, annual mean fluxes on the TM2 grid have been interpolated. The global annual net source is 5.3 Gigatons of Carbon (GtC). Compared to the biospheric and oceanic component, the uncertainty in this source is rather small. Hence we exclude this component by subtracting prior to the inversion from the observations the modeled seasonal cycle, linear trend and mean annual spatial gradient generated by the fossil fuel source alone.

In Eq. (2), as a priori estimate for f we employed the sum of the biospheric and oceanic components computed from high resolution models of both, the terrestrial biosphere [*Knorr and Heimann*, 1995] and the ocean[*Six and Maier-Reimer*, 1996; *Maier-Reimer*, 1993]. The global annual means of the surface flux fields from both models are zero.

The uncertainties assigned to the a priori estimates of the fluxes are crucial parameters in the inversion, because they constitute the weights in the cost function (Eq. (2)). In general, assuming large uncertainties on the a priori flux estimates (we choose values as large as 100% of the respective flux component) results in a solution that fits more closely the observations.

Globalview-CO_2 is a database of high quality atmospheric measurements coordinated by the NOAA/CMDL [*Globalview - CO2*, 1996]. This monitoring network comprises more than 60 sites for which weekly data together with standard deviations are available. have been prepared. For our inversion we use the data from the 26 sites (all stations are displayed in Fig. (1) except for KTL). Similar to *Tans et al.* [1990] we choose a target period of 6 years from January 1981 to January 1987 and extract the seasonal cycle, linear trend and spatial gradient from the observations.

The a posteriori estimate of the fluxes from January to June is displayed in Fig. (2). The cost function of Eq. (2) is the sum of two terms: The contribution of the misfit between modeled and observed concentrations is 10.9^2, while the contribution of the correction of the estimate of the a priori fluxes is $(11.9)^2$. This means that with a relatively small mean square correction of the a priori estimate of 0.001 standard deviations for the flux component a relatively small misfit of 0.35 standard deviations is obtained. Essentially this has two reasons: The a priori source estimate provides already a good fit to the observed concentrations. Furthermore, of course, the assumed uncertainty for the a priori estimate is large. Primarily the fluxes are corrected near several stations like BRW or CGO and also in some areas with large a priori values and thus large uncertainties. The uncertainties of the a posteriori flux estimate is not reduced significantly, except close to a few observing sites [see also *Enting*, 1993]. This is also reflected by the low model resolution [see e.g. *Menke*, 1989; *Tarantola*, 1987] of the present inverse problem [see also *Enting*, 1993].

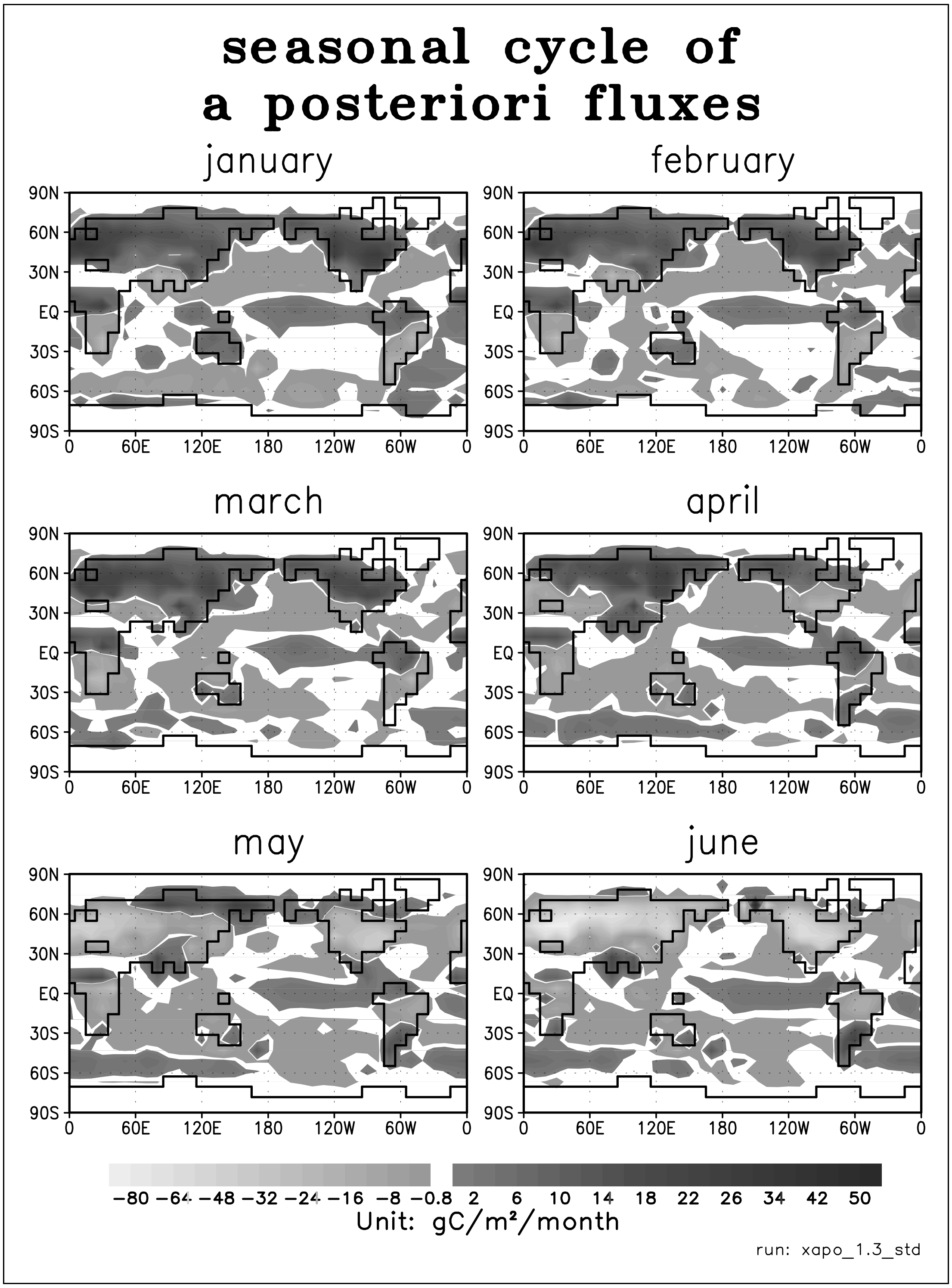

Figure 2. A posteriori estimate of the seasonal cycle of the sum of the biospheric and oceanic flux components

5. CONCLUSIONS AND PERSPECTIVES

We demonstrated the benefit of the adjoint approach for the computation of the Jacobian matrix for an atmospheric transport model in a particular setup. The computational cost is as low as 1 per cent compared to conventional forward modeling. For a higher spatial or temporal resolution of the fluxes, this percentage is even smaller.

In our example we employed the Jacobian to derive an estimate of the sources and sinks of CO_2 . However, the technique can be efficiently applied to other tracers in the same manner, as long as the number of observations is small compared to the number of flux components of interest.

If both, the number of observations and the number of flux components is large, or if a linearization around the a priori estimate induces a too large error, we recommend a different approach: The adjoint model can be used to provide the gradient of the cost function in Eq. (2) which is required by a class of powerful minimization algorithms. In an iterative procedure the cost function is minimized by variation of the fluxes [*Talagrand and Courtier*, 1987; *Giering and Kaminski*, 1996].

In the present study we characterized the sources and sinks by their net exchange fluxes with the atmosphere, rather than the processes causing the fluxes. After coupling the transport model (or its Jacobian) to process models such as the SDBM [*Knorr and Heimann*, 1995], the corresponding adjoint can be applied to estimate the internal parameters of the process models.

Furthermore an adjoint model constitutes a valuable tool for sensitivity studies. E.g. the adjoint of TM2 has been applied to efficiently decompose features such as the magnitude of the modeled seasonal cycle of the atmospheric CO_2 concentration with respect to the contributions of prescribed fluxes from all TM surface layer grid cells [*Kaminski et al.*, 1996].

6. ACKNOWLEDGMENT

The authors thank Wolfgang Knorr and Katharina Six for providing the flux fields from their models as well as Michael Voßbeck and Walter Sauf for preparing the figures. This work was supported in part by the Commission of the European Communities under contract EV5V-CT92-0120, European Study of Carbon in the Oceans Biosphere and Atmosphere (ESCOBA): Atmosphere Section. Computing support was provided by the Deutsches Klimarechenzentrum (DKRZ) in Hamburg.

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