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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Several inversion studies have been performed on the basis of three-dimensional models of the atmospheric transport (Tans et al., 1990; Enting et al., 1995; Brown, 1995; 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 (Heimann, 1995) 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. The adjoint has been derived for the base "coarse grid" version 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. 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. In this 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 $nc = 12 \times 26$ real numbers for the modeled monthly mean concentration at 26 observational sites of the NOAA/CMDL global monitoring network (Globalview - CO2, 1996). Since the transport of a passive atmospheric tracer in TM2 is linear, the model can be represented by its real $nc \times nf$ Jacobian matrix T and the application of TM2 can be written as $c = Tf$.The adjoint of TM2 has been derived directly from the model code based on the concept of differentiation of algorithms (Iri, 1991; Giering and Kaminski, 1997). Thereby the Tangent linear and Adjoint Model Compiler (TAMC, Giering, 1996) has been applied to automatically generate the adjoint code. On a Cray C916 vector machine the computaton of the Jacobian for 26 stations by the adjoint model takes the CPU time of less than 100 TM2 single tracer runs while using about 35 times as much memory as a single tracer run. The computing time scales with the number of observations nc.

The inverse problem associated with $c = Tf$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. The Bayesian approach allows to include an a priori flux field f in the inversion procedure to obtain a unique solution (see e.g. Menke, 1989; Tarantola, 1987). Assuming fluxes f and concentrations c_{obs} to have a Gaussian distribution with diagonal covariance matrices the a posteriori estimate of the flux field is characterized as the minimum of the cost function

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

where σ_f and σ_c are the uncertainties of the a priori fluxes and the observed concentrations respectively. 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. 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 (Andres et al., 1997) alone we exclude this component. In Eq. (1), as a priori estimate 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. (1)). In general, assuming large uncertainties on the a priori flux estimates (for most flux components we choose values as large as 100% of the respective component) results in a solution that fits closely the observations. 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. In the annual mean the a posteriori estimate of the net fluxes include large sinks over the northern hemisphere continents and the tropics over Africa whereas in the southern ocean the net flux into the atmosphere is increased compared to the a priori estimate. In addition localized sources are induced in the neighborhood of some of the stations (Cape Meares in Oregon, Point Barrow in Alaska), and localized sinks are induced around Cape Grim in Tasmania and Hawaii. These local sources and sinks most likely result from the fact that our model does not mimic the data selection procedures employed at the stations (see also Ramonet and Monfray, 1996). The uncertainties of the a posteriori flux estimate are 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.

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