

Time-dependent atmospheric CO₂ inversions based on interannually varying tracer transport

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ABSTRACT

The use of inverse calculations to estimate surface CO₂ fluxes from atmospheric concentration measurements has gained large attention in recent years. The success of an inversion will, among other factors, depend strongly on how realistically atmospheric tracer transport is represented by the employed transport model, as it links surface CO₂ fluxes to modelled concentrations at the location of measurement stations. We present sensitivity studies demonstrating that transport modelling should be based on interannually varying meteorology, as compared to the traditional use of repeating a single year's winds only. Moreover, we propose an improved procedure of representing the concentration sampling in the model, which allows consistency with the measurements and uses their information content more efficiently. In further sensitivity tests, we estimate the effect of different spatial transport model resolutions and different meteorological driver data sets. Finally, we assess the quality of the inversion results with the help of independent measurements and flux estimates, and preliminarily discuss some of the resulting features.

1. Introduction

Inverse techniques are increasingly used in atmospheric sciences to estimate surface exchange fluxes of greenhouse gases, since they offer global data-driven flux estimates with at least some temporal and spatial resolution. Unfortunately, there is still significant disagreement among inverse modellers on the most appropriate way to perform these calculations, mainly because the available data density is sparse and leaves room for many alternative choices in the methodological setup, the pros and cons of which are far from obvious. Several sensitivity studies (e.g., Gurney et al., 2002 and references therein; Gloor et al., 1999) explored a number of such details. However, most studies focused on inversions based on annual mean quantities or mean seasonal cycles.

The present paper considers time-dependent global Green's function CO₂ inversions. 'Time-dependent'

means that they also estimate the interannual variability of the CO₂ fluxes, rather than averaged seasonal cycles only, while the 'Green's function' approach refers to a scheme that also uses the relation of atmospheric concentrations to fluxes in previous months, rather than the same month only. This type of inversion was first performed by Rayner et al. (1999) and Bousquet et al. (2000). In their transport representation, both studies neglect the interannual variability of atmospheric transport. A sensitivity study by Dargaville et al. (2000) assesses this variability to be only a second-order effect in a mass balance inversion for 1985–1992. Here, we investigate the role of interannual transport variability for a global time-dependent Green's function inversion in the period 1983–1998.

Once the employed transport model is driven by interannually varying meteorological data from the 'true' years, it also becomes possible to represent the concentration measurement process in the model more consistently with the real measurements. We propose here a new treatment of this process, and show its impact on the inversion results by a sensitivity test.

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Exploring transport-related impacts further, we compare inversion results based on different spatial transport model resolutions, as well as results based on meteorological driving fields originating from different global weather prediction centers.

The ultimate goal is to present CO₂ flux estimates that we consider most reliable with respect to the factors considered here, as a necessary preparation to interpret inversion-derived flux estimates and their implications for the carbon cycle.

2. Inversion method

The inverse calculation determines monthly surface CO₂ fluxes that minimize the difference between modelled and measured monthly mean CO₂ concentrations at a set of stations. At the same time, the fluxes are required to stay close to what is known about them from other sources of information, such as models of the ocean carbon cycle and the land biosphere, independent flux measurements and fossil fuel statistics ('a-priori fluxes'). The individual contributions of these pieces of information to the minimized cost function are weighted according to a-priori assumed variances. This type of inversion is known as the 'Bayesian approach' (Tarantola, 1987).

In our particular inversion setup, atmospheric tracer transport is calculated using the TM3 global tracer model (Heimann, 1996). Specifically, we use an 'adjoint' of TM3 generated with the help of the TAMC software (Giering and Kaminski, 1998; Kaminski et al., 1999). The standard spatial resolution is approx. 4° latitude × 5° longitude × 19 vertical levels; however, most of the sensitivity runs were performed on a coarser resolution (approx. 8° × 10° × 9 levels) to make them computationally feasible. The transport model is driven by interannually varying meteorological fields derived from the NCEP reanalysis (Kalnay et al., 1996) which cover all of our inversion period (1983–1998) in a consistent manner. Modelled monthly mean concentrations are calculated by averaging over 'samples' that represent the concentrations at the same time instants as the real raw measurements (see next paragraph) were taken ('true sampling'). The sensitivity of the monthly concentrations to the monthly fluxes up to 3 yr before are calculated explicitly by the adjoint transport model, with a fourth year approximated by exponential decay towards uniform sensitivity.

Measured monthly atmospheric CO₂ concentrations are derived from raw data of NOAA/CMDL's station

network (Conway et al. 1994), omitting invalid values as flagged by NOAA/CMDL as well as a few additional 'obvious outliers' (as judged manually based on their distance to the long-term seasonal cycle and on NOAA/CMDL's soft flags). The assumed uncertainty of the concentrations (typically around 1 ppm) is the quadratic sum of a measurement error (estimated as the average spread of duplicate samples, with a minimum of 0.1 ppm) and a transport model representation error (estimated proxywise as monthly concentration variance simulated by the transport model). We use a set of 24 measurement stations (alt, asc, azr, bmw, brw, cba, cgo, cmo, gmi, hba, key, kum, mbc, mhd, mid, mlo, nwr, psa, rpb, sey, shm, smo, spo and stm: for full station names, coordinates and descriptions see Conway et al., 1994) that offer relatively homogeneous data records over the long target time span of our inversion.

The a-priori CO₂ fluxes comprise the following components: (1) fossil fuel CO₂ sources according to global statistics by Marland et al. (2000) with a global uncertainty (1 σ interval) of 6%, spatially distributed according to Andres et al. (1997) and Brenkert (1998); (2) ocean–atmosphere exchange fluxes based on CO₂ partial pressure difference across the air–sea interface (Takahashi et al., 1999, using a quadratic dependence of gas exchange on mean wind speed suggested by Wanninkhof 1992) with a global uncertainty of 0.5 PgC yr⁻¹ (with respect to a 4 yr sum); and (3) land biosphere fluxes according to the mean of four land biosphere models that took part in the Carbon Cycle Model Linkage Project (CCMLP) (McGuire et al., 2001), with a global standard deviation of 0.85 PgC yr⁻¹ (with respect to a 10 yr sum). Fluxes are assumed to be uncorrelated in space and time. This means that the global quadratic sum of the uncertainties of all the land and ocean fluxes, respectively, over 1 yr yields the corresponding global yearly uncertainties, where the spatial distribution of uncertainties is chosen proportional to the absolute fluxes (for the ocean) or to the spatial pattern of variance of the four CCMLP models (for the land), respectively.

The inversion acts on 'residual' monthly concentrations, after presubtraction of the modelled concentration response corresponding to all the prior fluxes. The residual monthly CO₂ fluxes are inferred for 23 large regions tiling the globe (as used in the TransCom project, Gurney et al., 2002). Within the land regions, the flux updates are assumed to be spatially distributed proportional to the NPP part of the CCMLP modelled fluxes, while evenly distributed flux updates are

assumed within the ocean regions. As two additional adjustable parameters, a scaling factor (constant in space and time) for the fossil fuel emission strength, and the initial concentration are estimated. The first 3 yr of fluxes are discarded as 'spin-up'.

As sensitivity tests, individual details are changed in turn, as described in due course.

3. Results

3.1. Sensitivity to interannually varying meteorology

The standard inversion based on 'actual' (i.e., interannually varying) meteorology was compared with five runs based on 'fixed' meteorology of the years

1987, 1988, 1990, 1993 and 1997, that was repeatedly cycled through. The chosen years span a range of circulation conditions, including El Niño, La Niña and 'neutral' years. Figure 1 shows the inferred CO_2 fluxes other than fossil fuel emissions, where the monthly fluxes inferred by the inversions have been further integrated into yearly fluxes, and the 23 regions have been aggregated into four latitude bands. While the runs agree with respect to some of the temporal patterns, there is large scatter in the individual yearly fluxes, sometimes exceeding 2 PgC yr^{-1} (e.g., 1997 both in North Temperate and Tropic Zones). The time-averaged RMS difference of all the 'fixed-meteorology' fluxes with respect to the 'true-meteorology' estimate amounts to 0.72 PgC yr^{-1} in

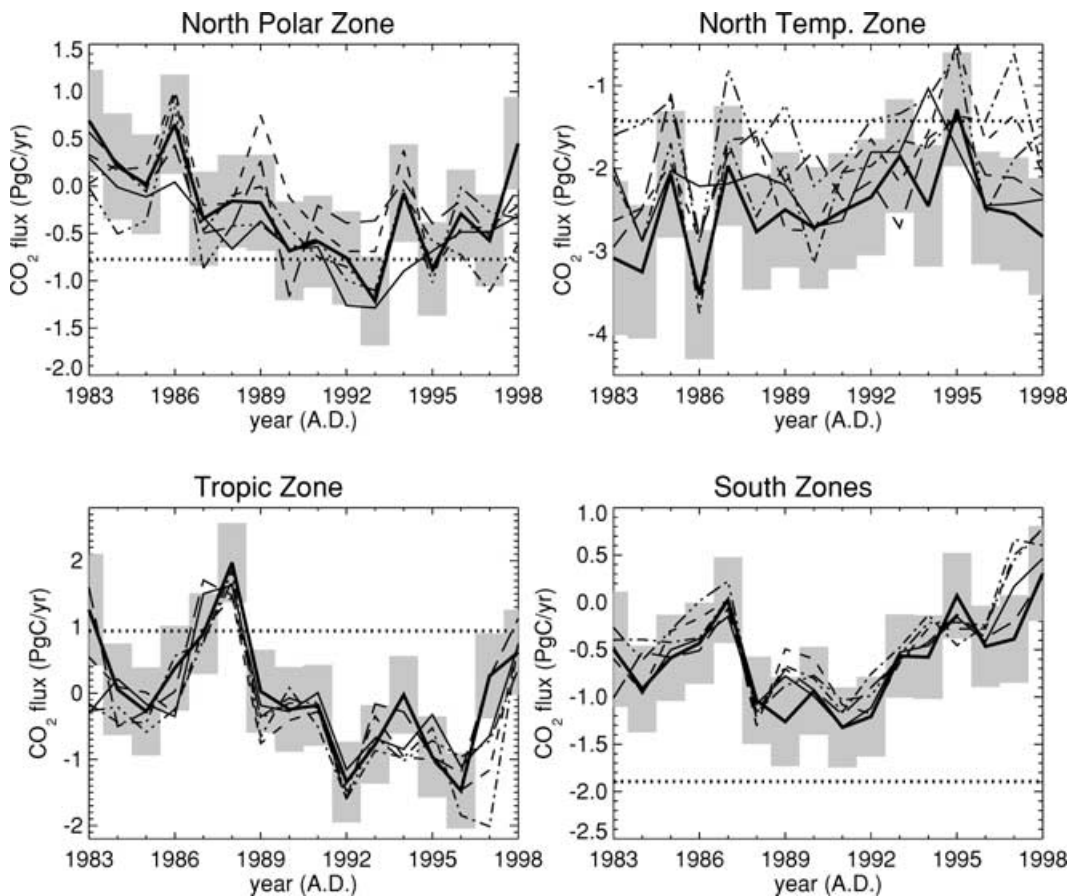


Fig. 1. Sensitivity of inferred yearly CO_2 flux estimates to transport modelling based on different meteorologies. [Meteorological year: (—) 'true' year, (---) 1987, (- · - ·) 1988, (—) 1990, (- · · · -) 1993, (- - -) 1997; (·····) a-priori assumed fluxes; shading: a-posteriori $\pm 1\sigma$ interval; transport model resolution here 'coarse' ($\approx 8 \times 10^\circ$, 9 layers)]. Fossil fuel component subtracted. North Polar Zone: $50\text{--}90^\circ\text{N}$, North Temperate Zone: $15\text{--}50^\circ\text{N}$, Tropic Zone: $15^\circ\text{S}\text{--}15^\circ\text{N}$, South Zones: $90\text{--}15^\circ\text{S}$.

the North Temperate Zone, which is slightly larger than the a-posteriori uncertainty in that region. We interpret this RMS difference as a measure of the flux variability that a ‘fixed-meteorology’ inversion spuriously attributes to the fluxes, in order to compensate the missing variability of transport. The discrepancies are lowest in the South Zone, still with an RMS difference of 0.31 PgC yr⁻¹ (or 68% of the corresponding a-posteriori uncertainty). Although we do not have an obvious explanation for the different sensitivities found in the Northern and Southern hemispheres, it might be related to the larger flux heterogeneity in the North (enhancing the impact of any differences in the timing or strength of the individual meteorological events), or to the higher a-priori uncertainties specified for the North (giving the inversion more freedom to change fluxes there).

Interestingly, our results do not allow to clearly trace the pattern of deviations from the ‘true-meteorology’ case to specific circulation conditions of the respective years (like Niño/La Niña). Thus, if an inversion based on fixed meteorology has to be done, say for computational reasons, the present comparison does not seem to favor any particular year.

The impact found here is larger than that reported by Dargaville et al. (2000) for the mass balance inversion technique. On a roughly comparable spatial scale, they found differences of maximally 0.6 PgC yr⁻¹.

To get an idea of the magnitude of the concentration signal which causes the differences in the inversion results, we compared modelled concentrations at station locations that result from the a-priori fluxes. Any difference in these values is exclusively caused by transport. At many stations (especially northern ones such as alt, brw, cba, mhd and stm), absolute deviations between the meteorologies often exceed 0.5 ppm, while much lower differences are found elsewhere (e.g., hba, mlo, psa and spo).

3.2. Sensitivity to concentration sampling scheme

Further, we compared different ways of calculating the monthly concentration in the model: Either modelled ‘measurements’ were taken exactly at the same time as the real raw measurements used in the inversion (‘true sampling’, our default), or simulated concentrations were just continuously averaged at every model timestep (‘continuous sampling’, traditional).

Success of ‘true sampling’ will depend on the ability of the transport model to reproduce the existing sub-month variability at the respective station loca-

tion (Houweling et al., 2000; Law, 1996; Ramonet and Monfray, 1996). We checked this by forward modelling, calculating the concentration response of the a-priori and a-posteriori fluxes, respectively. A typical example is presented in Fig. 2 (upper panel), comparing one year of modelled and measured CO₂ concentrations at the continental station Niwot Ridge. The results demonstrate that the transport model is well able to reproduce a considerable fraction of the within-month temporal patterns (even though the applied monthly fluxes miss any sub-month variability). Comparing now the monthly concentration averages resulting from ‘true’ or ‘continuous’ sampling, respectively, many months show a moderate difference (e.g., 0.1–0.2 ppm at Niwot Ridge). However, as seen in the enlargement in Fig. 2 (lower panel, including also a continuous modelled time series), there are also months where pronounced concentration excursions fall entirely between two measurement instants (see, e.g., the beginning or the second half of March). This means that, while both the measured mean and the true-sampling mean consistently ‘step over’ and ignore these events, the continuous-sampling mean includes the event and thus becomes inconsistent and biased (causing, e.g., a 0.6 ppm error in March 1998 at Niwot Ridge). Although also ‘true sampling’ can suffer from an error (of either sign) if the model happens to misplace such an event as much as to pass a measurement time (or if it grossly mispredicts the amplitude of an event that happens to be hit by a measurement instant), the bias of ‘continuous sampling’ will take place in any case. The figure further shows that a third alternative, namely taking a continuous mean over afternoon concentrations only (e.g., 11.00–17.00 local time), makes hardly any difference compared to the fully continuous mean. (Differences will, however, increase at continental stations that have larger diurnal cycles than the stations used here.) Note that any errors in the modelled diurnal cycle affect both ‘true’ and ‘continuous afternoon sampling’ in the same way.

At the other stations, a similar situation is found, with any differences becoming smaller at the more remote ones. As thus expected, the impact on the estimated CO₂ fluxes is moderate, causing differences up to around 0.5 PgC yr⁻¹ (Fig. 3). Nevertheless, as the forward simulations suggested, ‘true sampling’ provides the safer option. Moreover, since it allows modelled and measured concentrations to be matched at the level of the (preselected) raw data, it helps to avoid information losses due to the smoothing induced by curve-fitting of the data. The importance of ‘true

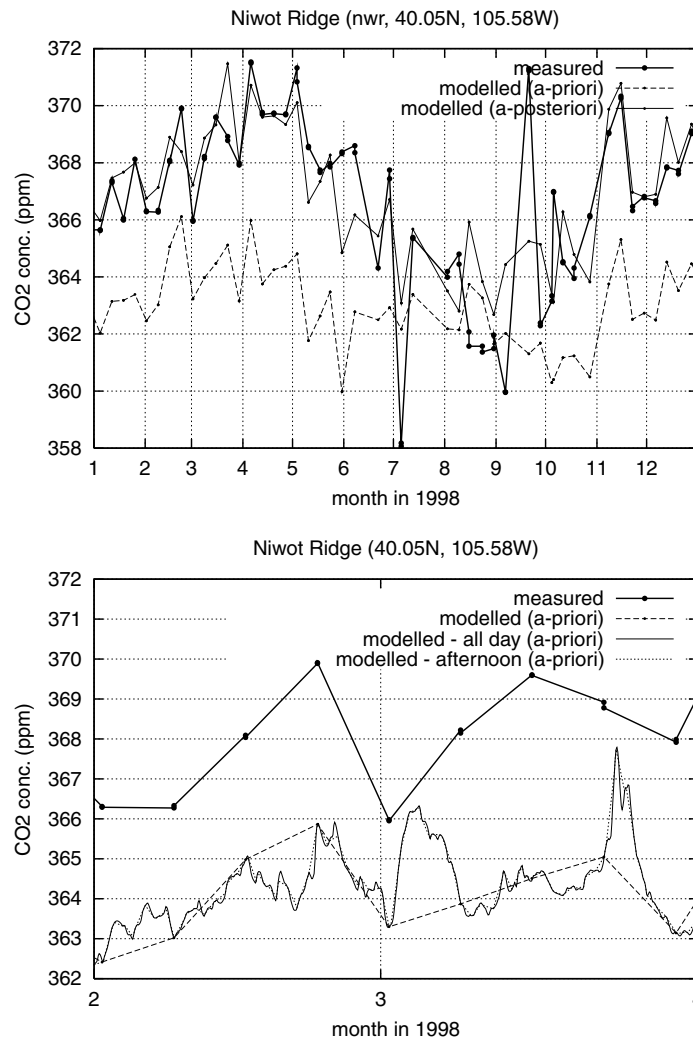


Fig. 2. Measured and modelled concentration time series at the station Niwot Ridge in 1998.

sampling' potentially increases for higher spatial and temporal model resolution, for stations with a high synoptic variability and/or a strong day–night contrast, or for stations closer to heterogeneous CO₂ sources/sinks. These cases might demand a careful re-consideration of which sampling procedure will be appropriate.

3.3. Sensitivity to spatial transport model resolution

Generally, the optimal model resolution represents a compromise between accuracy and computational

constraints. To test the potential gain in accuracy with increasing resolution, we compared our standard resolution ($\approx 4 \times 5^\circ$, 19 layers) with a coarser one ($\approx 8 \times 10^\circ$, 9 layers). One finds, e.g., considerable impact on how realistically the annual cycle of atmospheric concentrations can be reproduced (e.g., differences in amplitude up to about 3 ppm at station Barrow, Fig. 4). This indicates that the coarse-grid transport representation might, at least with the model employed here, lead to overestimating the amplitude of seasonal cycles of the inferred fluxes. Even in the annual fluxes, differences often lie outside the $\pm 1\sigma$ a-posteriori uncertainty range (Fig. 3).

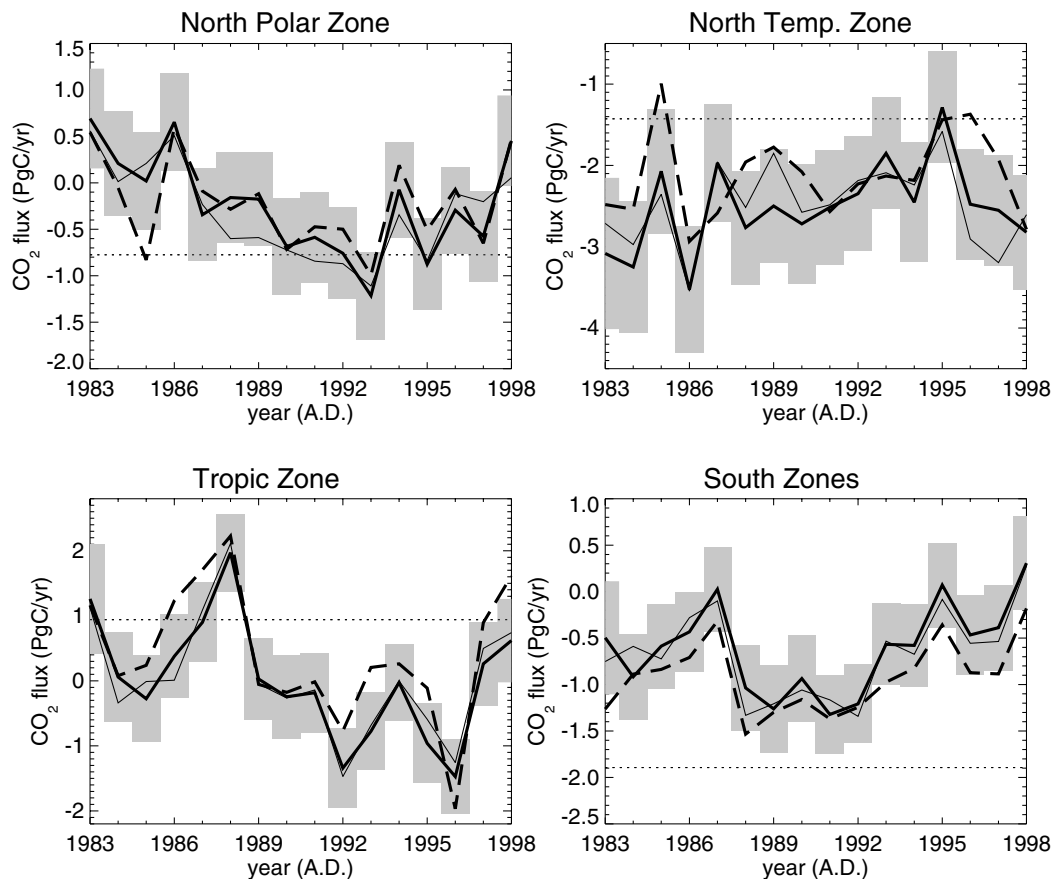


Fig. 3. Sensitivity of inversion results to concentration sampling scheme and atmospheric transport model resolution [(—) 'coarse-grid' version ($\approx 8 \times 10^\circ$, 9 layers) with 'true sampling', (---) 'coarse-grid' version ($\approx 8 \times 10^\circ$, 9 layers) with 'continuous sampling', (-.-) 'fine-grid' version ($\approx 4 \times 5^\circ$, 19 layers) with 'true sampling', (.....) a-priori fluxes, shading: a-posteriori $\pm 1\sigma$ interval]. Fossil fuel component subtracted.

3.4. Sensitivity to data source of driving meteorological fields

For the years 1979–1993, global meteorological fields are also available from the ECMWF reanalysis project (Gibson et al., 1997), as an alternative to the NCEP reanalysis normally used here. Figure 5 compares flux estimates when the transport model was driven with either of these data sets. The difference remains relatively small; largest effects are found in the partitioning between the tropical and the southern zones, the tropics being estimated to outgass about 0.5 PgC yr^{-1} more when using ECMWF data. A possible reason might lie in the different predicted strengths of convective activity (and hence vertical mixing) in the tropics. The smaller differences in the northern hemisphere are expected, since the global circulation

models are better constrained there by the denser network of meteorological observations.

4. Discussion

The present sensitivity study quantifies the impacts of some simplifications in the representation of atmospheric tracer transport on flux estimates derived by time-dependent global Green's function inversions. We find differences of an order of magnitude comparable to the a-posteriori flux uncertainty as well as to the update between a-priori and a-posteriori fluxes. Present-day inversion estimates may differ by more than that, due to different choices in other methodological details [e.g., flux aggregation into regions (Kaminski et al., 2001), the regularization method or

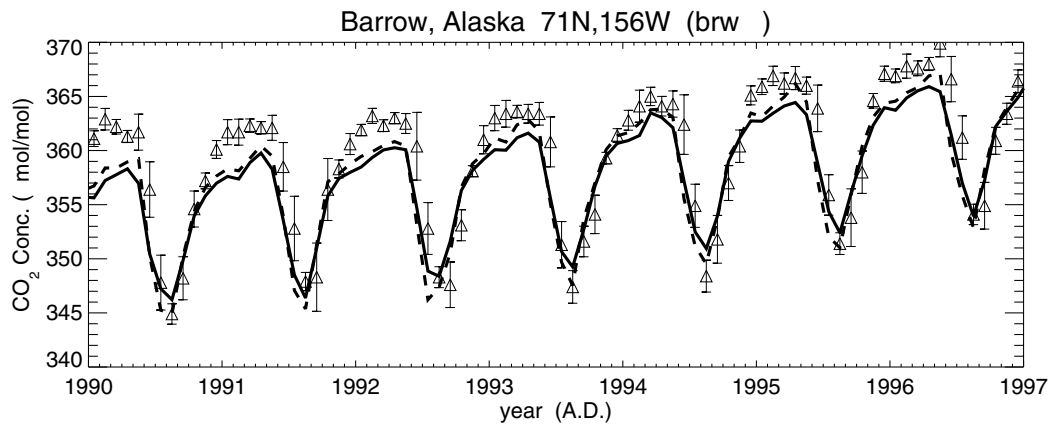


Fig. 4. Modelled monthly mean atmospheric CO₂ concentration at Barrow (Alaska), resulting from the a-priori assumed fluxes [(—) 'coarse-grid' version ($\approx 8 \times 10^\circ$, 9 layers), (---) 'fine-grid' version ($\approx 4 \times 5^\circ$, 19 layers), Δ measured concentrations with $\pm 1\sigma$ uncertainty interval].

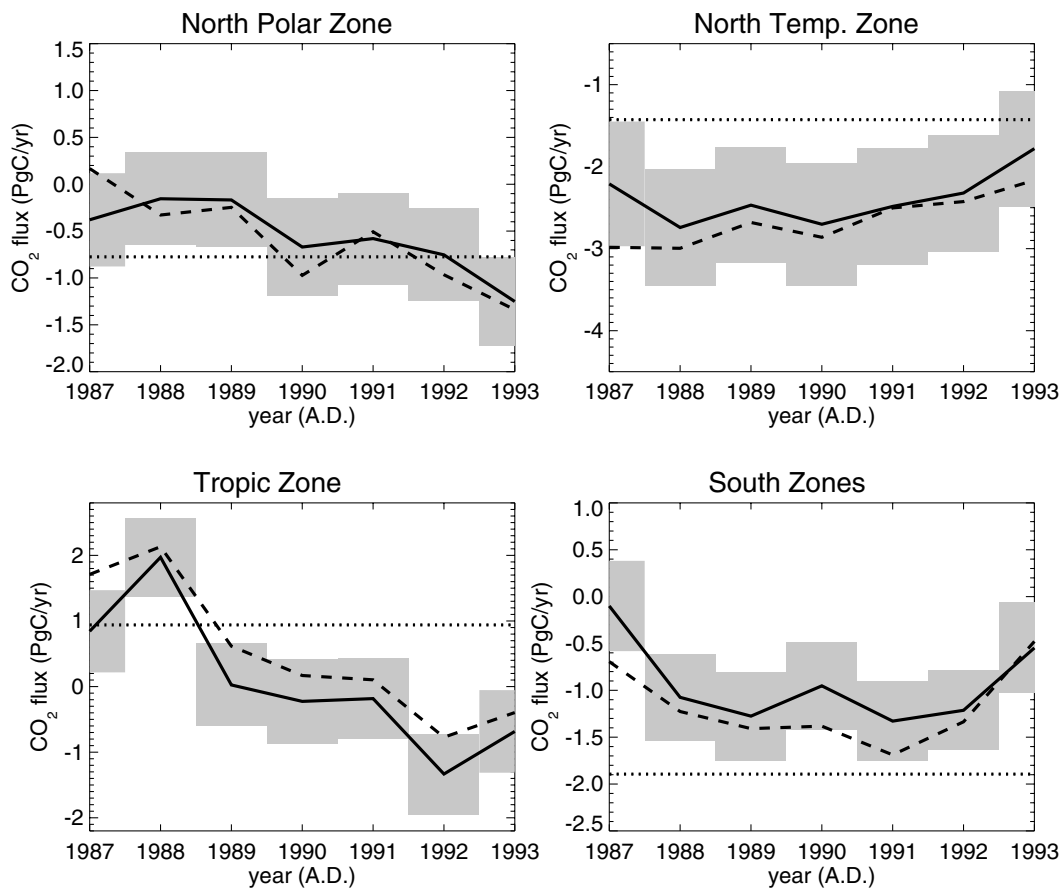


Fig. 5. Sensitivity of inversion results to meteorological driver data source [(—) NCEP reanalysis, (---) ECMWF reanalysis; both here with 'coarse-grid' transport model ($\approx 8 \times 10^\circ$, 9 layers)]. Fossil fuel component subtracted.

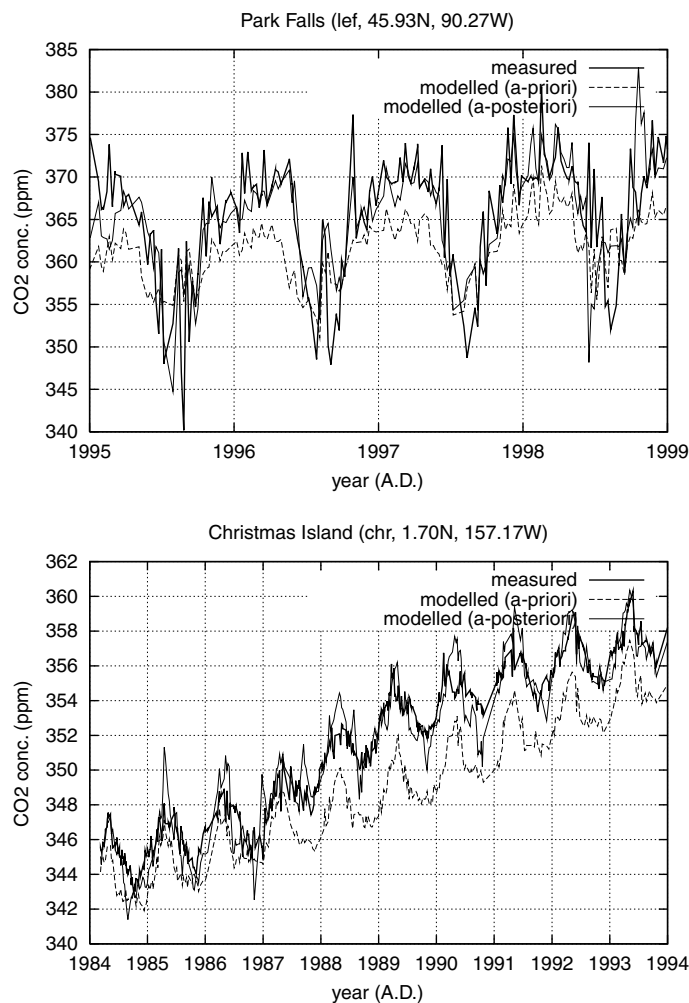


Fig. 6. Measured and modelled concentration time series at two stations that were not used in the inversion.

the poorly constrained assumptions on a-priori variances] or to different transport models (Gurney et al., 2002). This indicates that the sources of uncertainty considered here stay within the range of other uncertain aspects of contemporary inversions. In our opinion, they have the potential, however, to limit the progress of future atmospheric inversions.

Some confidence in the inversion results can be gained by comparing the modelled concentration response of the estimated fluxes with the corresponding concentration measurements, at stations that were not included in the inversion. While this comparison is expected to be most successful at remote stations, the rather good agreement e.g. at the continental station

'lef' (Fig. 6, upper panel) is encouraging. Although the seasonal cycle at the Pacific station 'chr' (Fig. 6, lower panel) gets overestimated, the observed interannual variability turns out to be well reproduced by the inversion.

As a further test, Fig. 7 compares our inversion-derived global ocean flux to the corresponding estimate by an independent global biogeochemical ocean model (Le Quéré et al., 2000, updated as described in Bousquet et al. 2000). Timing and relative strength of interannual flux variations are found to agree to good extent, while the amplitude of the inversion is more than twice that of the ocean model. The difference in the long-term averages is partly explained by the fact

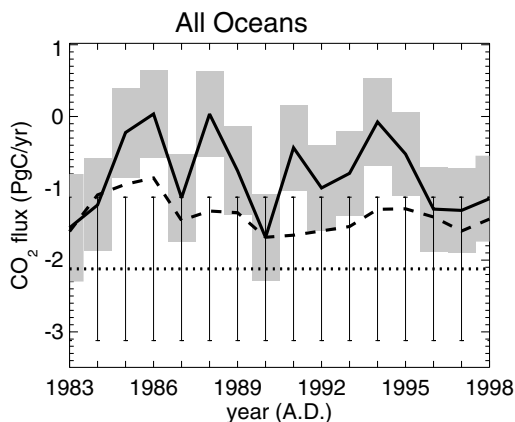


Fig. 7. Yearly ocean-atmosphere CO_2 fluxes as estimated by the inversion (—) and a global biogeochemical ocean model (---); [shading: a-posteriori $\pm 1\sigma$ uncertainty interval, (.....) a-priori fluxes (Takahashi et al. 1999), error bars: a-priori $\pm 1\sigma$ uncertainty interval]. Fossil-fuel component subtracted.

that the ocean model output does not include natural CO_2 outgassing of the ocean as a consequence of riverine input, which was estimated by Sarmiento and Sundquist (1992) to be about $0.4\text{--}0.7 \text{ PgC yr}^{-1}$. Less agreement is found for the distribution of the CO_2 flux among the different ocean regions.

Exerting the appropriate care in interpreting our inversion results, we find as some fairly robust features:

- Long-term mean ocean estimates generally stay close (within 1σ , typically 0.2 PgC yr^{-1} per region per year) to the prior fluxes of Takahashi et al. (1999), with two exceptions: North Pacific Temp. (0.0 PgC yr^{-1} compared to -0.5 PgC yr^{-1} predicted by Takahashi) and Southern Ocean (slight CO_2 source of 0.1 PgC yr^{-1} , compared to a sink of -0.9 PgC yr^{-1} ; cf. Gurney et al., 2002).
- For the continental regions, long-term flux estimates differ considerably from the a-priori fluxes. Largest updates result for Temperate Eurasia ($-1.15 \text{ PgC yr}^{-1}$ + fossil fuel) and Temperate North America (-0.7 PgC yr^{-1} + fossil fuel) in broad agreement with previous estimates (Tans et al. 1990; Bousquet et al. 2000; Gurney et al. 2002) and South America Tropical (-0.5 PgC yr^{-1} + fossil fuel).
- The interannual variability of continental flux estimates is on the order of 0.5 PgC yr^{-1} , more than twice that of the oceans (0.2 PgC yr^{-1}). Largest variability on land is found for North Africa, Eurasian Temperate, South Africa and North American Tem-

perate (std. deviation $\approx 0.7 \text{ PgC yr}^{-1}$). In line with Bousquet et al. (2000), for example, land fluxes show clear positive anomalies during Niño events.

5. Conclusion

Tentatively ranking their importance, the considered aspects of atmospheric transport representation influence the CO_2 flux estimates of the interannual inverse calculations as follows:

- Neglecting the interannual variability of atmospheric transport introduces a sizable error (similar order of magnitude as the a-posteriori uncertainties, up to 2 PgC yr^{-1} in our latitude bands). We therefore advise the use of true meteorology in future time-dependent inversions.
- Spatial transport model resolution has effects of almost the same order, when comparing our standard resolution ($\approx 4 \times 5^\circ$, 19 layers) with a coarser one ($\approx 8 \times 10^\circ$, 9 layers). Thus, the expense of higher model resolution seems well spent.
- Comparing meteorological driving fields from the NCEP reanalysis and from the ECMWF reanalysis, respectively, we mainly find a long-term redistribution of fluxes across latitudes. Largest effects (about 0.5 PgC yr^{-1}) result in the tropics.
- We find a moderate sensitivity to the concentration sampling procedure; however, as suggested by forward simulation, we consider the proposed ‘true sampling’ as the more straightforward and safer choice to avoid spurious anomalies. We expect ‘true sampling’ to be even more promising at higher transport model resolution and/or for non-remote stations, where, however, a careful re-evaluation is required.

Inversion results also depend on many choices in the inversion setup (uncertainty structure, choice of transport model, regularization, etc.), some of these causing differences similar or larger in magnitude than the effects considered here.

In summary, using interannually varying meteorology in time-dependent inversions has two advantages: it eliminates a significant source of error and allows a concentration sampling consistent between measurements and model.

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