Incremental approach to the optimal network design for CO2 surface source inversion

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[1] An algorithm for observational network design to obtain maximum constraints on CO2 flux estimate uncertainty by using inverse modeling and global transport model is presented. The extension to an existing network is made by adding new station locations one by one, based on their positive impact on the flux estimate uncertainty reduction. The approach is named Incremental Optimization (IO). This extension procedure performs equally well or better compared to the well known techniques, such as the simulated annealing, used in combinatorial optimization. We could reduce the estimated total CO2 flux uncertainty by 59%, 47%, and 29% relative to a reference network by using IO with additions of 3, 5, 12, and 20 stations, respectively. IO is shown to be efficient in studying various network configurations and re-emphasizes the need for CO2 measurements in continental Africa, South America, and Asia. INDEX TERMS: 0322 Atmospheric Composition and Structure: Constituent sources and sinks; 0394 Atmospheric Composition and Structure: Instruments and techniques; 0368 Atmospheric Composition and Structure: Troposphere—constituent transport and chemistry

1. Introduction

[2] The synthesis inversion is a useful tool to estimate the optimal CO2 source/sink strengths and their uncertainties for different geographic regions. It requires information on atmospheric observations and global transport model simulations of a priori fluxes [Tarantola, 1987; Enting et al., 1995]. Attempts have been made to improve our understanding of the key transport processes that control the tracer distribution [e.g. Law et al., 1996; Denning et al., 1999], and simultaneously to increase the network for atmospheric measurements. The extension of the CO2 measuring network to constrain inverse model results have gained considerable interest in the recent past [Rayner et al., 1996; Gloor et al., 2000]. In the present CO2 measuring network, most stations are positioned away from the source region to capture the background CO2 concentrations [Keeling et al., 1995; Masarie and Tans, 1995], allowing for a robust estimate of the meridional flux distribution. However, sources and sinks in the same latitude belt are difficult to discriminate reliably [Gloor et al., 2000]. Therefore, it is important to understand the influence of the observational sites on flux estimation and to identify the regions that are poorly constrained in our inverse modeling framework, so that strategies can be sketched towards enhancing the present day measurement capability. Finding an optimal solution for extending the existing network is a multivariate combinatorial optimization problem, and is often dealt with heuristics in computer sciences [Kirkpatrik et al., 1983]. One common approach is simulated annealing (SA) and has been applied to the problem of CO2 observational network optimization [Rayner et al., 1996]. Although SA is powerful and widely used, this technique is computationally expensive and probabilistic in nature.

[3] For a more comprehensive study on CO2 network design, it is beneficial to develop an optimization algorithm that is simple to implement, computationally inexpensive and deterministic (i.e. results in an unique solution). In this article, we discuss one such approach and evaluate its performance in comparison with a well established technique like SA. The Materials and Methods used in this study are described in section 2, followed by the Results and Discussion in section 3.

2. Materials and Methods

2.1. Synthesis Inversion

[4] In Bayesian time-independent inversion [Tarantola, 1987; Enting et al., 1995], the surface annual average fluxes of CO2 are optimally derived from its atmospheric observations and computed model responses of the fluxes under study. The source strengths are predicted by obtaining a least squares solution of the function \( GS = D \); where \( G \) is matrix of transport model simulated response functions at the observation stations for each source type, the vector \( S \) represents CO2 sources of different types on the earth and, \( D \) the atmospheric mixing ratio at the observation stations. The Bayesian synthesis inversion simultaneously minimizes the mismatches between both the initial and predicted sources as well as the gap between the predicted responses and the observations. Mathematically, the function to be minimised becomes,

\[
(S - S_0) C_S^{-1} (S - S_0)^T + (GS - D) C_D^{-1} (GS - D)^T
\]

where the elements of \( C_D \) are the data covariances, i.e. squared residual standard deviations (RSDs) of the high frequency CO2 data variability. Assuming that the elements of \( C_D \) are spatially uncorrelated, the solutions for \( S \) and its covariance \( C_S \) can then be found as (see Tarantola [1987] for details)

\[
< S > = S_0 + \left( G^T C_D^{-1} G + C_S^{-1} \right)^{-1} G^T C_D^{-1} (D - GS_0)
\]

\[
C_S = \left( G^T C_D^{-1} G + C_S^{-1} \right)^{-1}
\]

Note here that the predicted values of \( C_S \) does not depend on \( D \). This property of synthesis inversion will be exploited while producing synthetic atmospheric data for new candidate stations, as our target in this study is to constrain \( C_S \). The pseudo-inverse of the matrix \( G^T C_D^{-1} G + C_S^{-1} \) is determined by using singular value decomposition (SVD). The SVD of any general matrix \( A \) is factorization of the form \( U \Sigma V^T \), where the columns of \( U \) and \( V \) are orthogonal, and \( \Sigma \) is diagonal [Press et al., 1992].

2.2. Transport Model and Data Covariances

[5] The semi-Lagrangian NIES (National Institute for Environmental Studies, Tsukuba) FRSGC global transport model (see Maksyutov et al. [2001] for a detailed description) is used for computing the response functions. The model boundary layer
changes with the season, and transport due to cumulus convection is parameterized by a Kuo-type scheme. The model resolution is set to 2.5° × 2.5° in horizontal and it has 15 vertical sigma-layers. The cyclo-stationary transport is driven by the ECMWF (European Centre for Medium-Range Weather Forecast) meteorological data (operation analyses for 1997). As a test case, we use TransCom-3 setup for different CO₂ source types on the earth surface and definition of the land and ocean regions for the inverse model calculation [Gurney et al., 2000]. The TransCom-3 experimental protocol considers prescribed fluxes for (1) fossil fuels, (2) net ecosystem production (NEP), weighted by CASA Net Primary Production [Randerson et al., 1997] and (3) the oceans [Takahashi et al., 1996]. It also considers the regional fluxes from 11 land and 11 ocean regions as shown in Figure 1, in addition to the prescribed fluxes, which are used to correct the surface flux distribution in the inversion procedure for minimizing the mismatch between model and observations. Within the land and ocean regions, the fluxes are distributed according to terrestrial biosphere NEP and oceanic CO₂ fluxes. The prior source/sink distributions S₀ and associated uncertainties S₀ are assumed to be same as in TransCom-3 (also indicated on Figure 1).

[6] The regional flux signals G and data covariance C_D for new stations are estimated from the high frequency variability of daily outputs of the NIES/FRSGC model for a period of two years. The model was run by combining the fluxes from fuel combustion, ocean and net ecosystem production. The residuals are estimated from the high frequency data, by subtracting the CO₂ seasonal cycle calculated with a low-pass filter, as described in Nakazawa et al. [1997]. A comparison of the RSDs from the GLOBALVIEW-CO₂ data set [GLOBALVIEW, 2000] and model derived values show fairly good agreement Patra et al., [2001]. In general, the model somewhat underestimates the variability in the high latitude southern hemisphere and remote locations around 60° S.

2.3. Network Simulation Techniques

[7] Simulated annealing (SA) is the only technique that has thus far been applied to the problem of CO₂ network optimization [Rayner et al., 1996; Gloor et al., 2000]. In this technique, an objective function, here the flux estimate uncertainty (CS₀), is minimized by reconfiguring (n times) a desired number of locations with certain degree of freedom for movement. The movement is parameterized by a temperature (T) and a tunable Boltzmann constant (k_b) as in statistical mechanics. The new configuration is accepted if it has a positive definite influence on the exiting best network. Otherwise the new network accepted only with certain probability, which allows the system to escape from local minima. After a predetermined number of iterations n, the temperature is reduced in geometric progression (T_n = γT_{n-1}; 0 < γ < 1; N is the number of scheduling steps T_0 is the initial temperature). The values for both n and N are to be set by trial and error, and is often restricted by a trade-off between computational expense and finding the global minimum. Further details on our implementation of SA can be found elsewhere [Patra et al., 2001].

[8] For this study, data and RSDs for a basic set of 115 stations is derived from the GLOBALVIEW-CO₂ data set. We also prepared a candidate set of 446 stations, selected from more than 6000 surface meteorological observation stations that supply daily observational data to the World Meteorological Organisation (WMO). The criteria for this selection is the distance to the nearest existing station. Selecting a candidate from the meteorological observation network list guarantees minimum logistics, as opposed to working with the regular model grids which often includes inaccessible geographical areas. A set of 3, 5, 12, and 20 stations are then added to the basic set to formulate a new larger data space (D) for the simulated annealing procedure.

[9] The new approach for optimal network for CO₂ surface measurement is based on another classic heuristic to solve optimization problem — the ‘divide-and-conquer’ approach [Kirkpatrick et al., 1983] and has a rather straightforward implementation. In this case, the problem is divided into subproblems. At the first iteration, the subproblems are constructed by adding one of each candidate stations to the basic set. We perform the inverse calculation on 446 candidate data sets each consisting of 116 (115 + 1 new) stations. The data set that produces best total source estimate uncertainty is stored as the new basic set, and the new station location in the basic set is removed from the list of candidate stations. And a next set of

Figure 1. Network stations for measuring surface CO₂ mixing ratio for constraining the global flux estimate uncertainty. Indigo diamond: GlobalView, Green Square: Additions by IO (the numbers indicate the sequence of their entry into the basic set, see Figure 3 for exact location), Other symbols: 3 (red circle), 5 (orange triangle-down), 12 (blue triangle-up), and 20 (indigo cross) additions by SA. The approximate inverse model regions (prefix L stands for land regions, O for the Oceans; region names are given on Figure 1) are shown by the blue lines, and the numbers within parentheses are the associated prior flux uncertainties (in Gt C/year/region).
subproblem is constructed by adding remaining 445 candidate station to the new basic set containing 116 stations. Thus the basic set grows in size with an increment of one station, while the candidate set is depleted. This technique will be referred to as incremental optimization (IO). As the procedure is repeated, the number of subproblems will keep reducing until the basic set has evolved into another basic set including all the desired candidate stations. The process should be continued until the desired size of network for CO2 observations is reached. In contrast to simulated annealing, this method provides us with a continuous evolution of the observation network and is computationally inexpensive.

3. Results and Discussion

[10] Figure 1 shows the networks obtained by simulated annealing and by our approach. Both the networks suggest that the Tropical America, South America, Tropical Africa and South Africa are the most poorly constrained regions in the inverse modeling framework. The other regions that are loosely constrained turn out to be Temperate North America, Temperate Eurasia and Southeast Asia. Gloor et al. [2000] have also highlighted the need for measurements more or less in similar regions. The results are fairly consistent in both the network design models (SA and IO) as well as for different experimental realizations of SA. However, the individual stations in a network tend to deviate from one another when a bigger network is constructed, e.g. if network is enhanced by 12 stations or beyond. For the 12 station case, while IO continue to position stations in the poorly CO2 flux constrained regions, SA puts a couple of them in and around the Australasia.

[11] For simulated annealing we use $5 \times 10^4$ reconfigurations in each of the 10 scheduling steps for 3 new stations. However, number of reconfigurations up to about $5 \times 10^3$ has been used for the bigger network constructions. This demand in computational expense is commanded by the increase in complexity of the problem when worked on a bigger network, and at the same time fail to find the global minimum, even though the same network is obtained in successive test runs.

[12] The global total source estimate uncertainties obtained from IO and SA are compared with a benchmark (Figure 2). The SA apparently outperforms the benchmark result (random network) and appears to be in compliance with the previous works. Interestingly, our approach to observation network design seem to have constrained the global total CO2 flux uncertainty estimate more severely. It is also seen that IO is more efficient for constructing a larger network. The computation expense for iterative technique (e.g. simulated annealing) grows rapidly with the number of new observation sites under consideration. The global total flux uncertainies are found to be about 3.24, 2.57, 1.91, and 1.62 Gt C year$^{-1}$ by adding 3, 5, 12, and 20 new stations by IO, respectively, and about 3.24, 2.66, 2.23, and 1.96 Gt C year$^{-1}$ are obtained by SA for identical configurations; which was about 5.46 Gt C year$^{-1}$ for the initial ‘basic set.’ The ‘divide-and-conquer’ technique apparently wins in this specific application, probably due to the construction of naturally disjoint subproblems [Kirkpatrick et al., 1983] as described in section 2.

[13] It should be pointed out here that we have checked the results of both IO and SA against all the possible station combinations with a smaller basic set of 16 stations and only 44 candidate stations. The explicit permutation-combination (($^{445}_{116}$) are performed by picking 3 indistinguishable stations from the candidate set. The results are in complete agreement with those from IO and SA. Thus, we believe, that IO represents a correct approach to the CO2 network design problem. In addition, the results of IO agree perfectly well with SA even with larger number of additions (e.g. 5 and 8), but the total number of inversion increased approximately from 1400 (3 station case) to 4500 and 41,400, respectively. The results start deviating if the number of additions increased further. However, the gross features obtained from both the methods provide similar information.

[14] Finally, computationally less expensive algorithm helps in comprehensive study of the solutions to a problem like optimal network design. As the new network grows continuously in IO, the influence of every newly introduced station on the source estimate uncertainty for all the source regions can be visualized (see Figure 3). Generally, a station leads to maximum uncertainty reduction for the

![Figure 2. Comparison of reduction in global total source/sink estimate uncertainty for CO2 by introducing new sites for observation through IO (solid line) and SA (open circle) with a randomly generated network (dashed line).](image)

![Figure 3. Diagram showing the effect of new stations on the source estimate uncertainties for different regions of the inverse model. The location of the newly introduced stations are indicated in between the two panels.](image)
region where it resides, whereas the other regions linked through atmospheric transport only get peripheral benefit. Additionally, the incremental addition of the candidate sites provides us with a station ranking in terms of the source uncertainty reduction (see Figure 1) and an exact value of the uncertainty reduction gained (lost) by adding (removing) a particular station. This information is useful for actual implementation of observational programme expansion and/or reduction. However, it is desirable to test how IO and SA would perform in a more complex setting of high spatial resolution and time-dependent inversion.

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