NRA-00-OES-08: CARBON CYCLE SCIENCE

Global and Regional Carbon Flux Estimation Using Atmospheric CO_2 Measurements from Spaceborne and Airborne Platforms

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Abstract

We propose to develop methods for determination of surface sources and sinks of atmospheric CO2 using inverse modeling from spatially dense atmospheric data anticipated to be available in the near future. These will include ubiquitous column CO2 estimates made from infrared spectra measured by spaceborne sounders (AIRS in 2001, IASI in 2003), and high-precision measurements made from tall towers and aircraft over the continents as well as more traditional flask sampling. We anticipate that these data could be used to provide fully populated grids for global flux estimation, beginning with very low precision but improving over time. Although they provide a tremendous opportunity for the study of the global carbon cycle, these data challenge us to develop new methods to extract the information.

We will develop algorithms for both estimation of CO_2 mixing ratio from spaceborne measurements and for quantitative estimation of surface fluxes from concentration data by tracer transport inversion. The Colorado State University (CSU) General Circulation Model (GCM) will be used to simulate self-consistent hourly 3D grids of CO2 temperature, water substance and other meteorological variables. The CSU GCM is fully coupled to the Simple Biosphere Model (SiB2), which predicts exchanges of CO_2 with the vegetated land surface every few minutes and has been favorably compared to field data at many locales and scales. We will compute radiances at the top of the atmosphere in thousands of relevant bands in the infrared and fly "virtual satellites" through the model to sample these radiances. We will develop and test algorithms for CO_2 estimation in the column mean and in several atmospheric slabs from these simulated radiances, including cloud masking, water vapor interference, and a realistic diurnal and seasonal cycle. We will then use atmospheric inverse methods to estimate regional CO2 fluxes and uncertainty in these fluxes on a monthly basis from the concentration estimated radiometrically. We will also develop and test possible future strategies for spaceborne CO_2 sensors using dedicated hardware, including documentation of requirements for accuracy, sampling frequency, orbital considerations, etc.

We will also propose three "nested" regional experiments in the context of the hypothesized ubiquitous satellite CO_2 data. These will be high-resolution pseudo-data continents (North America, South America, and sub-Saharan Africa) simulated with a mesoscale model (SiB-RAMS) on a 40 km grid. We will sample these fields with "pseudo-aircraft" and "pseudo-tall-towers," and provide guidance about sampling strategies to provide maximum carbon budget constraints with limited resources. These regional optimization studies are seen as collaborative with regional aircraft sampling campaigns proposed in these regions (COBRA and LBA). The Amazon inversions will also require development of improved representations of transport by organized cumulus convection.

Statement of Relevance

Under Carbon Cycle Science, this proposal directly addresses the high-priority call for "*development of new techniques, algorithms, and/or analytical approaches for extracting important carbon cycle information from remotely sensed data*" on pages 6 and 18 of the NRA. We propose research to advance "*scientific readiness to evaluate the potential of new and exploratory measurements or data sets to provide critical information on carbon cycling dynamics*" that is "very strongly encouraged" on pages 18-19 of the NRA.

Introduction

Human activities release more than 7 GtC (1 GtC, or gigaton of carbon, equals 10^{12} kg C) each year, yet only about half of this annual increment remains in the atmosphere as CO_2 [*Schimel et al, 1996*]. The other half is dissolved into the surface oceans or incorporated into organic matter on the land surface, but the relative proportions of these sinks is uncertain. Carbon cycle science has made substantial progress in recent years, yet a mechanistic description and even the geographic distribution of the processes responsible for sequestering half of the anthropogenic CO_2 remain elusive. These sinks can be thought of as "Earth system services" of extraordinary value that currently provide the equivalent of a 50% CO_2 emissions reduction. Unfortunately, we can't say with confidence where or how these services work, or whether they will continue to work in the coming decades. Rational policy decisions depend on reliable predictions of the future behavior of these sinks, which will require better understanding and continued monitoring of CO_2 sinks.

A recent report sponsored by the US Global Change Research Program [*A U.S. Carbon Cycle Science Plan, Sarmiento et al, 1999*] recommended an expanded, systematic program of research on carbon cycle science. The Plan recommends a combination of process-based studies at the local level, intended to better characterize carbon exchange mechanisms from the "bottom up," and the application of mass balance constraints to land and ocean carbon budgets from the "top down." This approach allows mechanistic hypotheses to be developed from field experiments, leading to spatially explicit models extrapolated using remote sensing and other data, and the testing of model hypotheses against changes in CO_2 storage in the atmosphere and oceans.

Observations of atmospheric CO_2 contain information about exchange processes at the surface which can be quantitatively extracted using tracer transport inversion [e.g., *Tans et al, 1995; Enting et al, 1995; Fan et al, 1998; Bousquet et al, 2000*]At the largest of spatial scales (global, hemispheric), atmospheric data provide a very strong constraint on surface fluxes; these data are the basis for confident statement of the total source and sink magnitudes. The mixing ratio of atmospheric CO_2 is currently measured on flask samples collected weekly at nearly 100 stations located primarily at the surface in remote marine areas of the world, in deserts and on mountaintops [*Masarie and Tans, 1996*; Fig 1] Laboratory analysis produces data of very high quality (typical precision is better than 0.1 ppmv), with participating labs using international standards.

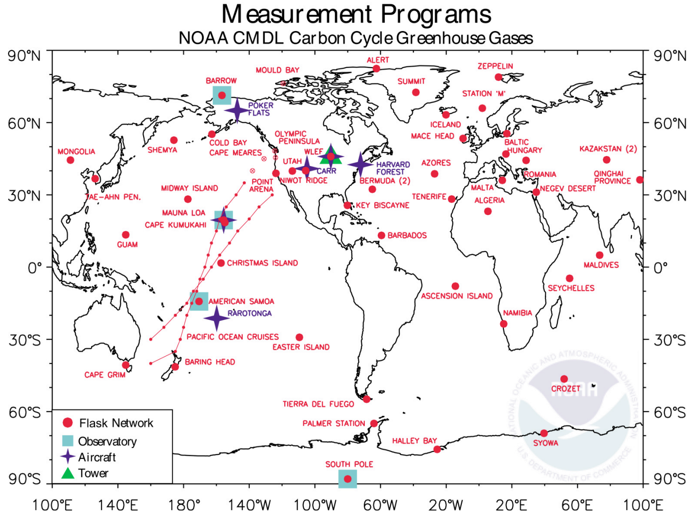

Figure 1: Flask sampling locations for CO_2 analysis

Estimation of regional sources and sinks from these data is accomplished by dividing the world into regions, each of which is assumed to emit or absorb CO_2 at an unknown rate. Atmospheric transport models are used to simulate the sensitivity of concentration measured at each sampling site as a function of the strength of these "basis" emissions. The inverse problem is to determine the magnitude of each basis flux that produces the best agreement with the observations.

Atmospheric inverse models have typically used subsets of the samples in Fig 1 to estimate surface fluxes for between three and 50 regions, but disagree sharply on the results. An international intercomparison study of inverse CO_2 models (IGBP TransCom, http://transcom.colostate.edu) is currently underway to elucidate the reasons for this failure to converge on a picture of current sources and sinks. When 15 transport models were run in a standard experiment, differences *between* models were smaller than the uncertainty in annual mean fluxes *within* models for nearly every region. This indicates that the inverse problem is currently *data limited* because within-model uncertainty reflects weak data constraint on fluxes. This is especially true over land in the tropics, where there are almost no samples collected. Furthermore, much of the difference in transport among models is due to parameterized subgrid-scale vertical motion (cumulus convection, for example), so model may agree in the marine boundary layer where data are dense at the expense of serious disagreement over the continents and aloft [*Denning et al, 1999*].

Network optimization studies using inverse models have demonstrated great potential for improved confidence in regional flux estimates with the addition of hypothetical sampling stations over the continents, particularly in the tropics [*Rayner et al, 1996; Gloor et al, 2000*]. This is problematic, because near-surface CO_2 concentration over land is extremely heterogeneous in both space and time, with vertical and diurnal variability an order of magnitude greater than exhibited by the global flask network. Point measurements in the surface layer reflect a tiny "footprint" or area of influence, which is why most flask samples are collected in the remote marine boundary layer, far from local sources and sinks. Measurements made from mountaintops or from very tall towers [*Bakwin et al, 1999*] provide an opportunity to collect representative samples over land, but are limited by availability of appropriate platforms. Sampling from airborne platforms [*Tans et al, 1996; Stephens et al , 1999*] is a powerful way to observe the regional atmosphere, but is very expensive, especially for routine data collection. Nevertheless, airborne sampling experiments are being conducted in the U.S., Europe, Asia, and Australia, with a potential to substantially reduce the uncertainty of regional carbon budgets.

Another potential source of new data on atmospheric composition for surface flux estimation retrieval of column integrated CO_2 from data collected by satellite sensors. Such data would have the advantage of global coverage, including continental areas that are currently so badly undersampled. The principle disadvantage is that such data do not exist! Nonetheless, several sensors soon to be flown have potential for use in CO_2 retrievals, and a dedicated mission is possible at some point (See attached letter of collaboration from James Abshire). [*Rayner et al, 2001*] have explored the potential constraint that could be provided by column mean concentration measurements analogous to satellite CO_2 data, and find that even low precision measurements (with random errors as large as 2 ppm or more) could add information to the inverse flux problem.

To evaluate the potential use of CO_2 retrievals from spaceborne sensors in atmospheric transport inversions of fluxes, we created a "pseudodata" atmosphere by prescribing known surface exchanges in a general circulation model (GCM). The model atmosphere was then sampled to represent data collected by both flask analysis and satellite retrieval. Flask samples were simulated using annual mean concentration from the model's planetary boundary layer (PBL), and satellite data were simulated as annual mean column mean concentrations. Gaussian "noise" of σ=1 ppmv was then added to the PBL values, and noise of various magnitudes was

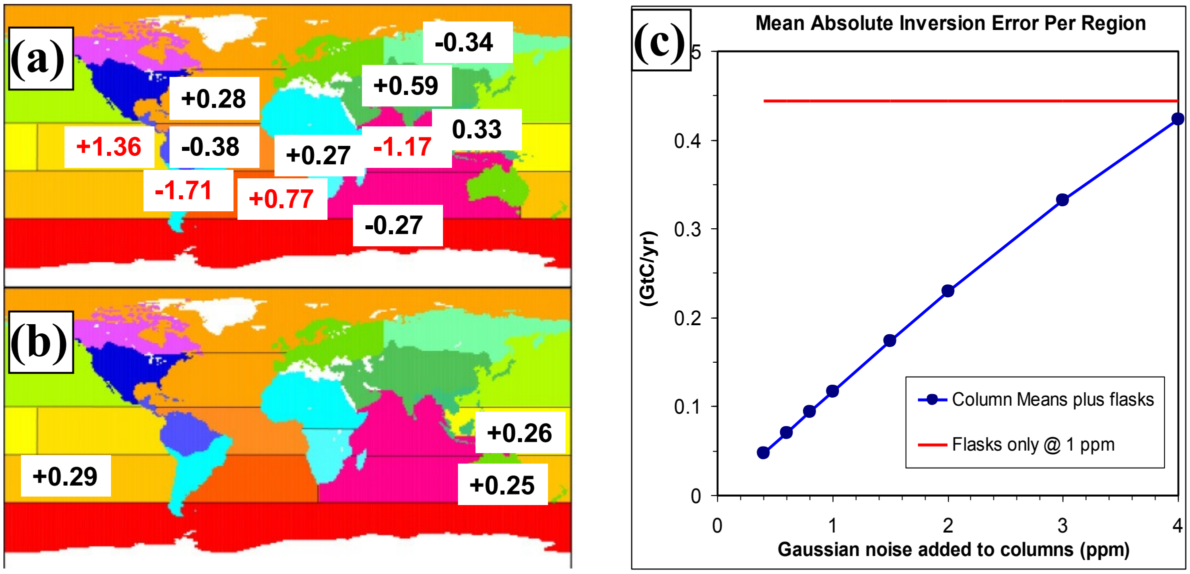

Figure 2: Errors in annual flux retrieved for each of 22 regions by transport inversion (a) using 67 NOAA surface flask stations sampled in the model PBL; (b) using column CO_2 pseudo-data. Gaussian noise with σ=1 ppm was added to both point and column data; regional errors less than 0.25 GtC/yr are not shown. (c) Average error in annual flux per region obtained by inverting flasks plus columns as a function of the standard deviation of Gaussian noise added to the column pseudo-data. For reference, the pink line shows the error for flask inversions alone using σ=1 ppm.

added to the column means to evaluate the effect of inaccurate retrievals. The combined “flask” and “satellite” samples were then used to estimate annual mean surface fluxes for 11 ocean and 11 continental regions by Bayesian synthesis inversion [*Enting et al, 1995*]. Error in the inferred surface flux was unambiguously evaluated for each region against the true flux, since these were prescribed.

The results of this simple observing system simulation experiment showed substantial improvement in the inferred sources and sinks relative to the flask-only case, even with very noisy column pseudodata (Fig 2). The flask-only inversions (Fig 2a and red line in Fig 2c) produced errors of more than 1 GtC yr^{-1} in several tropical regions, with unrealistic flux “dipoles.” With 4 ppmv of Gaussian noise added to the column measurements, very little extra information was obtained by the inversion, but as the error in the column pseudodata was reduced, the error in the inferred fluxes was dramatically reduced. For unbiased ubiquitous annual mean column CO_2 retrieval with a standard deviation of 1 ppmv, estimated fluxes for 19 of the 22 regions were within 0.25 GtC yr^{-1} of their true value (Fig 2b), with a mean absolute regional error of 0.12 GtC yr^{-1}.

Several important caveats must be emphasized with regard to the results shown in Fig 2. (1) The same transport model was used for both the “forward” and “inverse” parts of the calculation, which is analogous to inverting real atmospheric data with a “prefect” transport model. This is the reason the blue curve in Fig 2c approaches zero for zero noise, and is unrealistic. (2) The “error” added to the column data here is random and uncorrelated in space, whereas real satellite retrievals could suffer from spatially coherent errors related to clouds, water vapor, temperature structure, or other atmospheric properties. Any regionally coherent bias in the retrieval might be disastrous. (3) The pseudodata used here were true annual means based on hourly samples with no missing data. Real retrievals would be based on imperfect sampling due to clouds, viewing geometry, and orbital considerations. (4) These inversions were based on true column integrals, whereas actual retrievals from space would be associated with a weighting function that is unlikely to be uniform in the vertical. Most of the spatial structure in atmospheric CO_2 is in the PBL, but conceivable passive techniques for CO_2 estimation would probably be unable to "see" the PBL.

The somewhat surprising success of the pseudodata inversions shown here is due to the much larger number of observations in the satellite case than the 67 flask stations used. Even if the satellite data are of poor quality, the very large number of unbiased estimates in these simulations leads to a dramatic improvement in the flux inversion. These results compare only annual mean inversions for very large regions; very substantial improvement is also likely feasible for monthly mean flux estimation over smaller areas. Routine quantification of time-varying regional CO_2 exchange to 0.1 GtC yr^{-1} would change the nature of carbon cycle science. Such an improvement in the quality of the top-down constraint would enable meaningful hypothesis testing based on field measurements, process modeling, and "bottom-up" scaling with much greater confidence than is possible today.

A crucial aspect of any future carbon observing system using spaceborne sensors will be calibration and validation of the concentration retrievals. Continued high-quality analysis of flask samples will be imperative in this regard, but surface-only samples may insufficient, especially for a passive instrument whose weighting function does not include the PBL. Sampling and/or in-situ measurement from aircraft would be well-suited to pin down absolute concentrations, with spatial and temporal structure "filled in" from space. Measurements in the regional troposphere might also allow the extraction of information from synoptic-scale variations in space and time. The COBRA regional aircraft campaigns in August 2000 [S. Wofsy, personal communication] showed very strong, regionally coherent spatial patterns in CO_2 and other trace gas concentrations, for example, which could be interpreted quantitatively.

Making the most of ubiquitous CO_2 measurements from spaceborne and airborne platforms will require new approaches to inverse modeling. Previous studies have been based on very sparse, high-quality data, using "climatological" or very coarsely resolved transport. These surface flask data may soon be augmented with lower-quality estimates of atmospheric composition which are very dense in both space and time. Interpretation of these data may require much more detailed representation of actual atmospheric transport. Optimal extraction of surface exchanges will probably involve variation data assimilation [*Bengtsson and Shukla, 1988; National Research Council, 1991*]. One can imagine following CO_2 anomalies in evolving weather systems, and estimating surface fluxes from time rates of change in an airmass.

Project Objectives

We propose a series of observing system simulation experiments to investigate the feasibility of and requirements for future observing strategies. We will develop a pseudodata atmosphere in the CSU GCM including as much realism as possible (diurnal cycles, clouds, background spectral properties) to test these strategies. We will develop "nested" pseudodata at higher resolution (CSU RAMS) over selected regions to test aircraft observing strategies and their potential synergy with spaceborne sampling. We will develop algorithms for estimation of CO_2 from data already scheduled to be available in 2001 (AIRS) and 2003 (IASI). We will also investigate potential observing strategies (measurements, orbits) for possible future dedicated missions. Finally, we will develop and test new inverse methods within the model framework.

Observing System Simulation Experiments

Global modeling with the CSU GCM

Evaluation of new algorithms and sampling strategies will require the development of a pseudodata atmosphere that includes realistic distributions of CO_2, temperature, water vapor, and clouds. The model must also include self-consistent distributions of surface temperature, emissivity, and spectral reflectance. Exchange of CO_2 at the land surface is strongly diurnal, which could potentially introduce significant bias depending on satellite overpass times. The model pseudodata should therefore include realistic diurnal cycles of both CO_2 exchange and atmospheric transport.

The CSU GCM has been derived from the UCLA GCM over 20 years by David Randall and collaborators. Many changes have been made since the model left UCLA, including a new dynamical core and revised parameterizations of solar and terrestrial radiation, the planetary boundary layer, cumulus convection, cloud microphysical processes, and land-surface processes. Highly conservative finite differencing is performed in vorticity-divergence form on a unique geodesic grid [*Ringler et al, 2000; Randall et al, 2000*] eliminating the “pole problem.” Cloud microphysical processes include prognostic equations for three phases of water plus falling droplets and snowflakes and the transformations among them [*Fowler et al, 1996*]. Radiative transfer is based on [*Harshvardhan et al.,1989*] and is linked to the cloud microphysics. we are testing a new and more accurate radiation parameterization developed by Graeme Stephens and colleagues at CSU. The cumulus mass flux and the warming and drying of the free atmosphere due to cumulus convection are determined through the cumulus parameterization of [*Arakawa and Schubert, 1974*], as modified by [*Randall and Pan, 1993*]. Cumulus clouds can originate in any tropospheric layer [*Ding and Randall, 1998*].

The model is fully coupled to the land surface model SiB2 [*Sellers et al, 1996; Randall et al, 1996*] which includes a physiologically realistic interaction between the surface energy budget and photosynthetic carbon assimilation. It also includes prognostic calculation of the mixing ratio of atmospheric CO_2 based on prescribed emission scenarios and/or the carbon fluxes from SiB2, and has been shown to reproduce many aspects of the observed spatial and temporal variation of CO_2 [*Denning et al, 1996a,b*] and inert tracers [*Denning et al, 1999*]. The model is formulated terms of a modified sigma coordinate, in which the PBL top is a coordinate surface, and the PBL itself is identified with the lowest model layer [*Suarez et al, 1983; Randall et al, 1992*]. The mass sources and sinks for the PBL consist of large-scale convergence or divergence, turbulent entrainment, and the cumulus mass flux. Turbulent entrainment can be driven by positive buoyancy fluxes, or by shear of the mean wind in the surface layer or at the PBL top. This feature is a key to the model’s ability to simulate the CO_2 “rectifier” effect [*Denning et al, 1995, 1996b*].

The Simple Biosphere (SiB) Model, developed by [*Sellers et al, 1986*], has undergone substantial modification [*Sellers et al, 1996a*], and is now referred to as SiB2. The number of biome-specific parameters has been reduced, and most are now derived directly from processed satellite data [*Sellers et al, 1996b*] rather than prescribed from the literature. Another major change is in the parameterization of stomatal and canopy conductance used in the calculation of the surface energy budget over land. This parameterization involves the direct calculation of the rate of carbon assimilation by photosynthesis [*Farquhar et al, 1980*], making possible the calculation of CO_2 exchange between the global atmosphere and the terrestrial biota on a timestep of several minutes [*Denning et al, 1996a,b*]. Photosynthetic carbon assimilation is linked to stomatal conductance and thence to the surface energy budget and atmospheric climate by the Ball-Berry equation [*Collatz et al, 1991, 1992*]. Recent improvements include the introduction of a 6-layer soil temperature submodel based on the work of [*Bonan, 1996, 1998*], an explicit litter layer, and a revised surface energy budget that includes prognostic temperature and moisture in the canopy air space reservoir. We are adapting the surface parameterization to use continuous distributions of vegetation [*Defries et al, 1998, 1999a,b*]. Work is ongoing and proposed under separate support to define vegetation properties from EOS data [Asner *et al*, *1998a,b*] and soil texture using the new IGBP-DIS soils dataset [*Scholes et al, 1995; Bisher et al, 1999*]. Biogeochemical cycling in soils and litter and a new parameterization of seasonal plant growth are being implemented [*Kaduk et al, 1996; Friedlingstein et al, 1999*]. Particular strengths of SiB2 for this project include the treatment of carbon biogeochemistry and its links to surface energy budgets, the fact that the model has already been coupled to a suite of atmospheric models across a spectrum of spatial and temporal scales, and the ability to specify the vegetation parameters from globally-available satellite imagery. The coupled SiB2-GCM produced excellent agreement with the observed spatial and seasonal gradients, and is the only such global model that has yet been evaluated against local diurnal data [*Denning et al, 1996a,b*].

The specific tasks proposed for global observing system simulation experiments include

(i) *generate self-consistent 4-dimensional fields of atmospheric and surface properties (including CO_2) that could contribute to or interfere with the retrieval of CO_2 concentration from spaceborne sensors*

(ii) *archive relevant variables to large disk arrays every hour at every grid cell to facilitate rapid testing of retrieval algorithms and inversion methods*

(iii) *sample these variables according to actual or contemplated orbital paths for specific satellites. This strategy allows for masking of clouds, identification of diurnal or fair-weather bias in the retrievals, etc.*

(iv) *investigate algorithms for potential future dedicated CO_2 missions by testing different sampling strategies (e.g., influence of vertical weighting functions, polar versus high-inclination orbits, time of overpass for sun-synchronous orbits).*

Regional Modeling with CSU-RAMS

The CSU Regional Atmospheric Modeling System (RAMS) is a general purpose atmospheric simulation modeling system consisting of equations of motion, heat, moisture, and continuity in a terrain-following coordinate system [*Pielke et al. 1992*]. The model has flexible vertical and horizontal resolution and a large range of options that permit the selection of processes to be included (such as cloud physics, radiative transfer, subgrid diffusion, and convective parameterization). Two-way interactive grid nesting [*Walko et al. 1995*] allows for a wide range of motion scales to be modeled simultaneously and interactively. We have recently coupled RAMS to SiB2, and used the coupled model to investigate the influence of surface CO_2 exchange on the regional atmosphere. Figure 3 shows the simulated development of a CO_2-depleted mixed layer over the US upper Midwest during the course of a day and the subsequent decoupling of a stable surface layer enriched by ecosystem respiration.

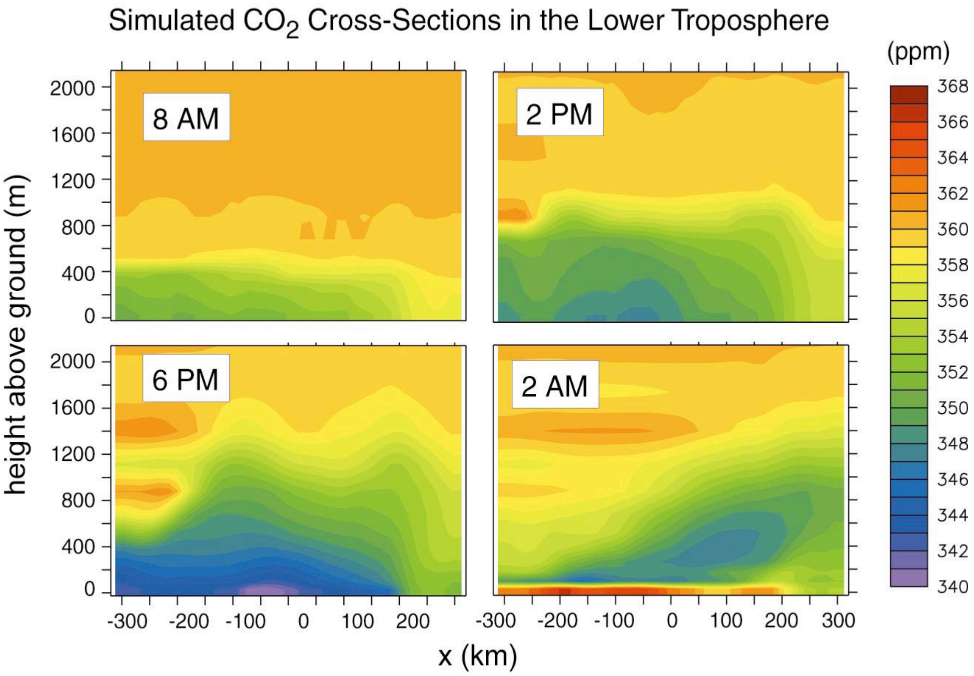

Figure 3: Diurnal evolution of atmospheric CO_2 as simulated by coupled SiB2-RAMS for a case in northern Wisconsin in July of 1997.

The first systems for quantifying CO_2 concentrations from space will have much lower precision and accuracy than existing laboratory analyses of flask samples. It is likely that tying regular sampling from aircraft could improve estimates of spatial and temporal variations in concentration by tying them to absolute standards. We will use the coupled SiB2-RAMS system to simulate mesoscale concentration fields over three continental areas: North America, tropical South America, and sub-Saharan Africa. North America is already the focus of intensive measurement campaigns (e.g., AmeriFlux, COBRA). It is likely to be preferentially sampled in future airborne missions because of its logistical advantages and interest by US government agencies. The tropical continents are currently the most poorly sampled regions in the world, and therefore contribute disproportionately to uncertainty in the distribution of carbon sources and sinks. Airborne measurements in these regions have the potential to substantially constrain carbon budgets on regional and global scales, with or without the context of spaceborne measurements.

The specific tasks proposed for regional observing system simulation experiments include

(i) *simulation of North America, tropical South America, and sub-Saharan Africa on a 40 km grid for an annual cycle. Lateral boundaries will be forced from NCEP analyses, surface properties will be prescribed from EOS data, and ecosystem carbon fluxes predicted on-line in SiB2*

(ii) *Sampling of the regional pseudo-data using satellite algorithms "virtual aircraft," and "virtual towers" to simulate various observing strategies*

(iii) *Evaluation of sampling schemes with respect to deep tropical convection by comparison of mesoscale experiments with cloud-resolving simulations of convective events*

Radiative Transfer Modeling and Algorithm Development

Here, we propose to explore the feasibility of retrieving atmospheric CO_2 concentrations from atmospheric infrared soundings likely to be available from space-borne instruments in the next several years. Two new infrared sounding instruments are currently being developed, the Atmospheric Infrared Sounder (AIRS) and the Infrared Atmospheric Sounding Interferometer (IASI). Both instruments will measure most of the infrared spectrum at high spectral resolution. IASI [*Diebel et al., 1996*] is a Michelson interferometer with a spectral resolution of 0.5 cm^{-1} in the spectral range between 645 and 2760 cm^{-1} and is expected to be launched on board of the first Meteorological Operational polar satellite (METOP) in 2003. AIRS [*Aumann and Miller, 1995*] is an echelle spectrometer that covers the spectral range between 650 and 2700 cm^{-1} with an average resolving power of 1200 and will be launched on board of EOS-Aqua in 2001. The satellites of both instruments will fly in sun-synchronous orbits providing 2 observations per day for each location on Earth (taking into account the cross-track scanning of the instruments).

The above 2 instruments have been designed to measure accurate temperature and water vapor profiles on a global scale, but their high spectral resolution observations offer great opportunities to measure other atmospheric gases as well. Two strong CO_2 absorption bands exist at 667 and 2350 cm^{-1}, respectively. The water vapor and CO_2 absorption spectra are shown in Figure 4a. In the past, these bands have been used to retrieve temperature profiles assuming a well-known atmospheric CO_2 concentration. However, with the above-mentioned high spectral resolution observations temperature, water vapor, and CO_2 can be retrieved simultaneously.

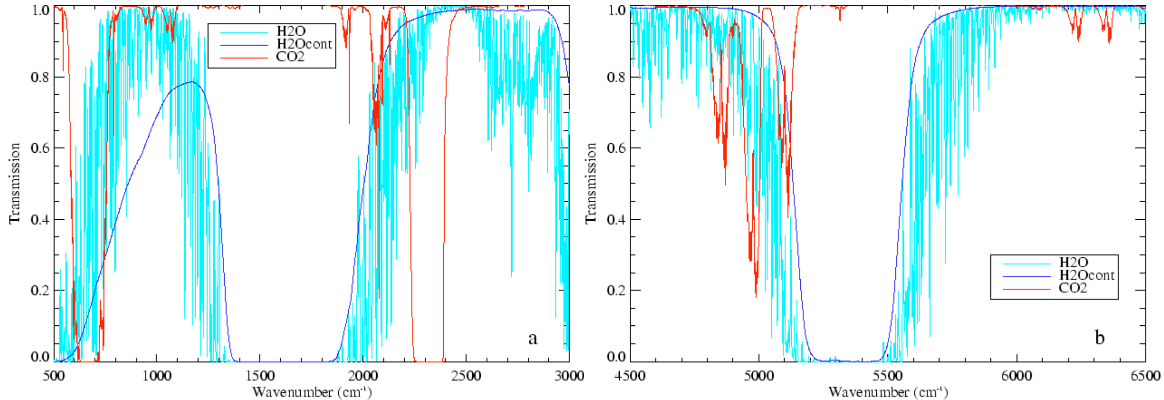

Figure 4. Absorption spectra of water vapor and carbon dioxide in the infrared (a) and near infrared (b) part of the spectrum.

Another technique to measure CO_2 that is being analyzed uses sunlight reflected in the near infrared (NIR). *Aoki et al. [1993]* describe a retrieval scheme that uses the reflected solar radiation in sun glint situations over oceans to retrieve several trace gases with high accuracy. In those situations the atmospheric contribution to the radiation observed at the top of the atmosphere is much smaller than the surface contribution and can therefore be neglected. This simplifies the radiative transfer considerably, which allows for accurate total column measurements of CO_2 and H_2O in the spectral region between 1.5 and 2.2 µm (4500 and 6500 cm^{-1}). Their absorption spectra in this spectral region are shown in Figure 4b. We propose to investigate the capabilities of this method not only in sun glint situations over ocean, but also over land. A key issue is the relative contribution of the atmospheric term in the radiative transfer with respect to the surface contribution.

Radiative transfer models and associated Jacobians

IR forward model and Jacobians

The model calculates the radiation at the top of the atmosphere for a given distribution of trace gases (CO_2, H_2O, O_3, N_2O, CH_4, and O_2) and temperature. Earlier versions of the model used to simulate TOVS/HIRS radiances are described by *Stephens et al. [1996]* and *Engelen and Stephens [1997]*. For the problem of relevance in this proposal, the equation for the monochromatic radiance (*I*) at the top of the atmosphere for a plane parallel non-refracted path in nadir view is

$$I = B(p_s)T_s + \int_{p_s}^{0} B(p)\frac{\partial T(p)}{\partial p}dp, \qquad (1)$$

where *B(p)* is the Planck radiance for the temperature at pressure level *p* and *T(p)* is the transmission from the top of the atmosphere to level *p*. To simulate the high spectral resolution radiance data the model uses a spectral integration ($\Delta\nu$) of 1 cm^{-1}. For this spectral band integration the Malkmus band model [*Malkmus, 1967; Goody and Yung, 1989*] was used, which expresses the transmittance as a function of pressure scaled absorber amount ($\tilde{u}$) and pressure ($\tilde{p}$) as:

$$T = \exp\left[-\frac{\pi\alpha_L\varphi}{2\delta\tilde{u}}\left(\sqrt{1+\frac{4S\tilde{u}^2}{\pi\alpha_L\varphi}}-1\right)\right] \qquad (2)$$

with

S = Average line intensity,

α_L = Average Lorentz line width,

δ = Average line spacing.

$\varphi = \tilde{u}\frac{\tilde{p}}{p_0}$

Broadband transmission is evaluated given suitable values of the band parameters α_L/δ and S/δ. These are obtained from line absorption data by requiring exact agreement in the weak-line and strong-line limits. Because the calculation from statistical line parameters provides band parameters that are not accurate enough [*Lacis and Oinas, 1991*], the Malkmus band model parameters were calculated by least squares fitting to HITRAN96 [*Rothman et al., 1998*] derived transmittances at a resolution of 1 cm^{-1} as a function of the optical path of the absorbers taking the statistical band parameters as a first guess. Individual absorption lines were cut off at 25 cm^{-1} to comply with the absorption continuum as defined by *Clough et al. [1989]*. Because the transmission is dependent on pressure through the pressure broadening of the absorption lines and on temperature through the line strength, the absorber amount and pressure are scaled according to the Van de Hulst-Curtis-Godson (HCG) parameterization [*e.g., Goody and Yung, 1989*] and the temperature effect is parameterized following *Rodgers and Walshaw [1966]*.

The Jacobian $\partial I / \partial q_i$, which is required for calculating the weighting function matrix, is obtained by calculating $\partial T_j / \partial q_i = -T_j \partial \tau_j / \partial q_i, j = i, N$ [*Garand et al., 1999*], where the surface is at level *N* and where there is no contribution from layers above *i*. The Jacobian follows analytically:

$$\frac{\partial \tau_j}{\partial q_i} = \frac{\pi \alpha_L}{2\delta \tilde{u}} \left[\sqrt{1 + \frac{4S\tilde{u}^2}{\pi \alpha_L \varphi}} - 1 \right] \left[\frac{\partial \varphi}{\partial q} - \frac{\varphi}{\tilde{u}} \frac{\partial \tilde{u}}{\partial q} \right] + \frac{S}{\delta \sqrt{1 + \frac{4S\tilde{u}^2}{\pi \alpha_L \varphi}}} \left[2 \frac{\partial \tilde{u}}{\partial q} - \frac{\tilde{u}}{\varphi} \frac{\partial \varphi}{\partial q} \right] \tag{3}$$

The Jacobian $\partial I / \partial T_i$ is obtained similarly, replacing $\partial \varphi / \partial q$ and $\partial \tilde{u} / \partial q$ with $\partial \varphi / \partial T$ and $\partial \tilde{u} / \partial T$, respectively. Most quantities are stored during the forward model run, making the calculation of the Jacobians very efficient.

The specific tasks proposed for forward IR radiative modeling include

(i) *Extend the fitting of band parameters to explicitly simulate the spectral response functions of future instruments (AIRS, IASI)*

(ii) *Evaluate the radiative transfer results of this study by comparing them with the radiative transfer of other existing codes being used for AIRS and IASI simulations*

NIR radiative transfer model

The radiative transfer model for the NIR retrievals is based on the work by *Gabriel et al. [2000]*. It is a very numerically efficient plane parallel atmosphere radiative transfer code that allows one to change the optical properties in a portion of the atmosphere (i.e. in one or more layers) without having to recompute all other layers whose optical properties remain the same. Therefore, Jacobians can be calculated extremely fast once a full forward calculation has been performed. This radiative transfer model is still under development, but will include full scattering, so the effect of aerosol and optically thin clouds can be simulated as well.

The specific tasks proposed for forward NIR radiative transfer modeling include

(i) *Fully develop the radiative transfer code to be used in the NIR CO_2 retrievals*

(ii) *Test the final radiative transfer code against other full scattering radiative transfer codes*

Retrieval method

The retrieval of atmospheric CO_2 from high spectral resolution radiance measurements is based on optimal estimation theory as described by *Rodgers [1976]*. An observation can be described as

$$y = F(x, b) + \varepsilon_y \tag{4}$$

where *y* is the observation vector of spectral radiances, *x* is the state vector one wants to retrieve including the CO_2 content, *F(x,b)* is the forward 'real world' model that links the state vector to the observation vector, b are all parameters that affect y but are not contained in x, and ε_y is the observational error.

For the characterization of the retrieval errors we linearize about the real atmospheric state x and the real model parameters b.

$$y(\hat{x},\hat{b}) = F(x,b) + \frac{\partial F}{\partial x}(\hat{x}-x) + \frac{\partial F}{\partial b}(\hat{b}-b) + \varepsilon_y \tag{5}$$

where the estimated state vector and model parameters are denoted by $\hat{x}$ and $\hat{b}$, respectively. The sensitivity of the radiances to deviations in the atmospheric profiles and the model parameters are thus described by $\partial F / \partial x$ (often called weighting functions K) and $\partial F / \partial b$, respectively.

The inverse model I describes how the retrieved state vector is obtained from the measurements. The linearized equation for the inverse model is

$$\hat{x} = I(y,b) + \frac{\partial I}{\partial y}(\hat{y}-y) + \frac{\partial I}{\partial b}(\hat{b}-b) \tag{6}$$

The sensitivity of the retrieved state vector to measurement errors, $\partial I / \partial y$, is called the contribution function $D_{y.}$

Because the inversion of the forward model is often very sensitive to noise (expressed by large values in the D_y-matrix), some constraint is needed on this inversion to obtain the optimal solution. Rodgers (1976) describes an optimal estimation technique in which a priori profiles are used as *virtual* measurements. The optimal (assuming Gaussian error statistics) solution is then obtained by minimizing the following cost function:

$$\Phi = (\hat{x}-x)^T S_a^{-1}(\hat{x}-x) + (y-F(\hat{x}))^T S_y^{-1}(y-F(\hat{x})) \tag{7}$$

where x_a is the a priori profile and S_a and S_y are the error covariance matrices of the a priori data and the forward model including measurement errors, respectively. The minimization results then in

$$\hat{x} = x_a + S_a K^T S_y^{-1}(y-F(\hat{x})) \tag{8}$$

The covariance matrix of the retrieved state vector can be written as

$$S_x = (S_a^{-1} + K^T S_y^{-1} K)^{-1} \tag{9}$$

Following Rodgers (2000), we can express the retrieved state vector as a linear combination of the real state vector and the a priori state vector

$$\hat{x} = Ax + (I-A)x_a + D_y K_b(\hat{b}-b) + D_y \varepsilon_y \tag{10}$$

with

$$A = D_y K_x \tag{11}$$

The rows of the matrix A are called the averaging kernels of the retrieval and describe the sensitivity of the retrieval to the real profile. They also are a measure of the vertical resolution of the retrieval by means of their width and overlap.

For the high spectral resolution infrared retrievals the state vector x consist of the temperature profile, the water vapor profile, the CO_2 profile or a CO_2 column amount, and possibly the O_3

profile or O_3 column amount. Retrieval simulations will be carried out using the above described retrieval theory. Error statistics will then be generated that allow us to study the effect of all error sources on the final retrieval product. Preliminary simulation showed that retrieval errors for a tropospheric CO_2 column retrieval are less than 2 ppmv, as shown if Figure 5.

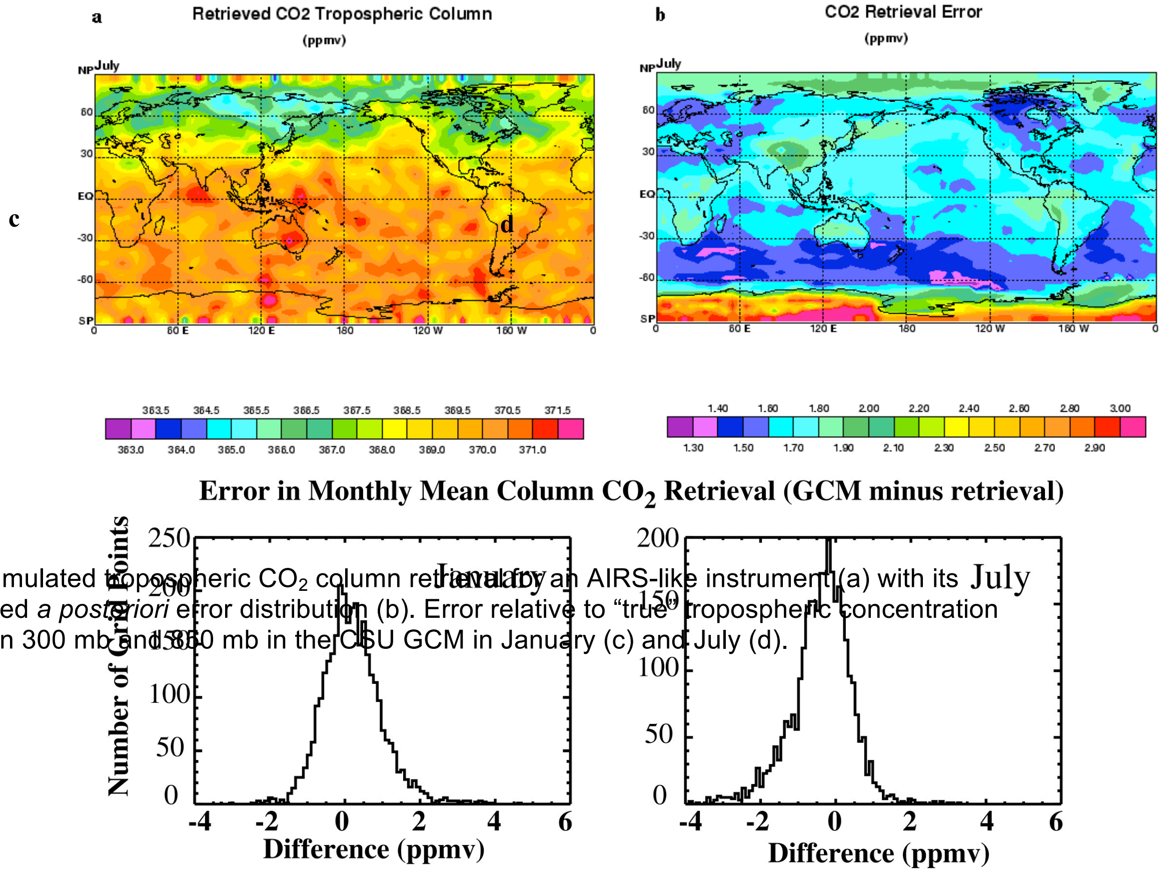

Figure 5. Simulated tropospheric CO_2 column retrieval for an AIRS-like instrument (a) with its estimated *a posteriori* error distribution (b). Error relative to "true" tropospheric concentration between 300 mb and 850 mb in the CSU GCM in January (c) and July (d).

Special attention will be paid to the effect of a priori constraints on the retrieval product. Using information theory concepts described by *Rodgers [2000]*, we also propose to study the possible improvements that can be made by using higher spectral resolution observations. The same information theory concepts can also be used to look at the optimal selection of channels in order to optimize the retrieval scheme.

Specific tasks proposed for CO_2 retrieval from IR data include

(i) *Perform sensitivity studies to estimate the accuracy of CO2 retrievals*

(ii) *Estimate the dependence of the retrieval on a priori information*

(iii) *Make recommendations for the use of additional observations to improve the retrieval performance*

(iv) *Use information theory to study the effect of spectral resolution on the retrieval and to optimize the retrieval scheme.*

(v) *Study the effect of the satellite sampling and the impact of the retrievals on the inverse CO_2 modeling (see following section)*

(vi) *Communicate our results with the AIRS team (see attached email from M. Chahine), and work with them to facilitate actual retrievals*

For the near infrared retrievals the state vector will initially consist of the CO_2 column amount. The retrievability of CO_2 profiles from these observations and possible other atmospheric information (e.g., H_2O and aerosol) will be considered as well.

The specific tasks proposed for CO_2 retrieval from NIR data include

(i) *Perform sensitivity studies for NIR retrievals over sea glint and high reflecting land surfaces in order to estimate the possible accuracy of these retrievals*

(ii) *Estimate the effect of aerosol on those CO_2 retrievals*

(iii) *Develop requirements for a satellite instrument capable to perform NIR CO_2 retrievals*

(iv) *Investigate the retrieval of vertical profiles of CO_2 from a "merged" product using both IR and NIR observations*

A priori data

Key in any satellite retrieval is the use of a priori data to somehow constrain the ill-posed problem. In case of the CO_2 retrievals in which the information content is low, it is crucial to have accurate a priori data and especially accurate a priori error statistics. For the infrared retrievals we propose to use forecast model temperature and water vapor profiles as a constraint for the temperature and water vapor profiles and CO_2 flask data to constrain the CO_2 concentrations. Several global forecast models do exist (DAO, NCEP, ECMWF) that can provide temperature and water vapor profiles with an estimated error of 1K and 20%, respectively [e.g., *Derber and Bouttier, 1999*]. CO_2 flask measurements have been carried out for years and could provide accurate monthly and zonal mean a priori data to be used in the retrievals.

The specific tasks proposed for development of a priori data include

(i) *Define the optimal a priori data sets for the infrared and near infrared CO2 retrievals*

(ii) *Estimate the impact of the a priori information on the final retrieval product*

Inverse Methods for Surface Flux Estimation

In the sort of data-rich world envisioned by the observing system simulation experiments proposed here, inversion of time-mean spatial patterns using "climatological" wind fields will probably be insufficient to extract available information about surface fluxes. We propose to develop and test several inversion methods within the framework of the global and continental pseudo-data fields described above.

At the global scale, we will estimate monthly surface fluxes for about 50 regions using Bayesian synthesis inversion [*Tarantola, 1987*] to recover the magnitudes of "pulses" of tracers released from each region for one month at a time [*Bousquet et al, 2000*]. The pulses will be tracked as Green's functions through atmospheric mixing until they are nearly uniform in space, and linear combinations of these will be used to fit the "observations" simulated using satellite algorithms, aircraft sampling, and tower-based approaches. The "forward" atmospheric transport simulation of each Green's function will be performed with both the CSU GCM and the MATCH transport model [*Rasch et al, 1997*], driven by GCM winds. The CSU GCM inversion is analogous to inverting real data using a "perfect" transport model (the same model is used to generate the pseudodata and transport the basis pulses). This will allow us to isolate the effects of the satellite algorithms and aircraft sampling strategies. The MATCH experiment will be more realistic in that an imperfect representation of atmospheric transport is inevitable. The Bayesian synthesis approach requires the use of prior estimates of regional fluxes, including their spatial structure, diurnal variability, and uncertainties. We propose to develop these a priori estimates using SiB2 driven by observed climate (NCEP analyses), using vegetation parameters derived from MODIS, ASTER, and other EOS data products.

The synthesis inversion approach requires a large number of forward transport simulations (12 months per year times *N* regions for which flux will be estimated). As the data constraint becomes more dense (with improved satellite retrievals and more airborne sampling), this may be computationally prohibitive at the global scale. At the regional scale, it is almost certainly untenable. We propose to test an alternative methods for data assimilation of CO_2 [*Bruhwiler et al, 2000*] which involves forward simulation with "known" fluxes followed by periodic correction of fluxes to match observations. This technique allows the inversion to focus on a rolling "window" in time, with repeated simulations of each time interval for which the observations are aggregated. Realistic forward modeling of the fluxes using SiB2 and EOS data are expected to improve the results of this method substantially. This method be tested for both global and regional experiments.

Finally, regional airborne sampling strategies will be evaluated using a new method based on Lagrangian particle dispersion analysis [*Uliasz, 1994, 2000; Uliasz et al, 1996*]. In this technique, imaginary particles are released at the surface into the transport model at every time step, and they are tracked as they advect and convect with the flow. Any atmospheric sample is then associated with a population of these particles, making it possible to track the conditional probability that an airmass last interacted with the surface at any given location. These "influence functions" are then treated as "basis functions" in a synthesis inversion, and the flux is optimized to produce the best agreement with the observed variations of CO_2 concentration in the

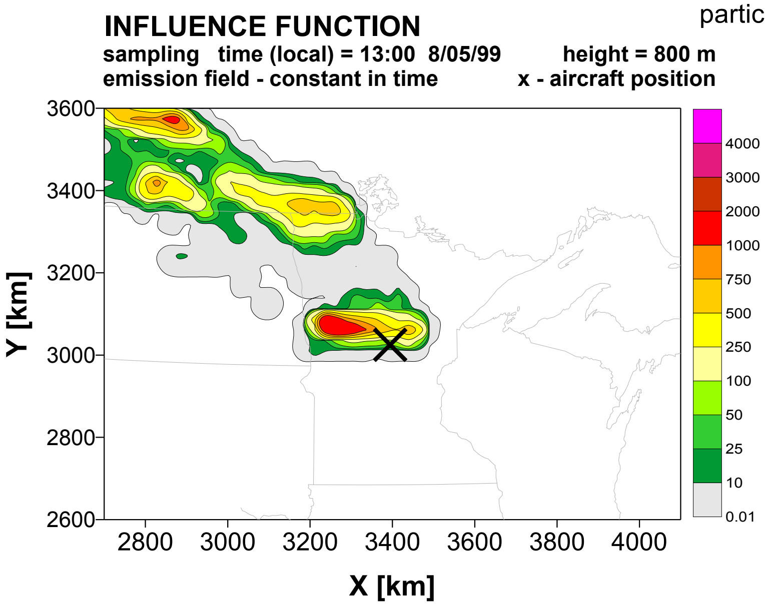

Figure 6: Influence function for an aircraft sample, derived from NCEP RUC analysis on a 40 km grid by Lagrangian particle dispersion modeling.

atmosphere. This technique has the advantage of being quite tractable for regional flows, and we expect it to help us evaluate strategies for combining aircraft with satellite observing strategies.

The specific tasks proposed for development and testing of inverse methods include

(i) *Perform global Bayesian synthesis inversion on monthly "pulsed" basis functions using transport from the CSU GCM and MATCH [Bousquet et al, 2000]*

(ii) *Develop global and regional CO_2 data assimilation methods using realistic boundary forcing with successive correction [Bruhwiler et al, 2000]*

(iii) *Use Lagrangian particle dispersion analysis to evaluate strategies for synergistic combinations of satellite and airborne sampling [Uliasz et al, 2000]*

Work Plan

In year 1 of the project, we will define the parameters of the forward flux calculation and create an archive of 4-D pseudo-data fields to be sampled and analyzed. We will use the forward IRT and NIR radiative transfer models to estimate top-of-the-atmosphere radiance in AIRS bands, and develop retrieval algorithms to estimate CO_2.

In year 2, we will use the CSU GCM and MATCH to perform global-scale Bayesian synthesis inversions on the retrievals from the RT algorithms, and analyze their effectiveness. We will also perform the regional simulations of North America, tropical South America, and sub-Saharan Africa using the coupled SiB2-RAMS system, and evaluate the results.

In year 3, we will develop and test inverse methods at higher resolution, including the data assimilation and Lagrangian influence function methods. We will communicate our results with instrument development teams (see attached letters of collaboration). If available, we will test our CO_2 retrieval algorithms using real AIRS data, and estimate surface fluxes from them.

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