

Assimilation, Surface Flux Estimation, and Error Analysis of Atmospheric CO₂ Observations from Space Using a Comprehensive Modeling System

Abstract

We propose to analyze GOSAT/Tanso data using a combination of existing models of CO₂ exchanges due to hourly photosynthesis and respiration (Baker et al, 2008), daily air-sea gas exchange (Doney et al, 2009), biomass burning (GFED, Randerson et al, 2007), Fossil Fuel Emissions (Gurney et al, 2009), and atmospheric transport (PCTM, Kawa et al, 2004). This comprehensive system allows direct comparison to the observed record of both in-situ and remotely sensed atmospheric CO₂ at hourly timescales. We have previously demonstrated that a lower-resolution version of the system has good skill at replicating diurnal, synoptic, and seasonal variations over vegetated land surfaces (Parazoo et al, 2008). The analysis system will be operated on a 0.5° x 0.67° grid ($\Delta x \sim 50$ km), providing global mesoscale coverage. The system is driven by meteorological output from the NASA Goddard EOS Data Assimilation System, version 5. Surface weather from the system drives calculations of terrestrial ecosystem metabolism (radiation, precipitation, humidity, temperature) and air-sea gas exchange (wind), with other input data coming from satellite data products (e.g., fPAR and LAI from MODIS, and ocean color from SeaWiFS and MODIS).

The result will be estimates of time-varying surface sources and sinks of CO₂ that are optimized with respect to in-situ flask and continuous CO₂ observations, TCCON data, GOSAT/Tanso retrievals, MODIS data, emissions inventories, and mechanistic models. We will use the modeling and analysis system (1) as a “smart interpolator” of non-satellite CO₂ observations that can be used to estimate systematic errors in GOSAT retrievals; (2) to map and interpret sources and sinks; (3) to quantify the effect of systematic errors in spectroscopic retrievals on source/sink estimates; and (4) to establish detection criteria for fossil fuel emissions.

1. Introduction

Despite the loss of the Orbiting Carbon Observatory (OCO) in February 2009, the global carbon cycle research community has been actively developing improved systems for analysis of carbon cycle data. The in-situ CO₂ observing network continues to expand (especially with respect to continuous observations). The Total Column Carbon Observing Network (TCCON) measures column abundances of CO₂ and other greenhouse gases using upward-looking Fourier Transform Spectrometers. Japan’s Greenhouse Gases Observing Satellite (GOSAT) is collecting data on atmospheric CO₂ column abundance, though at somewhat lower precision than was planned for OCO. A network of nearly 500 sites now reports hourly CO₂ exchanges with terrestrial ecosystems and air-sea gas exchange is estimated using in-situ observations, remote sensing of ocean color, and numerical modeling. Fossil fuel emissions are estimated with increasing

fidelity at high resolution in space and time using a combination of traditional inventories, remote sensing, spatial data, and demand modeling.

We propose to use a comprehensive forward modeling system to simulate variations of atmospheric CO₂ globally using mechanistic descriptions of sources, sinks, and transport processes. A combination of in-situ and remotely-sensed CO₂ observations will then be assimilated into the system to optimize source/sink estimates. The resulting CO₂ analysis product (along with comprehensive error covariance statistics) will then be analyzed to provide information about spatially coherent biases in the GOSAT products, and to help in the design of future spaceborne CO₂ measurements.

2. Model Descriptions

2.1. Simple Biosphere Model (SiB)

We propose to use the Simple Biosphere model (SiB), which is based on a land-surface parameterization scheme originally used to compute biophysical exchanges in climate models (Sellers et al., 1986), but later adapted to include ecosystem metabolism (Sellers et al., 1996a; Denning et al., 1996a). The parameterization of photosynthetic carbon assimilation is based on enzyme kinetics originally developed by Farquhar et al. (1980), and is linked to stomatal conductance and thence to the surface energy budget and atmospheric climate (Collatz et al., 1991, 1992; Sellers et al., 1996a; Randall et al., 1996). The model has been updated to include prognostic calculation of temperature, moisture, and trace gases in the canopy air space, and the model has been evaluated against eddy covariance measurements at a number of sites (Baker et al., 2003; Hanan et al., 2004; Vidale and Stöckli, 2005). Revised treatment of root zone hydrology and physiological stress has resulted in improved simulation of the seasonality of transpiration, photosynthesis, and ecosystem respiration at tropical sites in the Amazon (Baker et al., 2008) and Africa (Williams et al., 2007). Other recent improvements include biogeochemical fractionation and recycling of stable carbon isotopes (Suits et al., 2005), improved treatment of soil hydrology and thermodynamics, and the introduction of a multilayer snow model based on the Community Land Model (Dai et al., 2003). Direct-beam and diffuse solar radiation are treated separately for calculations of photosynthesis and transpiration of sunlit and shaded canopy fractions, using algorithms similar to those of DePury and Farquhar (1997). The model is now referred to as SiB3.

Until recently, ecosystem respiration was treated in SiB by scaling a temperature and a moisture response to achieve net carbon balance at every grid cell in one year by prescribing the size of a single pool of organic matter. This approach has recently been replaced by a scheme for allocation, transformation, and decomposition based on the Carnegie/Ames/Stanford Approach (CASA, Randerson et al., 1997). Stored photosynthate is allocated to leaves, stems, and roots in fractions that are constrained by changes in satellite vegetation index (NDVI). Carbon is tracked through biomass pools and released to the surface as dead litter, woody debris, and root litter, where it interacts with a microbial pool to produce several pools of soil

organic matter and CO₂. The interactive biogeochemistry module has been tested at dozens of eddy-covariance sites and found to improve simulations of the seasonal cycle of net ecosystem exchange relative to the single-pool model it replaces (Schaefer et al, 2008). Following previous work with CASA (van der Werf et al, 2006), we also plan to add a fire module to this model. The incorporation of the fire module is partly supported by NASA through a subcontract from Goddard Space Flight Center.

Historically, SiB has used prescribed vegetation parameters derived by remote sensing (Sellers et al., 1996b). At global scales, this approach allows realistic simulation of spatial and temporal variations in vegetation cover and state (Denning et al., 1996; Schaefer et al., 2002, 2005). At the underlying pixel scale, however, phenology products derived from satellite data must be heavily smoothed to remove dropouts and artifacts introduced by frequent cloud cover. An inevitable trade-off between cloud-induced “noise” in the leaf area and time compositing systematically stretches the seasonal cycle by choosing data late in each compositing period in spring, and early in each composite in fall. We have addressed this problem by developing and testing a prognostic phenology module for SiB (Stockli et al, 2008). We have assimilated vegetation imagery into the prognostic phenology model to estimate its parameters (e.g., growing degree day thresholds), rather than forcing it with the satellite data.

We have developed and testing an explicit treatment of phenology and physiology of agricultural crops, and parameterized of the crop model using data from flux towers, experimental farms, and agricultural databases (Lokupitiya et al, 2009). The model represents fluxes from multiple sub-grid scale “tiles” (e.g., corn, soy, wheat, pasture), and the revised model matches observed fluxes, leaf-area, and grain yield much better than the control (Corbin, 2008).

2.2. Global Fire Emissions Database (GFED)

Emissions of CO₂ due to biomass burning will be specified using the Global Fire Emissions Database (GFED v2.1, Randerson et al, 2007). The 8-day emissions data set was compiled using satellite data and the Carnegie-Ames-Stanford Approach (CASA) biogeochemical model. Burned area from 2001-2004 was derived from active fire and 500-m burned area data from MODIS (Giglio et al., 2006). ATSR (Along Track Scanning Radiometer) and VIRS (Visible and Infrared Scanner) satellite data were used to extend the burned area time series back to 1997 (Arino et al., 1999; Giglio et al., 2003; Van der Werf et al., 2004). Fuel loads and net flux from terrestrial ecosystems were estimated as the balance between net primary production, heterotrophic respiration, and biomass burning, using time varying inputs of precipitation, temperature, solar radiation, and satellite-derived fractional absorbed photosynthetically active radiation. Tropical and boreal peatland emissions were also considered, using a global wetland cover map (Matthews and Fung, 1987) to modify surface and belowground fuel availability.

2.3. Ocean Circulation and Biogeochemistry

Air-sea gas exchange will be a multi-decade (1979–2004) hindcast experiment conducted with the Community Climate System Model (CCSM-3) ocean carbon model (Doney et al, 2009). The CCSM-3 ocean carbon model incorporates a multi-nutrient, multi-phytoplankton functional group ecosystem module coupled with a carbon, oxygen, nitrogen, phosphorus, silicon, and iron biogeochemistry module embedded in a global, three-dimensional ocean general circulation model. The model is forced with physical climate forcing from atmospheric reanalysis and satellite data products and time-varying atmospheric dust deposition. Data-based skill metrics have been used to evaluate the simulated time-mean spatial patterns, seasonal cycle amplitude and phase, and subannual to interannual variability. Evaluation data include: sea surface temperature and mixed layer depth; satellite-derived surface ocean chlorophyll, primary productivity, phytoplankton growth rate and carbon biomass; large-scale climatologies of surface nutrients, $p\text{CO}_2$, and air–sea CO_2 and O_2 flux; and time-series data from the Joint Global Ocean Flux Study (JGOFS).

2.4. Atmospheric Tracer Transport (PCTM)

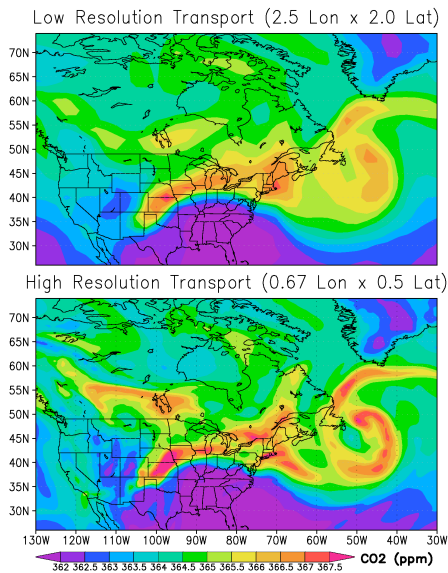


Figure 1: Simulated X_{CO_2} for March 5, 2004 using two different grids

The Parameterized Chemistry Transport Model (PCTM) will be used for forward global simulations of CO_2 transport (Kawa et al., 2004; Parazoo et al, 2008). This provides a diagnostic tool for studying synoptic interactions among weather and surface CO_2 flux. Transport fields will be provided by the NASA Goddard EOS Data Assimilation System, version 5 and include 6-hourly analyzed winds, temperatures, and convective/diffusive parameters for off-line transport (Rienecker et al., 2008). The GEOS-5 atmospheric general circulation model maintains the finite-volume dynamics (Lin, 2004) used for GEOS-4 and found to be effective for transport in the stratosphere and troposphere. The physical parameterizations include four major groups of processes and their submodules: moist processes, radiation, turbulent mixing, and surface

processes. Moist convective mass flux is calculated with a relaxed Arakawa-Schubert scheme (Moorthi and Suarez, 1992). Subgrid scale vertical processes also include a turbulent mixing scheme. GEOS-5 uses a new grid point statistical interpolation assimilation method that is a three-dimensional variational analysis applied in grid-point space.

CO2 Data Assimilation and Error Estimation

The comprehensive forward modeling system has been tested for multiyear simulations on both a $2^\circ \times 2.5^\circ$ (latxlon) and $0.5^\circ \times 0.67^\circ$ grid, driven by both GEOS-4 and GEOS-5 analyses (Figs 1 and 2). Synoptic variability is very well simulated on

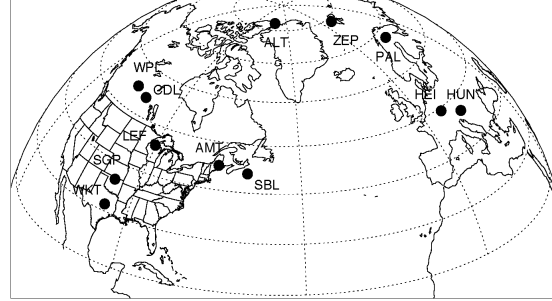
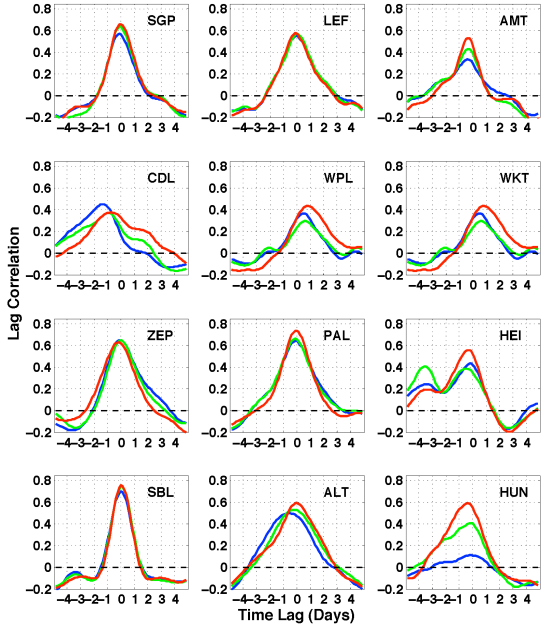


Figure 2: Lagged correlation analysis of synoptic variations of simulated and observed CO₂ at 12 in-situ stations (locations shown above). Abscissa is time lag (days). Blue is driven by GEOS-4 at $2^\circ \times 2.5^\circ$, green uses GEOS4 at $1^\circ \times 1^\circ$, and red uses GEOS-5 at $0.5^\circ \times 0.67^\circ$

the high-resolution grid, providing global mesoscale coverage and excellent fidelity to day-to-day variations observed at in-situ stations (Fig 2).

Global Flux Estimation by Ensemble Data Assimilation

We will use the component models described above to obtain an improved analysis of global sources and sinks of CO₂ at regional scales. For the first time, this analysis will include mechanistic treatment of all components of the carbon cycle (fossil fuels, air-sea gas exchange, biomass burning, photosynthesis, and respiration) and their error covariances, constrained by multiple data streams.

We will separate the well-understood “fast” processes driven by environmental forcing (temperature, solar radiation, precipitation, wind speed) from “slow” processes driven by less-understood biases in biogeochemistry and emissions. The total flux of CO₂ to the atmosphere from any grid cell at any time can be written as:

$$\begin{aligned}
 F_T(x,y,t) = & \beta_{FF}(x,y)FF(x,y,t) + \beta_{Fire}(x,y)Fire(x,y,t) \\
 & + \beta_{RESP}(x,y)RESP(x,y,t) - \beta_{GPP}(x,y)GPP(x,y,t) \\
 & + \beta_{Ocean}(x,y)Ocean(x,y,t)
 \end{aligned}
 \tag{EQ 1}$$

where x and y denote the spatial coordinates and t represents the time, which is at hourly resolution. Here FF , $Fire$, $RESP$, GPP , and $Ocean$ refer to the hourly gridded flux estimates described above. The β 's represent persistent multiplicative biases in the grid-scale component fluxes. A persistent bias in photosynthesis might result

(for example) from underestimation of available nitrogen, forest management, or agricultural land-use, whereas a persistent bias in respiration might result from overestimation of soil carbon or coarse woody debris. Sub-daily variations in the simulated component fluxes respiration and GPP are primarily controlled by the weather (especially changes in radiation due to clouds and the diurnal cycle of solar forcing), whereas seasonal changes are derived from phenological calculations parameterized from satellite imagery. Fine scale spatial variations are driven by changes in vegetation cover, soil texture, and soil moisture. It is reasonable to assume that the biases vary much more slowly than the fluxes themselves. Our method allows for component fluxes to vary on hourly, synoptic, and seasonal time scales, but assumes that biases in these fluxes persist for a period of approximately 2 months.

Optimization of the bias vector is accomplished using the Maximum Likelihood Ensemble Filter (MLEF, Zupanski, 2005; Zupanski et al, 2007; Lokupitiya et al, 2008). Important advantages of the MLEF are (1) that it can operate on fully mechanistic forward models of the component fluxes without requiring the derivation of their adjoints, and (2) it can be efficiently integrated in parallel on large computer clusters. The outcome of this calculation will be time-resolved maps of CO₂ sources and sinks at grid scale with mechanistic attribution that also optimally match observations of many kinds. Additionally, the MLEF will allow us to quantify uncertainty in sources and sinks.

We have tested the ensemble assimilation system using synthetic OCO data. Multiplicative biases (b) were specified to represent reasonable spatial patterns associated with CO₂ fertilization, atmospheric nitrogen deposition, forest regrowth, boreal growing season changes, and a saturating sink in the Southern Ocean. Random grid-scale perturbations were added to each of these biases in each month, and synthetic CO₂ data were created. Atmospheric columns were then sampled along the OCO orbit and masked for subgrid-scale clouds using NCEP-2 reanalyses. The resulting observation density is shown in Fig 3.

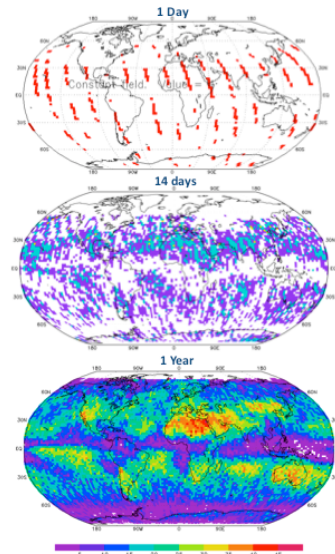


Figure 2: Sampling density for OSSE

A constant prior bias of $\beta(x,y,t)=0.0$ was assumed for all flux components, and new biases were estimated every month, with covariance propagation. Resulting fluxes were well-estimated (Fig 4) with excellent reduction of uncertainty over land. Ocean fluxes were somewhat less well-determined, due to the weaker fluxes there (Fig 5). One advantage of the MLEF system is that we are able to “post-aggregate” fluxes and their uncertainties a posteriori using the error covariance statistics that result from the optimization. Doing this shows excellent retrieval of annual fluxes over

TransCom regions (Fig 6). Note that prior fluxes over all land regions were precisely zero due to the net annual balance architecture of SiB.

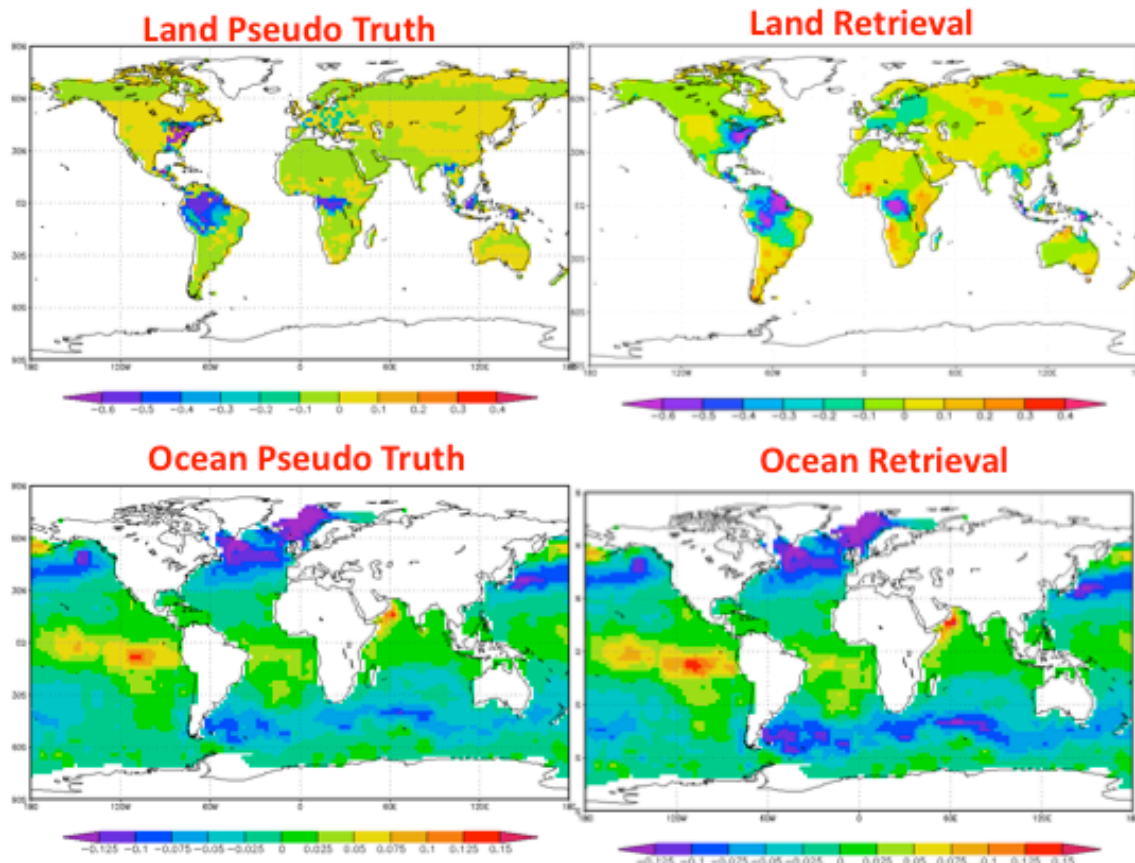


Figure 3: "True" and estimated fluxes ($\mu\text{Mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}$) recovered in OSSE

3. Specific Research Activities Proposed

3.1. Error analysis of GOSAT Level 2 CO₂ products

We propose to use our modeling system (SiB + CASA + GFED + FF + Ocean + GEOS5/PCTM) as a "smart interpolator" of the TCCON and in-situ observations, and use resulting model output to evaluate GOSAT L2 product. Specifically, we will analyze the flask sampling plus continuous in-situ plus TCCON observations using our ensemble data assimilation system. This will produce a global *a posteriori* estimate of atmospheric CO₂ which is available everywhere and optimized with respect to available non-satellite observations. The analysis system also produces error covariance statistics for every estimated CO₂ value.

We will then sample this CO₂ analysis to estimate column CO₂ (with an associated error estimate) for every GOSAT L2 retrieval, which we will compare to the actual satellite retrievals. Of course, the analyzed product cannot be considered the truth, but it should be considered a comprehensive interpolation of available observations using mechanistic process-based models.

We will then analyze the differences between our analyzed CO₂ product and the GOSAT L2 retrievals, focusing especially on spatial and seasonal patterns in model-

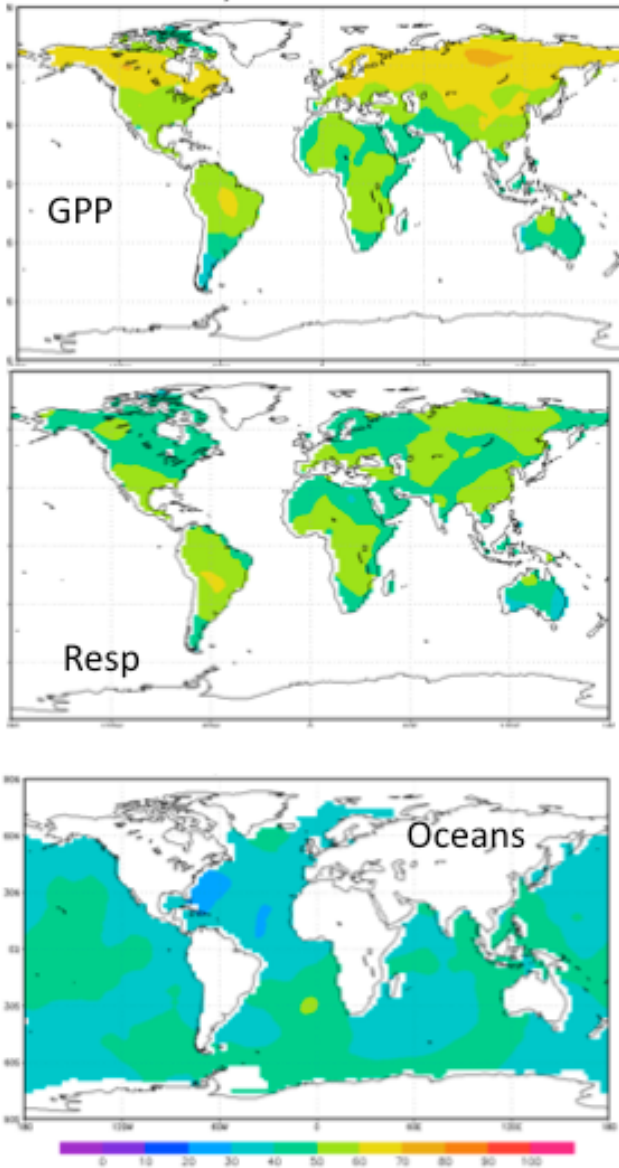


Figure 4: Uncertainty reduction (percent) relative to prior for OSSE

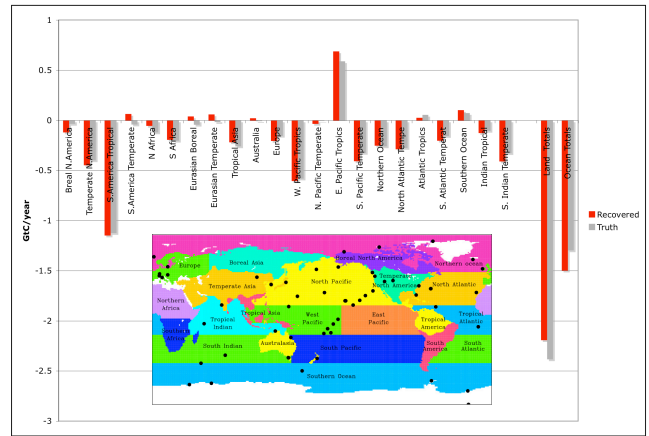


Figure 6: Post-aggregated flux estimates by TransCom region for OSSE compared to pseudo truth (inset shows regions). Note all land (but not ocean) priors were zero.

satellite differences. These will be interpreted in terms of aerosol optical depth, the presence and character of subpixel-scale cloud, atmospheric path length, solar illumination, surface albedo, and viewing angle effects that may introduce systematic error into the GOSAT retrieval.

Finally, this phase of the research will include close collaboration with the rest of the retrieval community in characterization of both random and systematic errors in retrieved column CO₂, to allow unbiased source/sink retrieval by transport inversion.

3.2. Comprehensive source/sink retrieval and analysis

We will assimilate the available in-situ, TCCON, and GOSAT L2 data into our comprehensive forward modeling system, optimizing the variable multiplicative bias terms (Eq 1). This will yield obtain time-varying maps of GPP, ecosystem respiration, fossil fuel emissions, biomass burning emissions, and air-sea gas exchange on a ~ 50 km grid globally on an hourly basis. These time-varying maps will be made available online for other researchers to use, and will be compared in detail with other estimates and analyses. These estimates will also be compared through the inversion intercomparison project proposed by David Baker and his colleagues, assuming that activity receives support. Otherwise we will seek to establish intercomparison through the international TransCom activities, with which the PI has been closely involved for the past 15 years.

Source/sink estimates will be evaluated against inventory data, aircraft observations, flux towers, and other available data sets. Interpretations of patterns in sources and sinks (for example, by in response to interannual climate variations) will be conducted as part of the larger carbon cycle community.

3.3. Impact of realistic satellite retrieval errors on source/sink estimates

We will use MLEF inversions of synthetic observations to investigate the potential impact of realistic patterns of spectroscopic retrieval errors on errors in sources and sinks. Mechanistic patterns of time- and space-varying sources and sinks (e.g., due to CO₂ fertilization, nitrogen deposition, forest regrowth, melting permafrost, or changes in ocean circulation) will be prescribed in the forward modeling system to obtain corresponding synthetic CO₂ observations. These will then be perturbed by assumed spectroscopic errors in column CO₂ due to atmospheric aerosol, subpixel-scale cloud, viewing angle, surface albedo, and other likely sources of satellite retrieval error. These incorrect synthetic observations will then be used in the MLEF system to estimate bias fields (Eq 1) to translate realistic retrieval errors in CO₂ (ppm) to errors in retrieved sources and sinks (GtC/month). It is anticipated that these simulation experiments will be useful to inform the design of future CO₂ missions as well as to better understand likely errors in real carbon cycle analyses.

3.4. Quantify ability of satellite CO₂ to detect errors in fossil fuel emissions

Observational data currently or soon available are sufficient to detect fossil fuel emissions from large sources, but it is debatable at what scales these emissions are better quantified by traditional inventory reporting or atmospheric inversion. To be useful for fossil fuel emission analysis in the future, transport inversions of satellite CO₂ retrievals must be able to detect not just the presence of fossil CO₂ plumes, but rather errors in our prior estimates. We propose to use our modeling and assimilation system in pseudodata mode to quantitatively analyze our ability to detect different levels of error in fossil fuel emissions maps. For example, we will prescribe a multiplicative error in certain parts of the world that might be associated with intentional underreporting of fossil fuel emissions in particular countries, and see whether the analysis system could detect that error. We will do this using both the existing space/time patterns of emissions and also experiment with detection of unreported large point sources that are not in the prior. We will use observing system simulations to analyze the degree of accuracy and precision needed to detect each kind of underreporting (ubiquitous scaling or unreported sources).

4. Synergy with/relationship to other research

Other research being conducted in the Department of Atmospheric Science at CSU (and in the related Cooperative Institute for Research in the Atmosphere, CIRA) are closely related and synergistic with the proposed work. See the Current and Pending Research document for details. Land and coupled model development is strongly supported by NSF under the Center for Multiscale Modeling of Atmospheric Processes (CMMAP). Ongoing collaborations with NASA Goddard (PI S. Randall Kawa) and GMAO (PI Steven Pawson) support development and evaluation of the PCTM with fluxes from SiB. A new project funded by NASA Terrestrial Ecosystems is scheduled to start in January 2011, leading to optimization of biomass and carbon pools rather than unknown biases (state variables rather than parameters) using SiB and PCTM. Regional experiments over North America using elements of the modeling system described herein are supported by DOE and NOAA. The Principal Investigator is one of the original organizers of the international TransCom inversion intercomparison activity, and continues to participate actively therein.

The global mesoscale version of PCTM (0.5°x0.67° grid) requires about 6 CPU days to integrate one simulated year. Large ensembles run in a “perfectly parallel” arrangement, so require no additional wallclock time, but do require large numbers of processors. We will seek NASA supercomputer time to perform the required calculations. We have been very successful in obtaining time in the past. We request powerful desktop workstations and large disk arrays for storing and analyzing simulation output.

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