Project Summary

Syntheses of carbon dioxide flux and mixing ratio measurements in support of the North American Carbon Program Midcontinental Regional Intensive

We propose to establish a multi-year regional flux measurement program in the Midwestern United States in support of the North American Carbon Program (NACP) and the NACP midcontinental intensive. AmeriFlux towers have contributed noticeably to our understanding of the terrestrial carbon cycle, but the areas represented by these flux tower measurements are limited to roughly one square kilometer, very small in a continental or even regional context. Following the successful "ring of towers" experiment conducted in northern Wisconsin in 2004, and the COBRA experiments in the upper Midwest and Maine, we propose to conduct a multi-year, high-resolution regional inversion experiment in the mid-continent region of the United States. We will conduct regional atmospheric inversions in the mid-continental region utilizing a variety of data sources including accurately calibrated CO2 mixing ratio measurements on AmeriFlux towers and a number of other tower sites in the region. During intensive measurement campaigns, we will use grid nesting to perform cloud-resolving (< 1 km) transport analyses, allowing direct comparison to aircraft and other experimental data.

The research will target a region that is relatively densely instrumented with AmeriFlux towers. Data sources not supported by this proposal but suitable for inclusion in our analyses include airborne mixing ratio measurements, and the NOAA tall tower and aircraft profile data. Since larger-scale boundary conditions are also necessary, this project will include maintenance and intercalibration of a broader net work of high-quality CO2 mixing ratio measurements on AmeriFlux towers. We have access to global and continental data assimilation products that will be used to process lateral boundary information, but we do not seek additional support for these products.

The analyses will provide information analogous in many ways to an AmeriFlux tower, but on a spatial scale of order 10^4 - 10^5 km2, several orders of magnitude larger than the flux footprint of a flux tower. The multi-year time span, and collocation with a dense array of AmeriFlux sites will enable evaluation of models of ecosystem-atmosphere carbon exchange at regional scales, and contribute to regional-scale understanding of the terrestrial carbon cycle. Research will be closely coordinated with the NACP's midcontinental regional intensive experiment, and the methods developed will be applicable to other regions.

Project Narrative

Syntheses of carbon dioxide flux and mixing ratio measurements in support of the North American Carbon Program Midcontinental Regional Intensive

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1. Introduction: The NACP and the Midcontinental Intensive

Northern hemisphere ecosystems play an important and highly variable role in the global carbon cycle (e.g. Bousquet et al., 2000; Gurney et al., 2002). Understanding the carbon cycling of northern terrestrial ecosystems is essential for reducing uncertainty in the future greenhouse gas burden of the atmosphere (e.g. Friedlingstein et al., 2003). In response to these scientific needs, U.S. scientists drafted the North American Carbon Program science plan (Wofsy and Harriss, 2002).

Overarching questions posed by the North American Carbon Program (NACP) include: 1) Diagnosis: What is the carbon balance of North America and adjacent oceans? What are the geographic patters of fluxes of carbon? How are these fluxes changing over time? and 2) Attribution: What processes control the sources and sinks of carbon, and how do the controls change with time? The NACP Science Implementation Strategy (SIS) was drafted to guide research towards answering these overarching questions.

The NACP Science Implementation Strategy (Denning et al., 2004) recommends, *"Major diagnostic studies…in which measurements of carbon storage on land and in the oceans between reservoirs will be made in a coordinated series of experiments. Process-based models will be used in conjunction with remote sensing and other spatial data to estimate net carbon fluxes and storage across the continent at fine spatial and temporal resolution. These gridded estimates will be compared…to independent estimates made from observations of atmospheric trace gas concentrations and trajectories. Mismatches between top-down and bottom-up flux estimates will be used to improve diagnostic and predictive models through innovative techniques such as data assimilation…Several "intensive field experiments" will be conducted as part of the diagnostic research program, intended to test each element of the "model-data fusion" framework with multiply-constrained estimates of regional fluxes. After the intensive period, the program will leave a network of systematic observations and analytical models in place that is optimally configured for continued monitoring of future carbon cycling over North America…"*

The Midcontinental Intensive (MCI) proposed by Tans in 2004 is the first such intensive in this program. The goal, as noted above, is to bring together so-called top-down (atmospheric inversion) and bottom-up (ecological models or inventory) estimates of the carbon balance of the upper Midwestern region of the United States in order to establish methods for long-term observations of the regional terrestrial carbon fluxes. Regional flux estimates are needed to bridge the gap in scales between detailed but difficult to extrapolate process understanding being gathered via eddy-covariance flux tower measurements (e.g. Baldocchi et al., 2001) and manipulative ecosystem experiments (e.g. Hanson et al., 2005), and the strong global constraints lacking mechanistic understanding which is provided by atmospheric budgets (e.g. Battle et al., 2000). Both the top-down and bottom-up approaches are challenging at regional scales, and successes to date are limited. This proposal seeks to implement an innovative atmospheric inversion study based heavily upon measurements made by the AmeriFlux network. The project will be a centrally important contribution to the NACP Midcontinental Intensive, and will yield fundamental and new methodological progress towards regional flux estimates using a synthesis of atmospheric inversions and flux measurements.

1.1 Inverse modeling and data assimilation

Spatial and temporal variations in the mixing ratio of atmospheric CO_2 are a rich source of information about the global carbon cycle, and have been analyzed by increasingly sophisticated inverse methods to infer regional sources and sinks (e.g., Enting et al., 1995; Rayner et al., 1999; Gurney et al., 2002, Rödenbeck et al., 2003). Such calculations can provide a critical integral constraint on regional flux estimates that are upscaled from local process understanding using remotely sensed imagery and other spatial data. Transport inversions from currently available atmospheric data inevitably face a trade-off between temporal and spatial aggregation and uncertainties in the estimated fluxes. Monthly mean fluxes over subcontinental-scale regions can be estimated over well-sampled parts of the world to a useful degree of confidence using now-traditional "synthesis inversion" methods (Peylin et al., 2005), and some insight into the likely impact of model transport error can be approximated by using a growing suite of such codes (Peylin et al., 2002; Gurney et al., 2003; Baker et al., 2006).

Synthesis inversion of atmospheric observations involves forward simulation of tracer pulses from regions with prescribed patterns of flux variations in space and time. Prescribing spatial patterns allows other forms of information to be brought to bear on the results of the inverse calculation (e.g., we expect little or no carbon exchange by the Sahara desert or the Greenland ice sheet). If patterns of flux variations are prescribed as *hard constraints* (not adjustable by the optimization procedure) and are incorrect, errors in subregional spatiotemporal variations are inevitably aliased into biases in the estimated fluxes in the regional and time mean (this type of error has been termed "aggregation error," and has been described quantitatively by Kaminski et al., 2001 and Engelen et al., 2002).

Given sufficient data, aggregation error can be greatly reduced by solving for fluxes on the smallest possible spatial grid and at the highest possible temporal frequency, though this approach necessarily entails greatly increased computational cost relative to the coarse resolutions in space and time that have been applied in the past. Backward-in-time transport from "receptors" defined at the time and location of each observation reduces the computational cost of high-resolution inverse calculations when the number of observations is smaller than the number of potential sources and sinks (e.g., Uliasz and Pielke, 1991; Uliasz et al., 1996; Kaminski et al., 1999; Rödenbeck et al., 2003; Gerbig et al., 2003b). In practice, the observational constraint for such calculations is still quite weak, so that meaningful information about upstream surface fluxes is only obtained fairly close to the time and location of the measurements. Rödenbeck et al. (2003) used monthly mean CO_2 mixing ratios at dozens of flask stations to estimate fluxes for every grid cell in their global transport model, for example, but uncertainty over most of the world was so high that production of interpretable results required very aggressive post-aggregation to much larger regions. This post-aggregation involved unrealistic assumptions about spatial covariance of surface fluxes: one scenario specified an autocorrelation length scale of 0.2 times the radius of the Earth over land, for example, though wildly heterogeneous fluxes are known to exist over land. Worse, temporal aggregation errors have scarcely been addressed by inversion studies to date. Rödenbeck et al. (2003) aggregate CO_2 mixing ratios to monthly means, and estimate surface fluxes only on monthly time scales as well. This aggressive temporal truncation is necessary for computational efficiency, but is justified only if covariance among transport, fluxes, and mixing ratio is negligible (Denning et al., 1995, 1996b, 1999). Local observations contradict this assumption, with terrestrial fluxes and concentration anomalies changing sign on diurnal, synoptic and seasonal time scales in synchrony with systematic changes in atmospheric mixing and convection (e.g., Bakwin et al., 1998; Davis et al., 2003; Gerbig et al., 2003a; Hurwitz et al., 2004; Yi et al., 2004).

1.2 Proposed project in relation to recent and ongoing research

This research team is finishing DOE TCP supported research, and has ongoing NASA supported research that provides the foundation for this proposal. In 2004 the investigators deployed the Ring of Towers experiment in northern Wisconsin, USA (Miles et al., in prep). The Ring consisted of five CO_2 mixing ratio measurements deployed for a few months of the growing season at 75 m above ground on cell phone towers in a ring of roughly 150 km radius arrayed around the WLEF tall tower carbon cycle observatory (Bakwin et al., 1998; Davis et al., 2003). The project has yielded robust and accurate instruments for CO_2 mixing ratio measurements, experience deploying and operating these instruments, interpretable observations of mesoscale gradients in atmospheric CO_2 (Miles et al., in prep), and modeling tools suitable for computing regional fluxes from such a field campaign. Simultaneously, Richardson and Miles have been instrumenting AmeriFlux towers with the same high-accuracy, high-precision CO_2 mixing ratio sensors in order to supplement the continental CO_2 observing network.

That backbone CO_2 network, consisting of tall towers, aircraft profiling sites (both supported by NOAA), and small-tower CO_2 flux and mixing ratio measurements (AmeriFlux, primary support from the DOE), intended to provide the terrestrial carbon cycle observing system described in the NACP SIS (Denning et al., 2004), remains untested. This project will test the design of the atmospheric inversion portion of this backbone network. The basic design is to greatly enhance the network of atmospheric CO_2 measurements in the MCI region for at least a year while maintaining CO_2 measurements on a more widely distributed set of AmeriFlux sites, and conduct atmospheric inverse estimates of midcontinental CO_2 fluxes during this period (spring 2007 through fall 2008). The methodology will be evaluated by comparison to independent regional flux estimates ongoing in the region, and via a simple but powerful data removal exercise. In addition to past DOE TCP support for this work, a current NASA NACP project at Colorado State is providing support for atmospheric transport fields throughout the continental U.S. in support of the NACP. These transport fields will be used in this study, simplifying the computational work required in this project substantially. The data collection proposed here is particularly important to the MCI given recent serious cuts in NOAA's funding to deploy the tall tower network.

2. Objectives

This project, therefore, aims to satisfy the following objectives:

1. Determine the level of precision and accuracy of our project's CO_2 mixing ratio networks, including both AmeriFlux long-term measurements and the MCI temporary towers.
2. Characterize and improve approaches for conducting atmospheric inversions. In particular, what ecosystem properties we should solve for, what are the spatial and temporal coherence of these properties, and how should AmeriFlux flux data be integrated into this methodology?
3. See whether or not these inversion results converge with independent bottom-up flux estimates.
4. Determine whether or not atmospheric transport models that parameterize cloud convection (horizontal grid scales of order ten kilometers) are sufficient for accurate regional flux estimation.
5. Determine the tradeoff between the density of atmospheric CO_2 mixing ratio measurements in the midcontinental region, and the accuracy of inverse estimates of regional terrestrial carbon fluxes.
6. Examine the robustness of the "virtual tall towers" method of interpreting surface layer CO_2 measurements derived at the WLEF tall tower by examining data from at least one additional tall tower with flux and mixing ratio measurements.

3. Hypotheses

We will endeavor to answer six main hypotheses.

1. Instrumental accuracy and network precision will be 0.2 ppm or better for the 18 months the campaign mixing ratio measurements are deployed.
2. The difference between modeled terrestrial net ecosystem-atmosphere exchange (NEE) of CO_2 and AmeriFlux NEE observations has a smoother distribution in space and time than the flux measurements themselves. The smoothness of this difference enables us to estimate fluxes at fine space/time scales using "fast" model biophysics, but to correct erroneous model state variables (e.g., wood, soil carbon, stand age), ecosystem parameters (Vmax, maximum LAI), or unmodeled processes (e.g., fertilizer application) using the atmospheric inversion.
3. Top-down and bottom-up regionally aggregated carbon fluxes within the MCI domain converge to within 0.2 gC m^{-2} d^{-1} during the growing season, and to within 20 gC m^{-2} yr^{-1} annually.
4. Continental inversions based on 20 km resolution transport fields, parameterized cloud convection in RAMS, and covariance smoothing using Maximum Likelihood Ensemble Filtering provide unbiased inverse estimates of NEE of CO_2. High resolution, cloud-resolving transport models are not necessary for the inverse problem at these space and time scales.

5. A network of similar density to the proposed NOAA network of roughly 15 tall towers, plus weekly aircraft, plus our own Ameriflux CO_2 measurements, is sufficient to yield regionally aggregated estimates of NEE of CO_2 with an accuracy of 0.2 gC m^{-2} d^{-1} for the growing season fluxes, and 20 gC m^{-2} for the annual cycle using SiB-CASA-RAMS plus MLEF.
6. The gradient functions describing the surface-ABL difference in CO_2 during well mixed conditions are found to be consistent with those derived from the WLEF tall tower.

4. Related recent and ongoing research

Several recent or ongoing projects have led to or are providing leverage for this proposal. DOE TCP DE-FG02-02ER63475, 9/15/02 – 9/14/05, *"Regional ecosystem-atmosphere CO_2 exchange via atmospheric budgets,"* and DOE TCP DE-FG02-02ER63654, 10/15/03 – 9/14/06, *"A virtual tall tower network for understanding continental sources and sinks of CO_2,"* have supported deployment and analyses of highly-calibrated CO_2 mixing ratio measurements on communications towers in northern Wisconsin (the Ring of Towers, 2003 and 2004 data collection), and on several AmeriFlux towers (deployment is finishing this spring). The Ring project also supported development of the regional inversion methodology to be applied and enhanced in this project. The virtual tall towers project supported substantial instrument development to improve the precision of the sensors deployed long-term to AmeriFlux sites. These projects are either ending or have finished. This proposal is a logical follow-on to these initial, ground-breaking efforts.

The ongoing NASA project *"Mesoscale data assimilation for NACP,"* is supporting development and testing of SiB-RAMS and the Maximum Likelihood Ensemble Filter (MLEF) for estimation of continental-scale exchange of CO_2 between the land and atmosphere. We have already demonstrated that the models, taken together, can optimize predictions of NEE and CO_2 given dense mixing ratio data (this was partly supported by DOE-TCP under the Ring project, above). We will run SiB-RAMS over the continental USA plus parts of Canada, Mexico, Atlantic, and Pacific Oceans for a year. Lateral boundaries will be nudged to weather from NASA GEOS or NCEP. Lateral CO_2 will be nudged from global simulations conducted via an additional NASA project with Randy Kawa, Goddard, using SiB/CASA with the PCTM. In year 2, we are running PCTM from NACP receptors (towers) and optimizing the bias in MLEF as was done for the Ring, but at a continental scale with 100 km horizontal grid sizes. This investigation provides the transport modeling to be used in this proposal.

Finally, a NOAA/CIRA research project involves archiving hourly 13-km analyses of weather and transport derived by NOAA RUC-13 model. Influence functions are calculated using the Lagrangian Particle Dispersion Model (LPDM) for all continuous NACP towers, and made available publicly via a web interface. This project provides the reanalyses needed for the cloud-resolving forward SiB-CASA-RAMS run proposed here.

5. Methods

This project requests support for continued maintenance of highly-calibrated CO_2 mixing ratio measurements at six AmeriFlux sites (see Figure 1) for the duration of this project as part of the continental CO_2 mixing ratio "backbone" observation system, as well as deployment of five highly-calibrated CO_2 instruments to cell phone towers (approximately 100m high) within the MCI study region (see red points, Figure 1, for potential locations) for roughly 18 months, spring 2007-fall 2008. This will greatly increase the density of mixing ratio measurements available in that region and allow us to establish what we hope is an "oversampling" intensive campaign that encompasses at least one full annual cycle. Inversions will be conducted for the entire intensive campaign period and will use these CO_2 data and any other data available in the MCI region. Further, SiB/CASA will be optimized prior to the inverse estimation with the AmeriFlux sites operating in the MCI region (see Figure 1). Fair use policies will be followed when working with AmeriFlux data. The high resolution forwards model runs will be conducted for one 2-week campaign when the largest density of atmospheric data are available (e.g. airborne measurements in addition to the MCI Ring). The following sections describe each of the tools we will use during this experiment in modest detail.

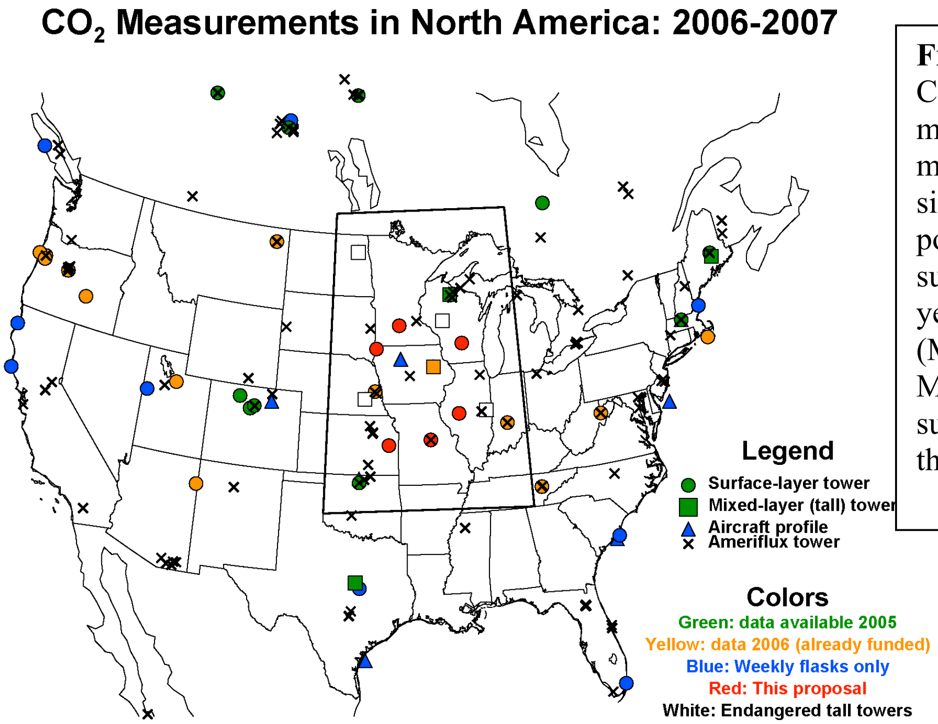

Figure 1: CO_2 flux and mixing ratio measurement sites. Red points and a subset of the yellow points (MT, WV, TN, MO, WI) are supported by this request.

5.1 Observations

As noted previously, as a first step towards implementing atmospheric budget or inversion methodology on a regional scale, a network of five relatively inexpensive CO_2 mixing ratio measurement systems were deployed, with support from TCP, on towers in northern Wisconsin between April and August 2004. Four systems were distributed on a circle of roughly 150-km radius, surrounding one centrally located system at the WLEF tower in Park Falls, WI. Additional data from the Sylvania, MI, AmeriFlux tower was incorporated into the dataset. The five systems used LiCor-820 infrared CO_2 analyzers and were calibrated every two hours using four samples known to within ± 0.2 ppm CO_2. Frequent calibration is necessary to characterize and remove the nonlinear response of the CO_2 sensor to changes in temperature and pressure. Before deploying the five CO_2 systems, their relative accuracy was tested by sampling air in parallel from a four-liter sample volume which had a fan actively circulating the air. For the tests, each system used its own set of calibration standards to accurately measure the relative accuracy in the field. The relative agreement between all systems was better than ± 0.3 ppm, which may include small errors in the field standards. A LI-7000 connected in series with one of the five systems revealed no systematic bias associated with the use of the LI-820.

As a further means to evaluate the accuracy of the systems, one system was deployed at the WLEF tower in Park Falls, WI, (Bakwin et al., 1998) where a NOAA-ESRL system also measured CO_2 mixing ratio. The PSU system sample line branched off from the NOAA-ESRL system 76-m sample line at the base of the tower to ensure that both systems were sampling identical air. The NOAA-ESRL and PSU systems had independent filtering and, more importantly, independent drying. In addition, the NOAA-ESRL system used a LI-6251. The difference between the CO_2 mixing ratio measured by the two systems for the times in which both systems were operational is shown in Fig. 2a.

The estimated uncertainty of the NOAA-ESRL system, calculated such that the actual value should be within one times the uncertainty estimate of the measured value 67% of the time, is also shown (A. Andrews, personal communication). The PSU estimate of the CO_2 mixing ratio is within one times the uncertainty estimate of the NOAA-ESRL value for 57% of the observations; the average ESRL uncertainty

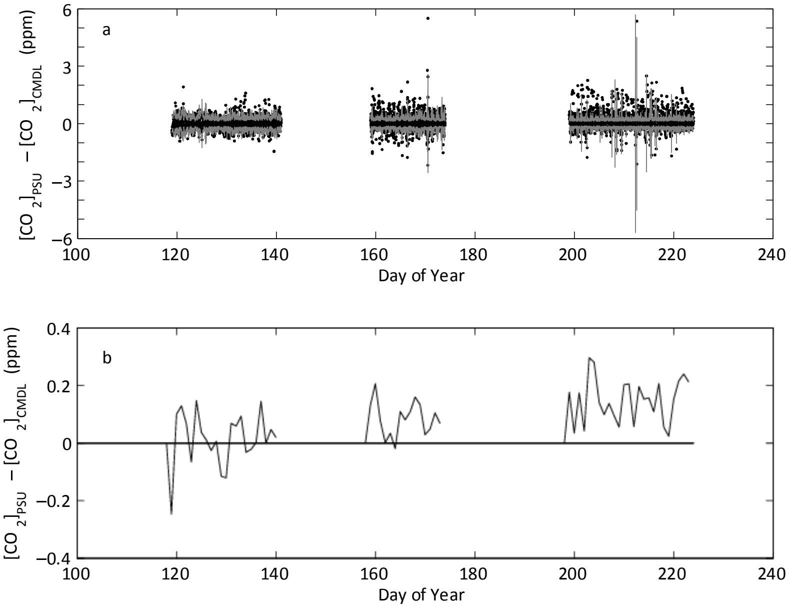

Figure 2. Difference between the CO_2 mixing ratio measured by the PSU and NOAA-ESRL systems at the WLEF tower (76-m level) during April–August 2004. **a)** 12-min data (solid circles) and uncertainty estimate of the NOAA-ESRL system (gray line), and **b)** difference between the daily average $[CO_2]$ measurements.

estimate is 0.29 ppm. The PSU value is within 0.5 ppm of the NOAA-ESRL value for 83% of the values, and 96% of the PSU values are within 1 ppm of the NOAA-ESRL values. The daytime-only percentages are similar. The difference between the daily mean PSU value and the daily mean NOAA-ESRL value (Fig. 2b) is consistently less than ±0.3 ppm.

To show the utility of such a regional scale network in determining the spatially- and temporally-varying regional flux, we calculate, in the simplest possible manner, the Lagrangian estimate of the daytime CO_2 flux on two days in which the wind direction was such that parcels traveled across the study domain and in which the wind speed was relatively constant for several hours. The days chosen for the analysis (19−20 June 2004) had simple CO_2 signals, i.e., no evidence of frontal passages or pollution events. The parcel transit times between upwind and downwind sites were about 6 – 8 hr for 19 June and 3 hr for 20 June. The change in CO_2 mixing ratio of parcels traveling between sites is at least 2.6 ppm, which is large compared to the accuracy of the systems, and typical of the horizontal gradients we might expect over a distance of 100-200 km under fair weather conditions. Using an estimate of the boundary layer depth based on temperature soundings and measured heat fluxes, and assuming the entrainment flux to be zero, the estimated flux is −10 to −11 μmol m^2 s^{-1} on June 19 and −18 to −19 μmol m^2 s^{-1} on June 20. We estimate the uncertainty of the flux, based on errors in the BL depth, transit times, and [CO2], to be at least 3 μmol m^2 s^{-1}. For comparison, the midday average net ecosystem-atmosphere exchange (NEE) measured at 30 m on the WLEF tower is −9 μmol m^2 s^{-1} on both 19 and 20 June. While the 122-m and 396-m data are generally used to calculate the flux on unstable days such as these, the data at those heights are, unfortunately, not available. A typical value for the difference between the flux measured at 30 m and the higher levels is −5 μmol m^2 s^{-1}; thus the actual NEE is likely closer to −14 μmol m^2 s^{-1}. This rough estimate shows that the Ring CO_2 measurements should yield very reasonable results when interpreted in a full inversion scheme. Those analyses are underway.

As another example of the data captured with a regional scale network, we show data during a frontal passage. Within the regional network on 29 April 2004, all six sites (with the possible exception of Wittenberg) show an abrupt increase in CO_2 mixing ratio followed by a gradual decline (Fig. 3). The timing of the increase in CO_2 mixing ratio coincides with a frontal passage through the region, from the northwest to the southeast. Prior to the frontal passage the CO_2 mixing ratio measured at 76 m at WLEF decreased from 386 ppm at 0230 GMT to 377 ppm at 0830 GMT (Fig. 3c). The frontal passage occurred during a calibration cycle of the PSU system so no data were recorded during the rapid change, but the CO_2 mixing ratio immediately before the frontal passage was 379 ppm and immediately after was 391 ppm. The ESRL system recorded two intermediate points between the prefrontal value and the postfrontal value 36 min later.

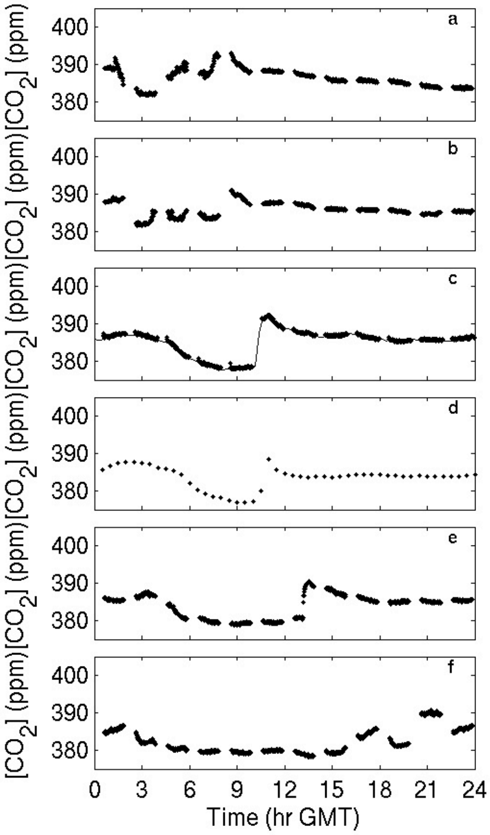

Figure 3. CO_2 mixing ratio measured at five sites within the regional network for 29 April 2004. **a)** Brule, **b)** Bayfield, **c)** WLEF, **d)**, Sylvania, **e)** Fence, and **f)** Wittenberg. All measurement heights are 76 m and data shown are 1-min averages, with the exception of Sylvania where the measurement height is 36 m and the data are available every 30 min. Both a PSU system (dots) and a NOAA-ESRL system (line) recorded data at the WLEF tower. The approximate times of frontal passage at each site (to the nearest hour) as determined from surface observations of pressure, temperature, and winds are a) 0600, b) 0900, c) 1000, d) 1000, e) 1300, f) 1300 GMT. Sunset at WLEF occurred at 0106 GMT, and sunrise at 1051 GMT.

After the frontal passage, the CO_2 mixing ratio then gradually fell to 386 ppm and remained relatively constant for the duration of the day. While the frontal case is not easily interpreted in terms of local biological fluxes, it clearly illustrates that the mixing ratio measurements on small towers capture coherent regional changes in CO_2.

5.1.1 Sensors

The measurements described in section 5.1 were made using an earlier system design and yielded excellent agreement with the NOAA-ESRL measurements made at the WLEF tower. The virtual tall towers DOE TCP project is deploying an updated version of this low cost CO_2 mixing ratio measurement systems at six Ameriflux sites across the continental United States (see Fig. 1). This design, developed collaboratively with NCAR-EOL (Britton Stephens), uses several new techniques to ensure data quality and accuracy, as well as simplify design, deployment, and maintenance. For example, the drying technique no longer requires the use of heavy and awkward N_2 tanks but uses two Nafion driers and two mole sieve moisture traps; this technique allows the sample air stream to be used as the purge gas in the Nafion driers. Note that this design requires infrequent maintenance as the mole sieve lasts for at least 12 months. Additional improvements include: monitoring the sample air stream dew point to ensure adequate drying of the sample, pressure controlling the sytem using a mini regulator, and testing the entire system for leaks into or out of the sampling lines thus ensuring that leaky valves will be immediately identified. The accuracy of the improved systems is approximately ±0.2 ppm CO_2. Finally, two additional calibration standards, termed target and archive tanks, are used to ensure system accuracy. The target tank is sampled every 30 minutes as if it were an air sample and provides a frequent test of the entire sampling system; the target tank is replaced every 6-12 months. The archive tank is sampled once a day and is designed to last over 10 years and ensures consistent measurements as the four working calibration standards are changed approximately every 12-24 months.

While the accuracy of the LI-820 sensor has been demonstrated, an opportunity to employ up to four state of the art sensors may present itself. We are currently working with Picarro, Inc., a small business in California, on a Phase II SBIR grant to evaluate the absolute accuracy of an instrument based on the Cavity Ringdown Spectroscopy (CRDS) method for determining CO_2 mixing ratio. The system accuracy is currently 1 part in 1000 (~0.3 ppm) and the goal of the project is to measure CO_2 with an accuracy of 1 part in 3000 (~0.1 ppm). Once calibrated, the systems require no calibration gas, although a target gas can be used to ensure the accuracy of the measurements. Picarro, Inc. currently has four systems available for field deployment and these systems could be used in place of, or in addition to, the proposed systems. The network design in this proposal is based on using the tested LI-820 systems but will be modified to include the use of the Picarro systems if possible.

5.1.2 Continental "Backbone"

i)Tall Towers

The National Oceanographic and Atmospheric Administration's tall tower and aircraft profiling programs are the core of the NACP's long-term atmospheric CO_2 sampling program. Current and planned sites are shown in Figure 1. Unfortunately, recent budgetary cuts have severly cut back the planned midcontinental expansion of the tall tower network, as indicated by the sites in white on the map (intended to be deployed in time for the MCI, but now delayed pending future budgets). Fortunately two tall towers are currently operating, and a third is likely to be instrumented in time to overlap with this project. The third site is likely to be Iowa or Illinois. These towers provide direct measurements of atmospheric boundary layer mixing ratios, and typically extend above the complex and difficult to interpret nocturnal boundary layer (Yi et al, 2001).

ii) Ameriflux Towers

Current support from TCP is funding installation of highly accurate CO_2 mixing ratio systems at five existing Ameriflux sites including Canaan Valley, WV, Chestnut Ridge, TN, .the WLEF tall tower near Park Falls, WI (or the NOAA Iowa site if possible), and sites in Missouri and Montana. In addition, separate funding has enabled several additional AmeriFlux sites to implement highly-calibrated CO_2 measurements (see Figure 1). All of these sites are intended to be long-term CO_2 mixing ratio measurements that will be used in atmospheric inversions. This network is being installed and will be in place by late spring, 2006. The current proposal seeks maintenance funds to ensure the Ameriflux-virtual tall tower network is operational for the Midcontinental Intensive. The mixing ratio measurements from these towers, when subsampled for midday conditions, are very close to the mixing ratio of the entire continental boundary layer. If desired, the difference between the surface layer mixing ratio and the mid-CBL can be estimated from micrometeorological scaling arguments that have been fitted to the detailed CO_2 flux and mixing ratio measurements from the 447 m tall WLEF tower (Bakwin et al, 1998; Davis et al, 2003). Data from these surface layer towers, subsampled for midday conditions, show abundant synoptic and seasonal structure (Davis et al, 2003; Hurwitz et al, 2004; Yi et al, 2004) that can be interpreted in inverse analyses. Nocturnal data are difficult to interpret, and the absence of these data is a distinct disadvantage to the tall tower approach. Nevertheless, the daytime data are valuable, and instrumentation and maintenance is relatively inexpensive.

5.1.3 Campaign Observations for the Midcontinental Intensive

i) Communications tower measurements

This project seeks to augment the continental scale Ameriflux CO2 mixing ratio measurements with a regional scale midcontinental intensive measurement campaign lasting approximately 18 months. Figure 4 shows the sites at which CO2 mixing ratio measurements are currently available (green and blue symbols), those that are in funding danger (white), those that will be available prior to the midcontinental intensive (yellow), and those proposed in this study (red). The sites proposed in this study will form a ring around the central Iowa site, much like the ring of towers deployed in 2004. As proved successful in the Wisconsin ring of towers in 2004, these temporary sites will be located on existing cell phone or communication towers, ensuring site access at a very minimal cost.

ii) Airborne measurements.

Campaign-style airborne mixing ratio measurements have been proposed for the MCI (see letter of support from S. Wofsy) and, for the limited times they would be collected, would be highly complementary to this study. Airborne measurements would add extremely high spatial resolution data over a large portion of the domain, albeit for a limited time. If funded, these data would become a focal point for our high resolution modeling efforts, and constitute an 'uber-oversampled' environment when added to the campaign style tower-based sampling we are proposing.

5.1.4 Ecological data

i) Flux measurements

The MCI domain is rich in AmeriFlux sites, as shown in Figure 1. These eddy-covariance flux towers measure continuous, long-term (often multi-year) time series of net ecosystem-atmosphere exchange (NEE) of CO_2 (e.g. Baldocchi et al, 2001; Davis et al, 2003). We intend to utilize the CO_2 flux (not mixing ratio) data from the AmeriFlux sites in the MCI domain to optimize the SiB/CASA terrestrial carbon cycle model, as described in further in this section. These flux measurements represent a rich constraint on hourly to interannual terrestrial carbon dynamics in the region.

ii) Inventory and land use data

Longer-term trends in terrestrial carbon fluxes are often governed by slowly changing carbon stocks, such as soil carbon pools and woody forest biomass (e.g. Caspersen et al, 2000). We will consider applying two sources of such data in our study, forest inventory data (via ongoing collaboration with P. Bolstad, U.Minnesota) and agricultural cropping and tillage information (see letter of support from Dr. Tris West). These data may serve to inform slower time scale processes in the SiB/CASA terrestrial carbon cycle model.

5.2 Numerical tools

The project will make use of a comprehensive suite of numerical models and analysis tools for the study of the continental carbon cycle. These tools have been developed and tested by the investigators over the past 15 years, partly with support from DOE TCP; some of them are also available through the current support of other agencies. The tools include:

- The **Simple Biosphere model (SiB)**, which represents ecosystem physiology, including photosynthesis, respiration, and decomposition on local, regional, and global scales;
- The **Regional Atmospheric Modeling System (RAMS)**, which simulates weather, winds, and atmospheric tracer transport as well as land-atmosphere interaction. The coupled SiB-RAMS model has been used to simulate gridded NEE and atmospheric CO_2 from the scale of large PBL eddies to the entire continent on a set of telescoping two-way nested grids;
- The CSU **Lagrangian Particle Dispersion Model (LPDM)**, which calculates backward-in-time trajectories to relate observed changes in CO_2 mixing ratio to surface fluxes upstream;
- A **Bayesian synthesis inversion algorithm (BSIA)** originally developed and optimized by Dr. Peter Rayner. The algorithm was previously used in the TransCom series of global experiments, and provides a fast and flexible testbed for prototyping new optimization problems;
- The **Maximum Likelihood Ensemble Filter (MLEF)**, a powerful ensemble data assimilation system useful for optimizing parameters or model state variables when the number of unknowns and observations is too large for the BSIA, and for studies of error covariance.

5.2.1 Forward Coupled Model of Land-Atmosphere Exchanges (SiB-CASA-RAMS)

The Regional Atmospheric Modeling System (RAMS) is a mesoscale meteorological (non-hydrostatic) model and contains time-dependent equations for velocity, non-dimensional pressure perturbation, ice-liquid water potential temperature (Pielke et al., 1992), total water mixing ratio, and cloud microphysics. Vapor mixing ratio and potential temperature are diagnostic. A significant feature of the model is the incorporation of a telescoping nested-grid capability, which enables the simulation of phenomena involving a wide range of spatial scales (Walko et al., 1995). A second-order advection scheme is employed. The turbulence closure scheme of Deardorff (1980) is used, which employs a prognostic sub-grid turbulent kinetic energy. The two-stream radiation scheme developed by Harrington (2000) is used. At regional scales for which individual convective elements (clouds) cannot be resolved, we use convective parameterizations (Grell, 1993; Freitas et al., 2000) that compute precipitation rates, atmospheric heating and moistening, and mass and tracer fluxes (including updraft and downdraft velocities) by unresolved cloud processes. The lowest level above the surface in the RAMS model is the reference level at which atmospheric boundary layer values of temperature, vapor pressure, wind velocity and carbon dioxide partial pressure are calculated. Additionally, the direct and diffuse components of short wave and near infrared radiation incident at the surface are provided from the RAMS radiation scheme.

RAMS has recently been coupled to the Simple Biosphere Model (SiB), 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). Other recent improvements include biogeochemical fractionation and recycling of stable carbon isotopes (Suits et al., 2004), 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.

The atmospheric surface layer, between the vegetation and the lowest level of RAMS is incorporated as part of SiB and is based on the scheme of Holtslag and Boville (1993). The input variables provided by RAMS to SiB are updated every minute of simulation time. SiB returns to RAMS, at the reference level, fluxes of heat, moisture, momentum and carbon dioxide, as well as the upwelling radiation. The coupled SiB-RAMS model has been used to study PBL-scale interactions among carbon fluxes, turbulence, and CO_2 mixing ratio (Denning et al., 2003) and the regional-scale controls on CO_2 variations (Nicholls et al., 2004; Wang, 2005; Corbin, 2005).

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 CO_2. 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 (Kevin Schaefer, unpublished simulations). Under separate support from NASA in collaboration with James Collatz, we also plan to add a fire module to this model.

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. Under separate support from NASA's

Energy and Water System program, we are addressing this problem by developing and testing a prognostic phenology module for SiB (and for the Community Land Model, CLM). We are assimilating 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. A separate proposal has been submitted to DOE-NICCR to develop and test an explicit treatment of phenology and physiology of agricultural crops, and to parameterize the crop model using extensive agricultural databases.

5.2.2 LPDM and Formulation of NEE and Mixing Ratio Variations

We have developed a method for regional CO_2 flux inversion using a Lagrangian Particle Dispersion Model (LPDM) driven by the output of SiB-RAMS. The method involves four steps: (1) forward simulation of photosynthesis, respiration, decomposition, and atmospheric transport using the coupled SiB-RAMS model; (2) calculation of a large number of backward-in-time particle trajectories from each observation point ("receptor") in space and time; (3) integration of the particle trajectories to quantify the "influence function" of each upstream grid cell at each previous time with respect to a particular observation; and (4) an optimization scheme that adjusts the fluxes so that simulated and observed mixing ratios differ by acceptable amounts. This method was developed partly with prior support from DOE TCP, and was tested using data from the Ring of Towers experiment (see results from prior TCP research described previously). The LPDM (Uliasz and Pielke, 1991; Uliasz, 1993, 1994; Uliasz et al., 1996) accounts for transport by resolved advection and by subgrid-scale stochastic motion (turbulence and clouds). Influence functions calculated by integrating upstream contact time with the surface quantify the partial derivative of a particular measurement with respect to all previous fluxes at all surface points in the domain (the method is nearly identical to that of Gerbig et al., 2003b). In general, influence functions are also calculated with respect to the initial distribution of CO_2 and the lateral boundary conditions, though with sufficient integration time the former become negligible.

We account for high-frequency time variations of photosynthesis and respiration by assuming that they are driven by well-understood and easily modeled processes (radiation, temperature, soil moisture), then solve for unknown multiplicative biases in each component flux after smoothing in space and time. This is accomplished by convolving the influence functions generated from LPDM with gridded photosynthesis (gross primary production, GPP) and ecosystem respiration (RESP) at each time step in SiB-RAMS. The net ecosystem exchange (NEE) is composed of these two component fluxes:

$$NEE(x,y,t) = RESP(x,y,t) - GPP(x,y,t) \qquad \text{(eq 1)}$$

where x and y represent grid coordinates and t represents time. Sub-hourly variations in the simulated component fluxes in time 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 variations in space are driven by variations in vegetation cover, soil texture, and soil moisture. To estimate regional fluxes from atmospheric mixing ratios, we assume that the model of the component fluxes is biased, and that the biases are smoother in time and space than the fluxes themselves:

$$NEE(x,y,t) = \beta_{RESP}(x,y)RESP(x,y,t) - \beta_{GPP}(x,y)GPP(x,y,t) \qquad \text{(eq 2)}$$

A persistent bias in photosynthesis might result from underestimation of leaf area, available nitrogen, or soil moisture, whereas a persistent bias in respiration might result from overestimation of soil carbon or coarse woody debris. In any case, it is reasonable that such biases vary much more slowly than the fluxes themselves.

To estimate slowly-varying biases β_{Resp} and β_{GPP} using SiB-RAMS and LPDM, we first generate surface flux influence functions by integrating the backward-in-time particle trajectories from LPDM. Using these, we can represent the mixing ratio observed at a given station k at time m as

$$C_{k,m} = \sum_{i,j,n} \left(\left(\beta_{R,i,j} RESP_{i,j,n} - \beta_{A,i,j} GPP_{i,j,n} \right) C^{*}_{k,m,i,j,n} \right) \Delta t_f \Delta x \Delta y + C_{BKGD,k,m} \qquad \text{(eq 3)}$$

where i and j are grid indices in the zonal and meridional directions, n is the time at which GPP and Respiration occurred (not usually the time at which the resulting change in mixing ratio was measured!). The influence function $C^*_{k,m,i,j,n}$ is then the discrete form of the partial derivative of the observed mixing ratio with respect to the NEE at grid cell (i,j) at time step n. The length scales Dx and Dy are the sizes of the grid cells in the zonal and meridional direction, and Dt_f is the time step over which the fluxes are applied. The term $C_{BKGD,k,m}$ represents the contribution of "background" CO_2 flowing into the model domain from the larger scales. With a little algebra and a healthy dose of computer time, we obtain a simpler representation more practical suitable for optimization:

$$C_{obs} = \sum_{cell=1}^{nCell} \beta_{RESP,cell} C^*_{RESP,obs,cell} + \sum_{cell=1}^{nCell} \beta_{GPP,cell} C^*_{GPP,obs,cell} + C_{BKGD,obs} \qquad \text{(eq 4)}$$

where obs is an observation number (combines indices k and m), and $cell$ is a grid cell number (combines indices i and j). The influence functions have been convolved with the GPP and RESP terms from the forward model and integrated over the time period over which the bias terms are assumed to apply:

$$\begin{aligned} C^*_{RESP,obs,cell} &= \Delta t_f \Delta x \Delta y \sum_n RESP_{cell,n} C^*_{obs,cell,n} \\ C^*_{GPP,obs,cell} &= -\Delta t_f \Delta x \Delta y \sum_n GPP_{cell,n} C^*_{obs,cell,n} \end{aligned} \qquad \text{(eq 5)}$$

We have experimented successfully with 10-day time scales for the bias terms, which allow influence functions on hourly fluxes and observations to be integrated for 240 hours. This approach has two important advantages: (1) the area and strength of upstream influence over 10 days is much greater than for a single hour, so the inverse problem of estimating the bias terms $\beta$is much better constrained than the estimation of the fluxes themselves; and (2) the storage of the influence functions in (eq 5) is 240 times smaller than would be required to store all the $C_{obs,cell,n}$!

Equation 4 is a linear system which can be written simply as

$$\vec{y} = h\vec{x} \qquad \text{(eq 6)}$$

where $\vec{y}$ is the vector of observations C_{obs} and $\vec{x}$ is the vector of unknown bias terms $\beta_{\text{GPP,cell}}$ and $\beta_{\text{Resp,cell}}$. The Jacobian matrix h contains the influence functions $C^*_{GPP,obs,cell}$ and $C^*_{RESP,obs,cell}$. The rows of h correspond to each observation, and each column corresponds to an unknown bias term β_{RESP} or β_{GPP} at a given grid cell over the 10-day integration period. In practice, we treat the background mixing ratio by prescribing lateral inflow from a larger scale model. We treat errors in this boundary condition additively by augmenting the vector of unknowns $\vec{x}$ with lateral boundary concentrations and "transporting" them to the receptor by augmenting matrix h with additional influence functions for these fluxes.

5.2.3 Estimation of Bias Terms from Atmospheric Mixing Ratios with MLEF

For relatively small numbers of unknowns and observation, the inverse problem of estimating $\vec{x}$ from $\vec{y}$ in (eq 6) is straightforward and can be solved by matrix methods involving singular-value decomposition (SVD). We minimize a cost function that penalizes model-data mismatch and is regularized by imposing a weak prior constraint:

$$J = (\vec{y} - h\vec{x})^T r^{-1} (\vec{y} - h\vec{x}) + (\vec{x} - \vec{x}_p)^T p^{-1} (\vec{x} - \vec{x}_p)$$

here r is the observation error covariance, and p is the prior error covariance of the unknown β's. The solution is given (e.g., Rodgers, 2000) by

$$\vec{x} = \vec{x}_p + (h^T r^{-1} h + p^{-1})^{-1} h^T r^{-1} (\vec{y} - h\vec{x}_p) \qquad \text{(eq 7)}$$

and the *a posteriori* error covariance of the b's is given by

$$c = (h^T r^{-1} h + p^{-1})^{-1} . \qquad \text{(eq 8)}$$

To solve (eqs 7 and 8), we use a fast and flexible algorithm for this “analytical” inversion, originally derived by Peter Rayner (pers. comm.), and implemented in the IDL programming language. Continental inversions of hourly data from 11 towers for 10-day biases in GPP and RESP on a 100-km grid with (4408 unknowns with 2640 observations) take about 10 minutes of CPU time using this routine on a fast Linux machine. Unfortunately, the computing requirements for the analytical solution to the inverse problem scale roughly as the square of the number of unknowns or observations, and large problems will not fit in computer memory. This method is also limited to linear models with (assumed) Gaussian errors. To overcome these obstacles and for more flexibility with respect to optimizing structures in the error covariance in the bias terms β, we have implemented the model described above into the Maximum Likelihood Ensemble Filter (Zupanski, 2005; Fletcher and Zupanski, 2006), which is closely related to the Ensemble Kalman Filter (Peters et al, 2005). The MLEF is very flexible, allowing for nonlinear models of arbitrary complexity and for non-Gaussian errors. It has been adapted for separate estimation of model error as well as optimal control parameters. The essence of the ensemble data assimilation approach is that an ensemble of sets of systematically perturbed control parameters (the β’s in our case) are generated by the algorithm from an initial forward simulation and calculation of model-data mismatch ($\vec{y} - h\vec{x}$ in our case). An ensemble of forward model integrations (for us, the simple matrix multiplication $h\vec{x}$) is then performed, and the optimization algorithm estimates values and uncertainties of each control parameter from the resulting dependence of model-data mismatch on parameter values, subject to specified prior values and error covariance.

The ensemble yields an approximation of the full error covariance matrix of the β’s, the accuracy of which depends on the size of the ensemble. Theoretically, the MLEF estimation approaches the analytical solution (eqs 7 and 8) when the size of the ensemble is equal to the number of unknowns (this is called the “full-rank” problem). We have verified this behavior for continental and regional inversions of SiB-RAMS fluxes by comparing estimates of β (x,y) and its error covariance computed with full-rank ensembles to the analytical solution. The MLEF algorithm includes a strong preconditioning step that reduces the size of ensembles required. In our experiments with estimation of SiB-RAMS biases for the Ring of Towers, we have found that ensembles of 100 members produce results that are almost indistinguishable from the full-rank solution (1800 members).

A key advantage of the estimation of β (x,y) using the MLEF is that spatial covariance and correlation between biases in GPP and respiration can be propagated from one 10-day “assimilation cycle” to the next, so that spatial patterns in the bias emerge over time. In any given time window, the model is terribly underconstrained by observations, but the system “learns” about the model biases and their spatial structure over successive cycles as new observations are assimilated. Without spatial patterns of error covariance, inverse methods are prone to creating unrealistic flux patterns determined by the placement of the observations. Alternatively, one can assume that model biases are determined uniquely by vegetation type (Gerbig et al, 2003b, 2005), but this risks extreme aggregation error. Biases due to incorrect soil nitrogen or forest stand age, for example, are very unlikely to be constant across all pixels of a given vegetation type.

5.2.4 Regional Evaluation of SiB-RAMS-LPDM-MLEF for the Ring of Towers

We have evaluated the ability of the MLEF to estimate biases in SiB-RAMS fluxes given influence functions generated by the LPDM using synthetic observations for the Ring of Towers experiment in the summer of 2004. A forward simulation of a 70-day period starting on 1 June, 2004 was performed in SiB-RAMS on a domain somewhat larger than the conterminous USA on a grid of *Dx*=40 km. A finer nest was run on a 1000 km x 1000 km subdomain centered on WLEF with *Dx* =10 km. Influence functions were generated by running the LPDM backward in time for two-hour mean “samples” from six surface layer towers in the Ring, plus five levels on the WLEF tower (all but the 11 m level). We then sought to estimate the bias factors every 10 days (seven assimilation cycles) on a 20-km grid over a 600 x 600 km area centered on the tall tower.

We created a "true" field of the biases in SiB-RAMS simulations of GPP and ecosystem respiration (β_{RESP} and β_{GPP}) by dividing the domain in half. On the east side, we set the mean value of both β's to be 1.1, and on the western half we set them to 0.5. To make the problem more difficult, we also included random deviations in each β chosen from a Gaussian distribution with a mean of 0 and a standard deviation of 0.1. Because we are gluttons for punishment, we applied these deviations with different decorrelation length scales: 80 km in the southern and 160 km in the northern halves of the domain. We then used these perturbed β's to generate synthetic mixing ratio data by multiplying them by the LPDM influence functions (eq 6), which were already convolved with the modeled photosynthesis and respiration from SiB-RAMS, as two-hourly averages assuming that the model bias is constant over periods of 10-days. The data were also perturbed by Gaussian noise, with a mean of 0 and a variance that depended on tower height and time of day. The error assigned to the data ranged from 1 ppm above 200 m during daytime to 45 ppm below 50 m at night. Note that this formulation only allows about three "observations" per day from the surface-layer towers under well-mixed conditions, and very strongly deweights night-time and transitional values.

As a "first guess" of the unknown distribution of model bias, we assumed a uniform field of $\beta = 0.75$ in every grid cell. This value was assumed to be known to within 0.2 (at 1-sigma). Our initial estimate of the spatial decorrelation length-scale was 120 km. Successive cycles in the assimilation used the estimated β's and covariance matrix from the previous cycle as a background field, constituting a "persistence forecast" for both the β's and their covariance structure. No further smoothing was applied. After the first cycle, the spatial covariance of the errors in β's was determined from the synthetic mixing ratio data. Results (Fig 4) are very encouraging. The estimated β (x,y) clearly distinguish the east-west structure in the "true" field, and also capture much of the random finer variations, including the smoother patterns in the south than the north. The constraint is weak over the Great Lakes, because both GPP and Resp are zero there. Overall uncertainty in the model bias was less than 5% over most of the interior of the Ring.

5.2.5 Assimilation of AmeriFlux measurements into SiB/CASA

Unlike the previous Ring of Towers project, here we will assimilate AmeriFlux observations of CO_2 fluxes in the MCI region into SiB/CASA *prior* to the atmospheric inversion. This step will allow us to derive a mechanistically sound probabilistic reconstruction of the carbon fluxes over the considered region and to test our hypotheses. The formulation of the likelihood function will follow previous (Braswell et al., 2005; Hargreaves and Annan, 2002), with one potentially important improvement. These past studies typically assume uncorrelated model residuals. We will account for potential autocorrelated residuals using a modified likelihood function approach (cf. Zellner and Tian, 1964). We will characterize the statistical properties of the assimilation problem and test two assimilation methods. Specifically, we will test (i) the MLEF and (ii) the Metropolis-Hastings algorithm (Hastings, 1970; Metropolis et al., 1953). The MLEF (see above) is a very efficient assimilation method but relies on a number of assumptions. On key assumption for the MLEF is that the estimated probability density function of the parameters is approximated by a unimodal distribution. It may well be that our likelihood function will show several maxima. Nonlinear models forced by seasonal and interannual variability often show this property (Athias et al., 2000; Hurtt and Armstrong, 1999; Rayner et al., 2005; Schartau et al., 2001; Vukicevic et al., 2001). Indeed, two studies focusing on the interannual variability of the terrestrial carbon cycle show strong evidence for a multimodal likelihood function (Rayner et al., 2005; Vukicevic et al., 2001). Finding the appropriate data assimilation method is an important technical point. Some data assimilation methods are prone to converge to merely a local (as opposed to the global) maximum of the likelihood function and can yield biased estimates. We will carefully test for multimodality and compare the MLEF results with the results derived from the Metropolis-Hastings algorithm. The Metropolis-Hastings algorithm is simple and has been shown to be relatively robust (Qian et al., 2003).

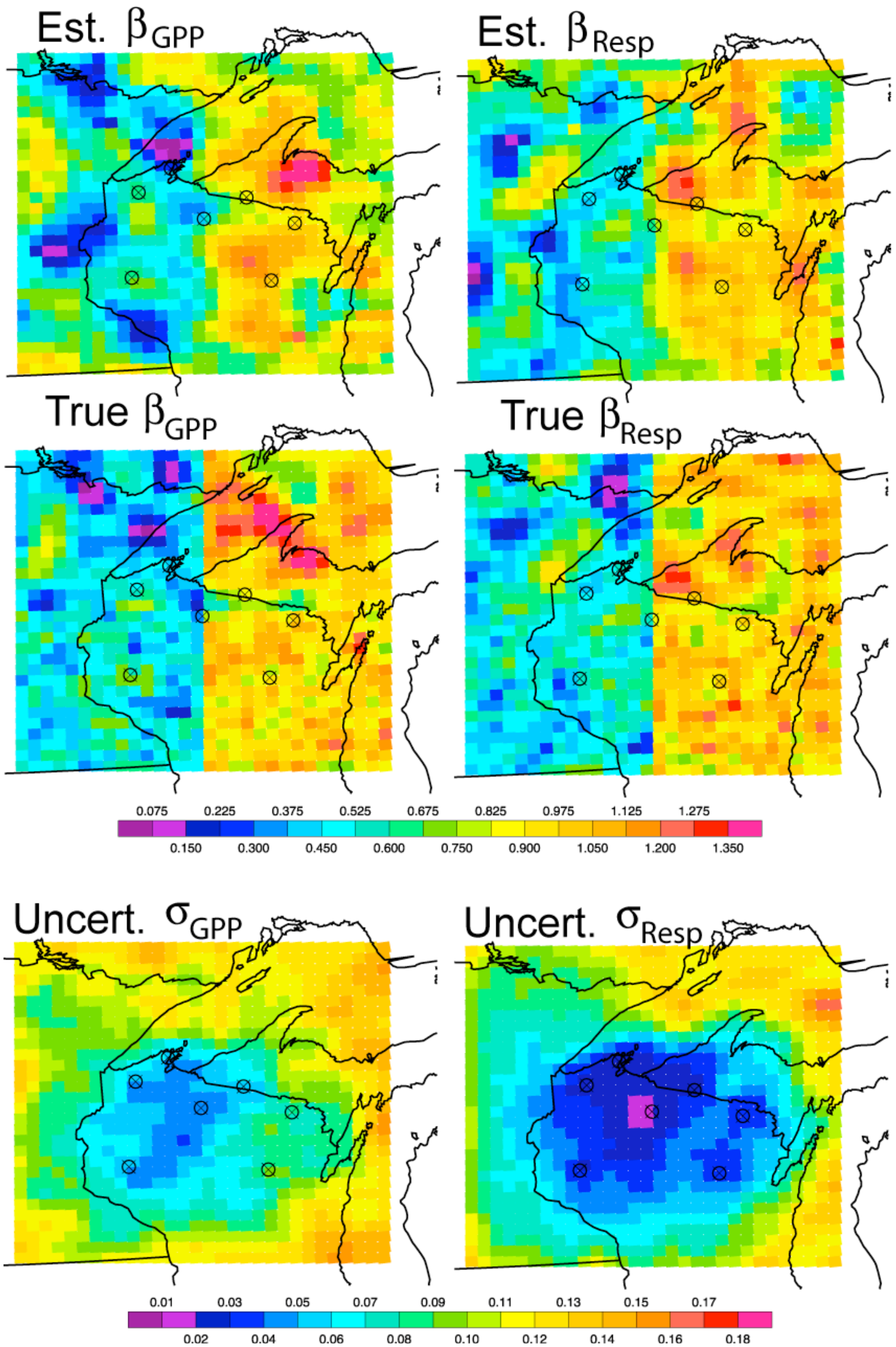

Figure 4: Assimilation of synthetic Ring [CO_2] using SiB-RAMS-LPDM-MLEF. Top panels show gridded estimates of biases in GPP (β_{GPP}) and ecosystem respiration (β_{Resp}) on a 20-km grid after 7 assimilation cycles of 10 days each. Small circles with X's indicate sampling sites. Prior guesses for both biases was a uniform value of 0.75. Middle panels show the prescribed "true" distribution. The lower panels show the estimated uncertainty (1σ). See text for details.

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5.2.6 Cloud-resolving model

We will use terrestrial ecosystem CO_2 flux estimates from the inversions described above (continental scale provided by the NACP NASA project at CSU, merged with fluxes derived via this project from the higher data density in the MCI) plus RUC-13 analyses to perform short (e.g., 2-week) forward RAMS simulations of the central MCI domain (central Iowa) with 500 m horizontal resolution. Crop coverage will be specified according to data provided by West (see letter of suport). Other vegetation types and land use will be specified from MODIS. Fossil fuel emissions scaled by population will be taken from Gurney et al's NACP NASA project.

5.3 Experimental plan

5.3.1 Tower Network Inter-calibration

Ensuring the agreement between the systems and their absolute accuracy is essential to this project, as even small biases can introduce significant errors into inversion studies of the carbon budget. Several measures to ensure accuracy, including the use of a target tank, pressure tests, and monitoring the sample dew point, are employed at each site individually. In addition, inter-calibration activities among the sites are proposed, including installing one system at a well-established NOAA-ESRL site, providing an archive tank for each site, and transporting a roving system with independent calibration tanks to each site. A system was deployed at WLEF during the summer of 2005, collocated with a NOAA-ESRL long-term CO_2 mixing ratio measurement site for cross-network calibration purposes. This system will be re-deployed to a newer NOAA tall tower (e.g., central Iowa) once it is established. The use of an archive tank and roving system are discussed below.

An archive tank will be provided at each site and sampled once a day. The life span of the archive tanks is expected at least 10 years, but the tanks require recalibration every 3 years. The primary purpose of an archive tank is to act as an accurately known concentration to detect any long term drifts of the four calibration gasses due to frequent extraction, especially toward the end of their life time. Any abrupt changes in the measurements caused by replacement of the working tanks will also be signaled by errors in the retrieved value of the mixing ratio of the archive tank. Note that archive tanks will be used only for the "backbone" AmeriFlux sites, and not for the campaign instruments set out for the midcontinental intensive.

The roving system will have its own set of five (small) high-precision NOAA-ESRL tanks. Four of the tanks will be used as calibration tanks and one as a target tank. The roving system will be transported to each site for duration of 3 – 4 days twice per year during maintenance visits. Ideally, at each site a separate sample line will be placed parallel to existing sample line, so that the simultaneous measurement can be done by both systems completely independent of each other. Depending on the sample height, completely separate tubing may not be feasible. In that case, a tee with the same length tubing to each instrument (to avoid introducing lags) will be used. The roving system method will be able to detect errors due to leaks anywhere within the system, working tank drifts, problems with flow rates, or insufficient drying of the samples. A roving system will ensure that each site in the network is in good agreement with the NOAA precision requirements.

5.3.2 Inverse estimation methodology

One of the most challenging aspects of this project will be evaluating the inversion methodology. Section 5.2 describes the methods that have been used in the Ring of Towers experiment. As noted, SiB was run as a prior flux estimate, and the atmospheric inversion solved for respiratory and photosynthetic bias factors on ten day time steps. While the Ring project resulted in development of the regional inversion tools, and showed that the regional inversion using the Ring observations is a viable approach (Figure 4), it did not examine the method of inversion in detail. This project will analyze and refine the inversion methodology in hopes of determining recommended approaches to conducting these regional inversions.

We will not experiment, in this project, with our flux prior (SiB/CASA), or the atmospheric transport model (RAMS). While valid, this is beyond the scope of this investigation. The ways the inversion can be varied that we will consider include:

i) the spatial and temporal resolution of the quantities that are solved for;
ii) the method of assimilation (e.g. Markov Chain Monte Carlo or MLEF);
iii) the quantities that are estimated (e.g. model parameters, flux corrections);
iv) the spatial and temporal coherence of the quantities that are solved for;
v) estimation of SiB/CASA using AmeriFlux observations in the region.

We will focus on estimating and correcting for three sources of error between SiB/CASA and the true terrestrial fluxes: (1) errors in model parameters (e.g. Vcmax, the maximum photosynthetic rate); (2) errors in poorly observed state variables (e.g. soil carbon pools); and (3) missing processes (e.g. application of fertilizer, time since logging or plowing) that cannot be represented in SiB/CASA as it is currently formulated. We hypothesized that these sources of error have different spatial coherence, and lead to errors of varying temporal coherence. We therefore propose the following approach towards the effective use of the available data and to move towards an accurate regional inversion.

SiB/CASA will be optimized by assimilating AmeriFlux eddy-covariance flux records from the midcontinental region. Model complexity will be reduced so that the number of remaining parameters is fairly well matched to the information content of the flux tower data sets. We will carefully benchmark these different choices of model complexity using cross validation. We hypothesize that a small number of universal parameters will explain much of the region's flux tower record. Success of the VPRM model (D. Matross, personal communication) in explaining data from multiple flux towers suggests that this is likely to be the case. We will test this by seeing if the estimated model parameters (e.g. Vcmax) from multiple towers converge. If this is the case, then the estimated parameter can be used to derive a reasonable description for the study region. If not, then there is a source of variability which is not captured in the model. This step in the analyses will address the hypothesis about the spatial and temporal coherence of the flux model-observational bias. A second test whether the model succeeds in finding a coherent parameter set consists of comparing two assimilation experiments. One experiment will estimate the joint pdf of the model parameters separately for each flux tower. A second experiment will estimate a joint pdf of the model parameters valid for all towers. If the model succeeds in describing these fluxes coherently, then the predictions of the joint assimilation will be a reasonable representation ($r^2 > 0.9$) of the predictions derived from the separate assimilations.

We will study the space-time coherence of the model-data differences computed as part of this assimilation step. The coherence of these differences will guide the space-time coherence of the quantities which we solve for when running the inversion. The coherence of observed state variables such as woody biomass or disturbance patterns from forest inventory, and soil types and tillage patterns from agricultural databases (e.g. letter of support from Dr. Tris West, collaboration in the forests of northern Wisconsin with Dr. Paul Bolstad) may also serve to guide our choices regarding coherence of our inversion method.

Finally, we will conduct the atmospheric inversion. We expect that the best approach will be, like the Ring of Towers, to solve for an unresolved model bias. We further expect, however, that the assimilation of flux tower data will have shown that the model-data bias is consistent over time and space, justifying a bias that is coherent in time and space. We will, in addition, consider the possibility of optimizing a state parameter, such as soil carbon content, in addition to, or in place of, a model bias.

This algorithm, which we anticipate to be the "best" approach for conducting the inverse estimate, will be compared to several alternative approaches including:

i) proceeding without assimilating SiB/CASA with the regional AmeriFlux towers;
ii) assuming highly coherent vs. highly incoherent bias factors, rather than using coherence suggested by the statistics of the model-data differences;
iii) inverting for model parameters, or a combination of model parameters and bias factors, instead of inverting for simple photosynthetic and respiratory bias factors;
iv) using Markov Chain Monte Carlo vs. MLEF assimilation methods for the SiB/CASA model.

The success of these various approaches will be evaluated in two ways. First, the error structures of the solutions will be examined. The temporal autocorrelation structure of the residuals (at any given tower site) will be analyzed using ARIMA time series models. The spatial autocorrelation structure will be estimated by estimating hyper-parameters in a class of general correlation functions (Gneiting, 2002).. This characterization of the autocorrelation structure will yield two important insights. First, this will allow us to correct for the effects of autocorrelation in the formulation of the likelihood function (cf. Zellner and Tian, 1964). Second, this provides an important input for the estimation of bias factors in the atmospheric inversion. Since certain assumptions (e.g. highly coherent bias) will imply a very well-constrained solution whether or not the assumed coherence is correct, however, this measure is of limited value. Our second means of evaluating our various inversion methods is to aggregate fluxes and compare the aggregated fluxes to independent, bottom-up flux estimates created as part of the broader NACP midcontinental intensive. An obvious choice in this study region is to compare to seasonal crop yield data (see letter of support from Dr. Tris West, ORNL). While ecologically we are more interested in annual terrestrial fluxes, seasonal fluxes such as crop yield are large, can be measured with good accuracy, and are independent of our inverse method, thus are a good choice for evaluating our methods.

5.3.3 Comparison of inverse estimates of regional terrestrial CO_2 fluxes to bottom-up fluxes

As noted above, our inverse estimates will be aggregated to regional fluxes at various temporal and spatial scales, and compared to available bottom-up flux estimates from the midcontinental intensive. These comparisons, when independent, will serve as a measure of confidence in the various methods.

This top-down, bottom-up comparison is the primary purpose of the MCI, and proves or disproves the overall NACP concept. This is central to both MCI and the NACP, and is explicitly called for in the NACP science implementation strategy. The density of sampling available via the regional experiment maximizes our chances of successfully validating the NACP concept.

5.3.4 Data density test.

Our hypothesis concerning that degree to which the proposed "backbone" atmospheric CO_2 monitoring network is sufficient to derive fluxes in the midcontinental region will be examined in a very simple fashion. We will systematically eliminate data sources from our inverse estimates, and show uncertainty in regional fluxes as a function of the density of observations in the region. This test of the atmospheric sampling required to yield successful regional flux estimates is also central to the NACP science implementation strategy.

5.3.5 Sensitivity to high resolution transport

The CO_2 flux and mixing ratio fields will be compared in detail to tower and airborne flux and mixing ratio data. NOAA airborne profiling and tall towers, continuous CO_2 data at towers funded via this project, airborne mixing ratio surveys (see letter of support from Dr. Steven Wofsy), and airborne and tower flux measurements are all candidates for comparison to these high resolution model runs.

The logic for this experiment is as follows: Consistency between observed and simulated flux and mixing ratio fields implies that the methods used to derive regional fluxes (the inversion methods described above) were successful, and that the spatial and temporal resolution of the atmospheric transport used to derive those flux estimates was sufficient. If, on the other hand, there are systematic biases between the modeled mixing ratio fields and the observations, this suggests that the fluxes derived are dependent upon the resolution of the atmospheric transport model used to perform the inverse estimate.

5.3.6 VTT evaluation at other tall towers

Surface layer towers, either cell phone or flux towers, are used extensively in this study. Questions remain, however, regarding the gradient in mixing ratio between the mid-boundary layer and surface layer, which must be simulated by an atmospheric transport model or eliminated from the data via a micrometeorological method. This gradient function has been computed at the WLEF tall tower, but evaluation at one or more additional towers would be beneficial. We will therefore evaluate the top-down and bottom-up gradient functions for at least one other tall tower hosting flux and mixing ratio measurements (e.g. South Carolina if funded; Norunda, Sweden).

6. Management Plan/Evaluation Phase

6.1 Management. The project can be divided into 5 logical units of work:

6.1.1 Instrumentation. This covers instrument manufacture, instrument deployment and maintenance, intercalibration and data collection. This will be managed by **Richardson** and **Miles**, who have developed the instrumentation, deployed the Ring of Towers project, and currently manage the network of AmeriFlux sites with PSU's highly-calibrated CO_2 instruments.

6.1.2 Data management. Includes data processing, archiving, and dissemination. This will also be managed by **Richardson** and **Miles** who will participate in supervision of the project graduate research assist, and who will be primarily responsible for supervision of a technical programmer in years 2 and 3, who will ensure careful data processing and broad dissemination of the mixing ratio data from the experiment. Data (CO_2 mixing ratios) will be reported to a PSU web site, and be submitted to NOAA's Globalview-CO_2 data archive.

6.1.3 Flux assimilation. This involves gathering AmeriFlux flux observations and regional carbon stock data, assimilation these data into SiB/CASA, and evaluating the SiB/CASA – flux data residual to study the character of the model bias. This activity will be directed by **Keller, Denning** and **Davis**, with contributions from Miles and the PSU and CSU graduate students. Joint analyses will ensure ample analyses and comparison of a complex topic.

6.1.4 Atmospheric inversions. Includes running the inversions, and analyses and archiving of the inversion results. **Denning** and **Zrukanski** will port their methodology to PSU where the entire senior staff will take part in the analyses and supervise the project graduate student. Inversion experiments will also be run at CSU. Join analyses will ensure strong model-data intergration and ample analyses of this complex topic.

6.1.5 High-resolution forwards modeling. Denning will lead this effort, supervising the graduate research assistant at CSU.

6.2 Evaluation metrics. Project metrics are closely linked to the project objectives. The project will be successful if, through peer-reviewed publications and dissemination of project data:

1. The AmeriFlux and "new Ring" CO_2 measurement networks are both operational in early 2007. The sites should collect more than 80% of possible data at each site. The level of precision and accuracy of the CO_2 mixing ratio measurement network is established via intercalibration activities, and is small enough to be of use for inversion estimates.
2. We establish characteristics of flux model – flux data mismatch in the MCI study area, particularly the characteristic length and time scales of this bias.
3. The flux model – flux data mismatch suggests optimal strategies for conducting inversions that successfully assimilate both regional, continuous CO_2 observations and AmeriFlux eddy-covariance observations.
4. We determine whether or not the NACP approach – convergence of top-down and bottom-up regional flux estimates, can succeed given the available resources.
5. We establish whether or not, and to what degree cloud-resolving atmospheric transport models are necessary to determine regional flux estimates via atmospheric inversions.
6. We quantify the tradeoff between the density of atmospheric CO_2 mixing ratio measurements in the midcontinental region, and the accuracy of inverse estimates of regional terrestrial carbon fluxes, and rank the value of various observation types, including aircraft profiles, tall towers, and surface layer towers.
7. We learn if the surface layer to mid-ABL CO_2 gradient measured at the WLEF tower follow the same micrometeorological scaling laws at a second tall tower site.

In addition to the scientific progress metrics, we also intend for the products of this investigation, especially the CO_2 data, to serve a broad community of researchers. To that end, we propose the following additional metrics:

8. Project CO_2 measurements will be readily available to the scientific community and utilized by at least five additional research groups within the span of this project
9. Inverse flux estimates produced for the 12-18 month intensive will also be available to the community, and used as a source of comparison by at least three independent bottom-up modeling efforts.

7. Project Performance Site

Research will take place at multiple sites across the United States, with a focus of work in the upper Midwest. Analyses will be conducted primarily at Colorado State and Penn State.

8. Merit Review Criterion Discussion and Expected Results

1. Scientific merit of the project: The success of the "Ring of Towers" approach at reducing inversion uncertainty (see Figure 4) suggests that this project will arguably provide the best potential for success of the NACP approach of convergent bottom-up and top-down regional flux estimates. This is true because of the data density this project brings to the MCI. Regional inversion is a data limited problem. Excellent inverse modeling in the absence of data cannot succeed. Oversampling the regional is an essential element of testing the data density required for the NACP approach to succeed, and oversampling at long time scales (more than 12 months) is most applicable to evaluating the ability to derive annual regional carbon balance with the proposed NACP observing backbone. Thus project represents a central and essential methodological test for the NACP. The project will also make substantial progress into the intellectually rich domain of optimal data assimilation methods, particularly in terms of how to best utilize networked AmeriFlux observations. This is a major scientific conundrum in the inverse modeling community.

2. Appropriateness of the proposed method or approach: This work builds directly upon past DOE TCP support, and relies heavily upon the infrastructure of AmeriFlux, consistent with the intent of the RFP. The methods proposed are central to the NACP science plan, and arguably the best tools available for characterizing terrestrial carbon cycling at regional scales.

3. Competency of the applicant's personnel and adequacy of the proposed resources: Project personnel have a long history of collaboration and productivity, and extensive experience with the proposed experimental methods.

4. Reasonableness and appropriateness of the proposed budget: The budget for the project is large, but it should be recognized that this represents an integrated modeling/measurement proposal from two institutions, and that observations should serve a much broader MCI (Ring deployment) and NACP (AmeriFlux backbone CO_2 measurements) carbon cycle science community. The research questions are modular to a degree, and the budget could be cut back with a concomitant limit of the scope of the project. Limited observational resources, however, are putting the basic viability of the MCI in danger. This project will bring much needed observations to the intensive.