Reporting Categories: Checklist

1. Participants: Who has been involved?

•What people have worked on the project?

Mel Nicholls, Lara Prihodko, Marek Uliasz, Scott Denning, Lixin Lu, Ian baker, John Kleist, Connie Uliasz, Chris Eller, Amy Dykstra, Jason Rist, and Owen Leonard

•What other organizations have been involved as partners?

Closely related research activities at CSU supported by NOAA, NASA, and DoE (A. S. Denning, PI)

•Have you had other collaborators or contacts?

Ken Davis (Penn State Univ)

Peter Bakwin (NOAA CMDL)

Steve Wofsy (Harvard U)

2. Activities and Findings: What have you done? What have you learned?

•What were your major research and education activities?

We have developed and tested a set of atmospheric inverse methods for estimation of the regional exchange of CO2 with the land surface (from the "top down") and modeling the linkage of biophysics, biogeochemistry, meteorological, and atmospheric transport processes to be tested against various observables (from the "bottom up"). The methods we have developed are also applicable to other carbon cycle models and to new data sources (e.g., COBRA, and measurements made under the North American Carbon Program).

All of the work described in this section has been performed with support from other agencies in addition to the relatively modest contribution from NSF-IRC (including US DoE/NIGEC, DoE/TECO, NASA, and NOAA).

Major research activities included:

1) development of a method for quantitative estimation of regional surface CO_2 exchange and its uncertainty from continuous atmospheric [CO_2] measurements;
2) investigation of information content in eddy correlation timeseries and consequent ability to quantify physiological parameters in a spatially-explicit regional carbon cycle model (SiB2);
3) quantification of time-varying uncertainty in simulated fluxes of heat, water, and carbon on hourly and seasonal time scales that results from uncertainty in ecophysiological parameters;

4) coupling of a numerical model of ecosystem physiology (SiB2) to a mesoscale model of weather and atmospheric CO_2;
5) evaluation of mesoscale simulations of surface CO_2 exchange and atmospheric CO_2 mixing ratio against measurements made at a tall tower, over both eddy-resolving local and 1000x1000 km regional domains; and
6) investigation of the sensitivity of regional coupled simulations of land-atmosphere carbon exchange to the resolution of satellite imagery used to derive spatial variations of ecophysiological parameters.

Educational activities supported under the NSF-IRC grant **(also listed below under "training and development")**:

1) several years of graduate study and research by Lara Prihodko, leading to a PhD in Ecology (Colorado State University) in 2004;
2) Contributed to a summer mini-course on Carbon Cycle Data Assimilation at the National Center for Atmospheric Research (NCAR), summer 2002; and
3) Contributed to a summer mini-course on Carbon Cycle Modeling and Data Assimilation at the Colorado State University (Program for Interdisciplinary Study of Mathematics, Ecology, and Statistics (PRIMES), summer 2003).

•What are your major findings from these activities?

1) Modeling Framework for Regional Inversions

We have developed inverse modeling techniques for the estimation of regional-scale CO_2 fluxes from atmospheric concentration measurements. The Bayesian inversion method is commonly used to estimate surface CO_2 at continental scales. However, the application of this approach to the limited domains used in mesoscale or regional scale modeling is more challenging. In addition to the estimation of surface CO_2 flux, it is necessary to evaluate unknown CO_2 fluxes through lateral model boundaries. This is critical for understanding CO_2 fluxes, as the inflow flux may be several orders of magnitude larger than the CO_2 flux from the surface of the regional modeling domain.

A modeling framework has been developed to examine regional scale inversion problems and has been preliminarily tested using model-generated pseudo-data. The proposed approach is based on the Lagrangian Particle Dispersion Model (LPDM) (Uliasz, 1994) applied in a receptor-oriented mode to derive influence functions for concentration sampling data. This framework allows us to estimate values for the unknown inflow (lateral) fluxes in regional or mesoscale domains. Three options are provided on how to obtain these inflow fluxes. They can be 1) estimated from observations, 2) obtained from larger scale models (eg. GCMs) where such concentrations are known, or 3) included as unknown parameters in inversion calculations.

Within the framework, with the aid of an adjoint equation technique, a concentration sample, $\Phi(C)$, can be expressed as the sum of contributions from different sources (Uliasz and Pielke, 1991):

$$\Phi(C) = \underbrace{\int_0^T \int_0^{L_x} \int_0^{L_y} qC^*\Big|_{z=0} dxdydt}_{\Phi_1} + \underbrace{\int_0^T \int_0^{L_y} \int_0^H C_W \tilde{u} C^*\Big|_{x=0} dydzdt}_{\Phi_2}$$

The first term provides a contribution from the surface source, q, while the second term is a contribution from the inflow flux, where C_W is the tracer concentration and $\tilde{u}$ is the wind velocity at the upwind boundary. For simplicity, only the inflow flux through western boundary is considered here. C^* is the influence function describing potential contributions from different potential sources into concentration at the receptor. Both terms are integrated over the entire modeling domain $L_x \times L_y \times H$ and time period of the simulation.

The influence function is derived from model particles released from the receptor and traced backward in time. The total mass of particles released from a given receptor is equal to 1. Different volumes and release times can be considered to represent samples from various observational systems. The influence function in the first and second term is derived in by counting particle mass, m_p or $m_p\tilde{u}$ in layers adjusted to the surface or the lateral upwind boundary correspondingly.

A series of numerical experiments was performed in order to test the framework. Different sampling strategies were tested, including aircraft vertical profiles through the boundary layer and time series of concentrations from a tall tower. Tracers included those constant in time flux, and those variable in time flux, which correspond to CO_2 diurnal fluxes. The simulations were performed over 500x200 km regional domain using the idealized 1-D simulation of diurnal cycle of the planetary boundary layer over homogenous terrain (roughly corresponding to the WLEF tall tower location in Wisconsin). Since the modeling domain was limited, all calculated concentrations can be interpreted as regional perturbations from large-scale fields.

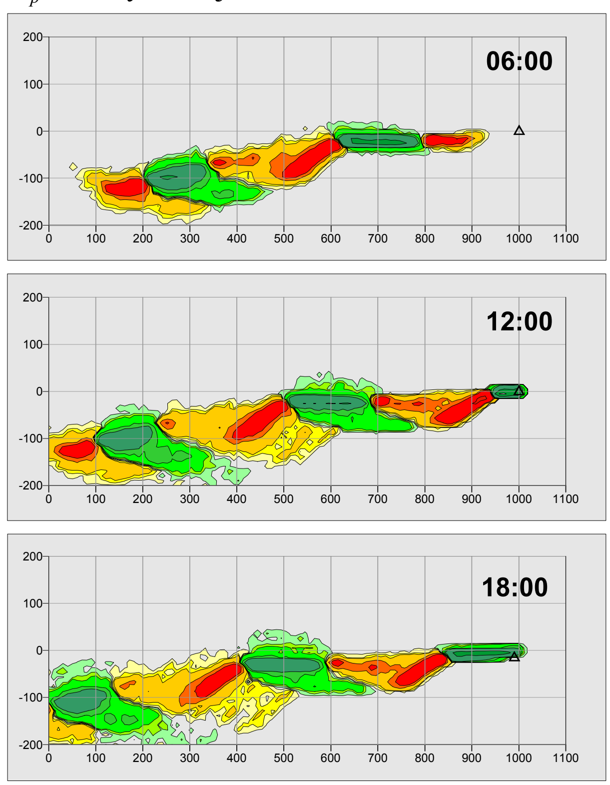


Figure 1: Examples of influence functions calculated for the CO_2 concentration samples at different times of day.

The influence functions derived from the Lagrangian particle model linked to RAMS are an essential part of the modeling framework developed to estimate surface fluxes from concentration data and evaluate different sampling strategies. The influence function provides information on contributions from different source areas into the concentration observed at the receptor. Figure 1 presents examples of influence functions calculated for the CO_2 concentration samples taken at a 400m height at different times of day. The red and green areas indicate positive (respiration flux) and negative (assimilation flux) contributions respectively.

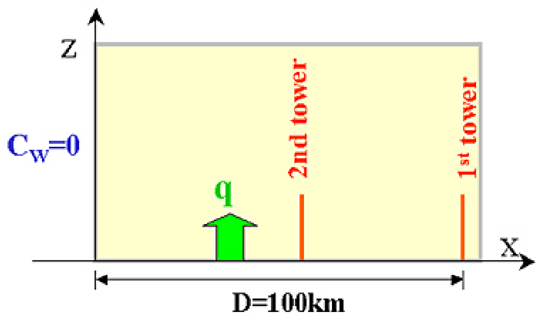


Figure 2 shows an example of an estimation error (RMSEflux) for a 24 hour net CO_2 flux from a 100km upwind source using different amounts of information from two tall towers with five levels of concentration measurements up to 400m. No inflow flux at the upwind boundary was taken into consideration. The 24 hour time concentration time series are used starting from the lowest level (30m) of the first (downwind) tower. The blue and red lines correspond to observational data of different accuracies (standard deviation equal to 0.2 and 1 ppm respectively). The inversion calculations become successful when at least 24-hour concentration data from the downwind tower are included. This figure also demonstrates how much the accuracy of flux estimation is improved when additional data from upper levels and finally data from the second tower in the middle of the source are added. The example was created using an idealized simulation of the boundary layer diurnal cycle and model generated concentration pseudo-data.

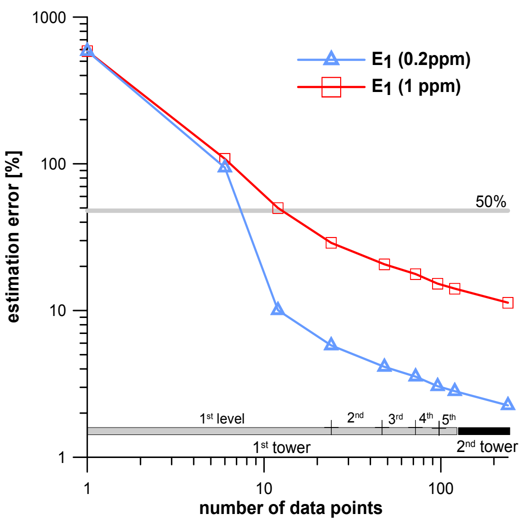


Figure 2: Example of estimation error for net CO_2 flux.

2) Parameterization of an ecophysiological model (SiB2) using measured fluxes

In a series of analyses, sources of error, potential for bias and impacts of model and data choices in the context of regional carbon cycle modeling of temperate, forested ecosystems were evaluated. A comprehensive sensitivity analyses was conducted to evaluate the sensitivity of a commonly used, complex biophysical land surface model to its parameterization through time (Simple Biosphere Model - SiB2.5). Parameter sensitivity was assessed with respect to the ability of SiB2.5 to predict fluxes of latent and sensible heat as well as the net ecosystem exchange of carbon as measured on a flux tower at both monthly and annual time scales.

In conducting the sensitivity analysis, in which tens of thousands of simulations were run with randomly varying but realistic parameter sets, it was found that there was an irreducible level of mismatch between the simulated and observed fluxes. This minimum possible error reflects a difference between simulated and observed fluxes that cannot be

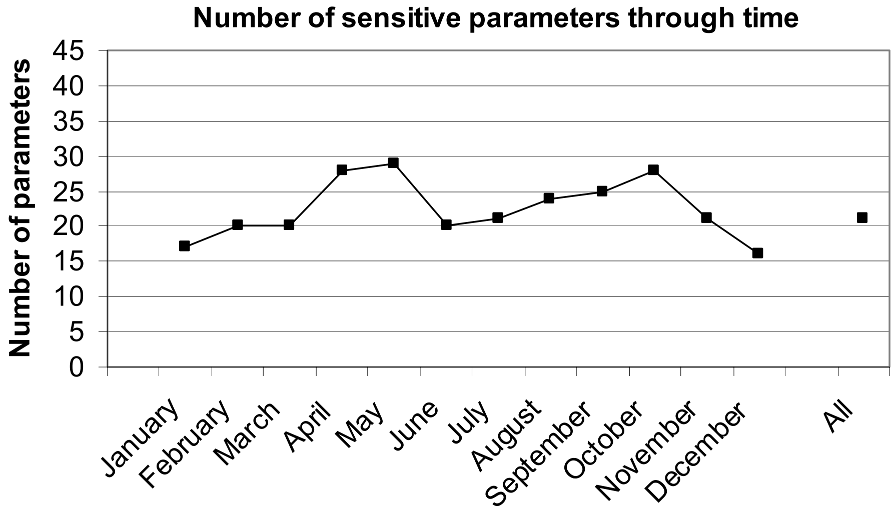


Figure 3. Number of parameters the SiB2.5 model was sensitive to through time for a temperate mixed forest. The model was conditioned on observed fluxes of latent and sensible heat and the net ecosystem exchange of carbon.

overcome through optimization due to variability (or noise) in the observations and/or structural problems with the model. The sensitivity analysis also revealed that the number and identity of influential parameters varied considerably by month. The greatest sensitivity to parameters, both in the magnitude of the sensitivity as well as in the number of parameters, occurred during those periods of rapid land surface change surrounding leaf-on in the spring and leaf-off in the autumn, the shoulder seasons (Figure 3).

3) Uncertainty analysis of simulated surface fluxes with respect to model parameters

The results of the sensitivity analysis were then used within a Bayesian framework to calculate the uncertainty of land surface fluxes predicted by the model attributable to the parameterization.

The uncertainty analysis indicated systematic biases in predicted fluxes. Uncertainties in the simulated fluxes were quite large relative to measured fluxes during the shoulder seasons. This was attributed to the estimation of time-varying vegetation parameters with a single, monthly maximum-value-composited satellite product and linear interpolation between months. When model parameterization was allowed to vary monthly, much of the uncertainty was reduced (Figure 4). However, there were still within-month biases indicating that information at a finer time scale resolution could reduce uncertainties further for these sensitive periods.

Our results reveal a quantifiable level of model-data mismatch that could be used as a prior uncertainty in regional atmospheric inversions, and suggest that the potential for reduction in uncertainty appears to be greatest during the periods of rapid land surface change surrounding leaf-on in the spring and leaf-off in the autumn.

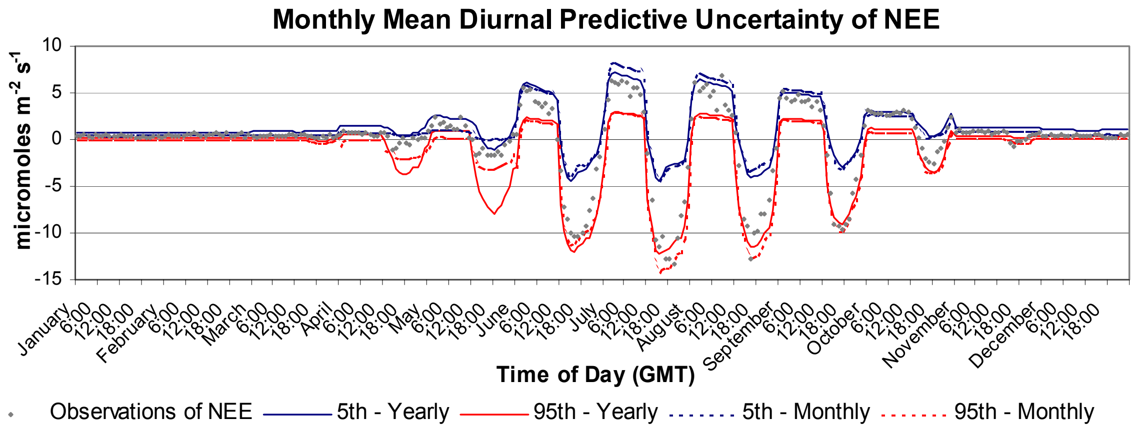


Figure 4. Monthly mean diurnal uncertainty in simulations of net ecosystem exchange conditioned on fluxes of latent and sensible heat and net ecosystem exchange for a temperate mixed forest.

4) Evaluation of High-Resolution 2D Coupled SiB-RAMS Simulations at Local Scales

In addition to the "inverse" modeling studies described above (estimating surface fluxes from measured atmospheric CO_2 and physiological parameters from observed fluxes), we have performed "forward" experiments of fully coupled atmosphere-ecosystem interactions using SiB2 in the Regional Atmospheric Modeling System (RAMS). We have published two simulation experiments investigating some of the mechanisms leading to CO_2 variability, both on local (Denning et al, 2003) and regional (Nicholls et al, 2004) scales. We were interested in exploring the signal to noise ratio of CO_2 variability to ascertain to what extent meteorological processes versus biological processes lead to atmospheric variations in CO_2 concentrations. To the extent that hey cannot be correctly captured by the transport model used for atmospheric inversion, variations of CO_2 concentrations due to meteorological processes can be considered as "noise" in the measured signal. This is an important consideration if meaningful interpretations of CO_2 measurements at tall tower sites and by aircraft are to be made.

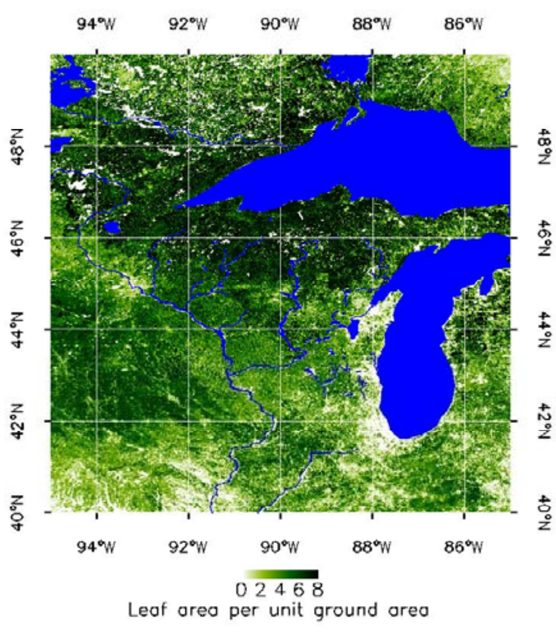


Figure 5: Leaf area per unit ground area (LAI) for the mesoscale domain, July 1995. Leaf area index is one of 8 time-varying parameters required by SiB2

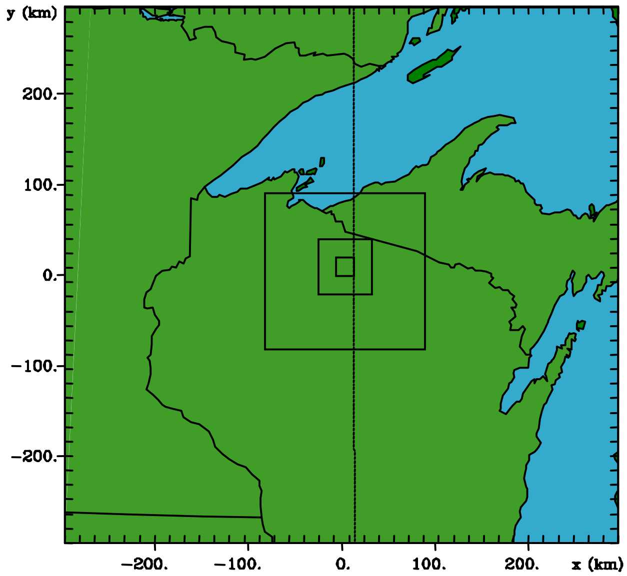


Figure 6: Model domain and outline of 3 nested grids.

Mesoscale parameter sets were generated on a 1 km grid for a 1200 x 1200 km area surrounding the WLEF tower (see Figure 5 for an example). Soil moisture was not known over the entire grid, so as an alternative we used the initial moisture from WLEF and weighted it across the domain by soil type. Soil respiration was parameterized by biome rather than at each point since the parameterization we use requires an annual simulation and more than one million simulations would have been required.

The simulation was run for a five-day period from July 26 to July 30, 1997 (for which we have excellent, continuous measurements of fluxes and CO2 concentrations at the WLEF tower). Multiple nested grids were employed, which enabled mesoscale features to be simulated and which resolved small-scale features in the vicinity of the WLEF tower. Figure 6 shows the coarse grid domain and outline of the three nested grids used by the coupled SiB2-RAMS model. The horizontal grid increments were 16km, 4km. 1km and 333m, for grids 1,2,3 and 4, respectively. There were 45 vertical levels. The vertical grid increment was 20m next to the surface and was gradually stretched to the top of the domain at 7.2km. Vegetation classes and the 47 SiB2 parameters were determined for the region. Surface elevation was obtained from 30-second data sets supplied by the United States Geological Survey (USGS). Atmospheric fields of pressure, potential temperature, relative humidity and winds were obtained from 2.5 degree National Centers for Environmental Prediction (NCEP) reanalysis data and interpolated by the RAMS analysis package to the coarse grid mesh at six hourly intervals. The gridded data files produced were used to initialize the model and to nudge the lateral boundaries and the upper levels of the domain during the simulation.

Simulated values of short wave radiation, potential temperature, water vapor, wind velocities, sensible and latent heat fluxes, carbon dioxide concentration, and carbon dioxide fluxes for the fine grid, were compared with observations made at the WLEF tower. Overall the agreement with observations was reasonably good.

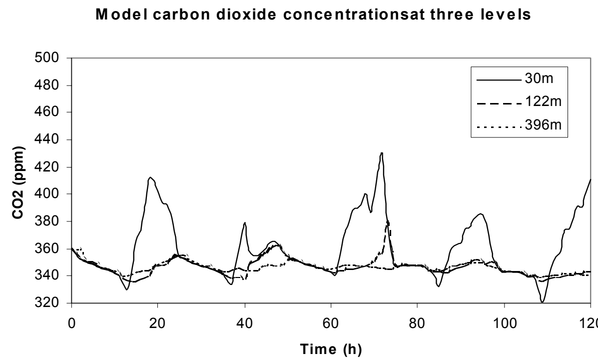
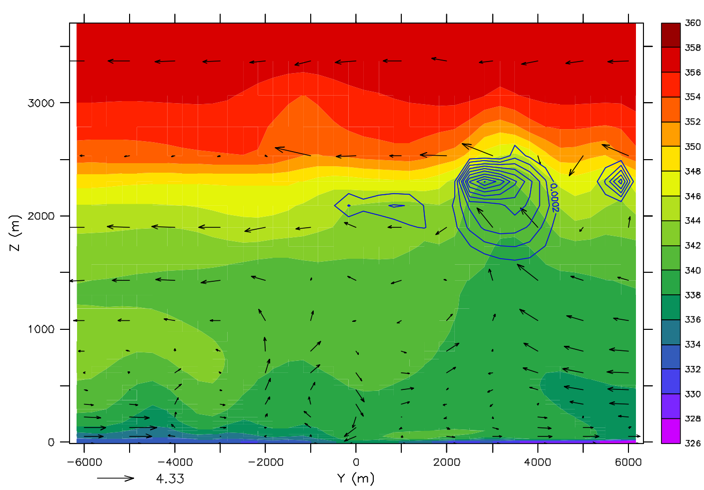


Figure 7: Observed and simulated carbon dioxide concentrations

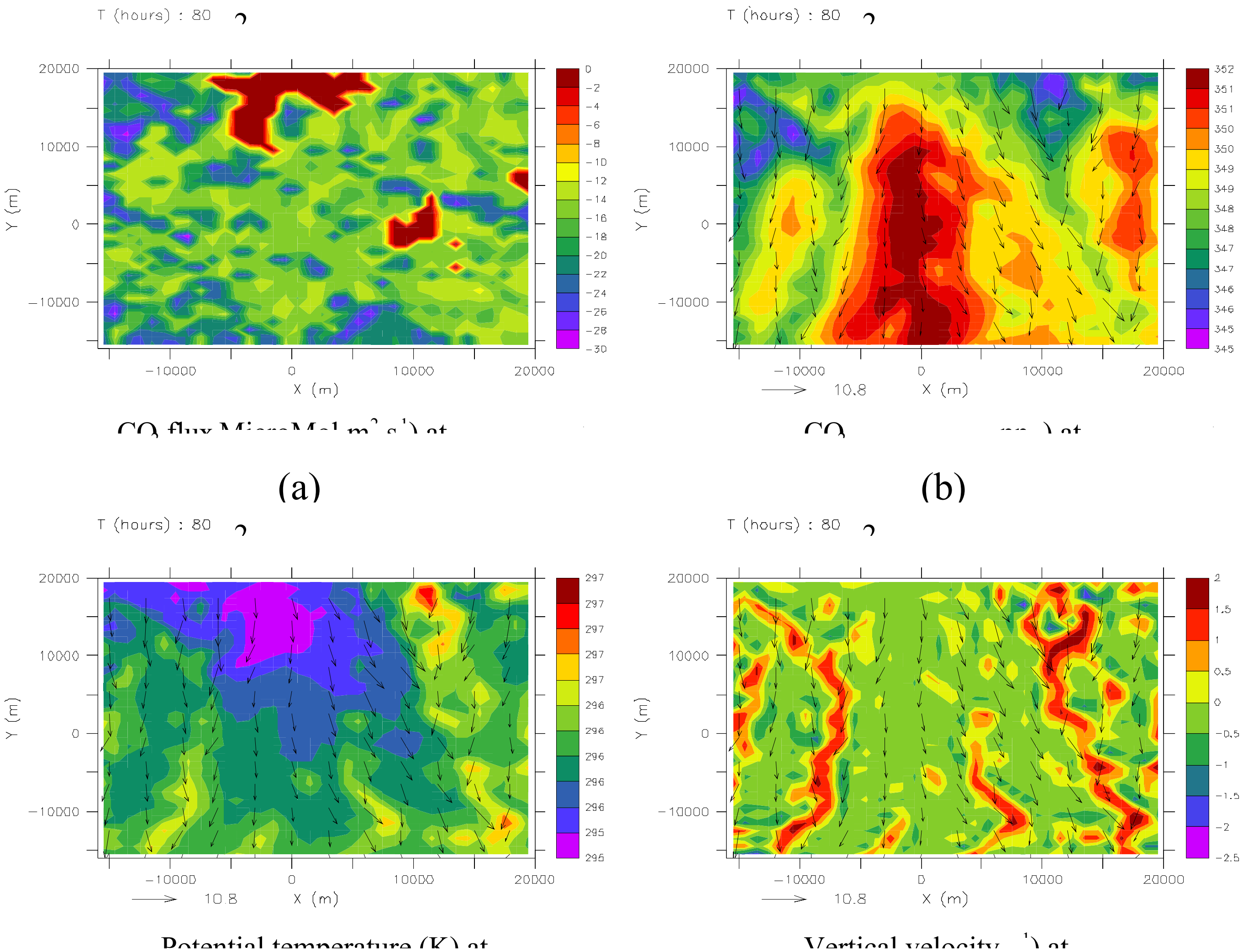
As an example, the observed and simulated values of carbon dioxide at three levels above the surface are shown in Figure 7. The model and observations show decreasing values of CO_2 during the daytime due to photosynthesis, occurring through a deep layer. During the night, respiration typically leads to high values in a shallow stable layer next to the surface. One discrepancy is the development of a minimum in a shallow layer next to the surface, just before sunset. This phenomenon may be attributable to misrepresentation of the extinction of direct beam radiation in SiB2 (Denning et al., 2003). Figure 8 shows a vertical cross-section through a cloud in the fine grid, at 5 p.m. LST. The cloud updraft has lifted air depleted in CO_2, resulting in an approximately 4 ppm difference in concentration between the cloud free air at the upper levels of with boundary layer. Also evident are small-scale turbulent boundary layer eddies which are resolved by the fine scale grid.



CO_2 concentration (ppm) and cloud contours

Figure 8: Vertical cross-section of CO2 concentration (ppm), wind vectors and contours of cloud water mixing ratio (kg/kg)

5) Evaluation of 3D Coupled SiB-RAMS Simulations at Regional Scales



(a) (b)

(c) (d)

Figure 9: Horizontal cross-sections at 396m above the surface for grid3.

We now move up in scale to the next grid, which has a grid increment of 1km. Figure 9a, b, c, and d, shows horizontal sections of the CO_2 flux at 30m above the surface and CO_2 concentration, potential temperature, and vertical velocity, respectively, 400m above the surface for grid 3 at 2 p.m. LST, during the fourth day. The lakes are clearly evident in Figure 9a since the fluxes from the water are zero. At this time there is a strong drawdown of CO_2 over the land. At 400m above the surface, relatively high concentrations are advected from the northern lake, where there is no CO_2 uptake, over the WLEF site. The temperature of the air above the lake is considerably cooler than over the land, which has warmed due to strong sensible heat fluxes. This colder air advects southward and slowly sinks bringing down higher values of CO_2 from aloft, which contributes to the CO_2 anomaly at this level, At the same time air is lifted on the margins of the cold sinking air, leading to narrow lines of upward motion. The upward motion lifts air depleted in CO_2 from nearer the surface. The contrast in CO_2 concentration between high and low values at this level is 6ppm, which is quite high for this relatively small area. These results indicate that small lakes could have significant local impacts on CO_2 concentrations, suggesting that interpretations of concentration anomalies at the WLEF site should be made with caution since they can be produced by purely physical advective effects on a scale of about 10km.

We now proceed to examine the larger regional scale variability. Figure 10a and b shows spatial variations of simulated CO_2 flux at midnight and noon during the fourth day of the simulation for grid 1. During the night there is stronger respiration to the south. This is quite highly correlated with temperature that tends to be warmer to the south. During the daytime the strongest uptake of CO_2 is focused near the center of the domain and occurs for the deciduous broadleaf vegetation class. Sensitivity tests indicate that the uptake tends to be more for the deciduous broadleaf class than for the mixed forest class since it has a higher temperature stress factor. Therefore, these trees are not as stressed by the warm temperatures that occurred during this period.

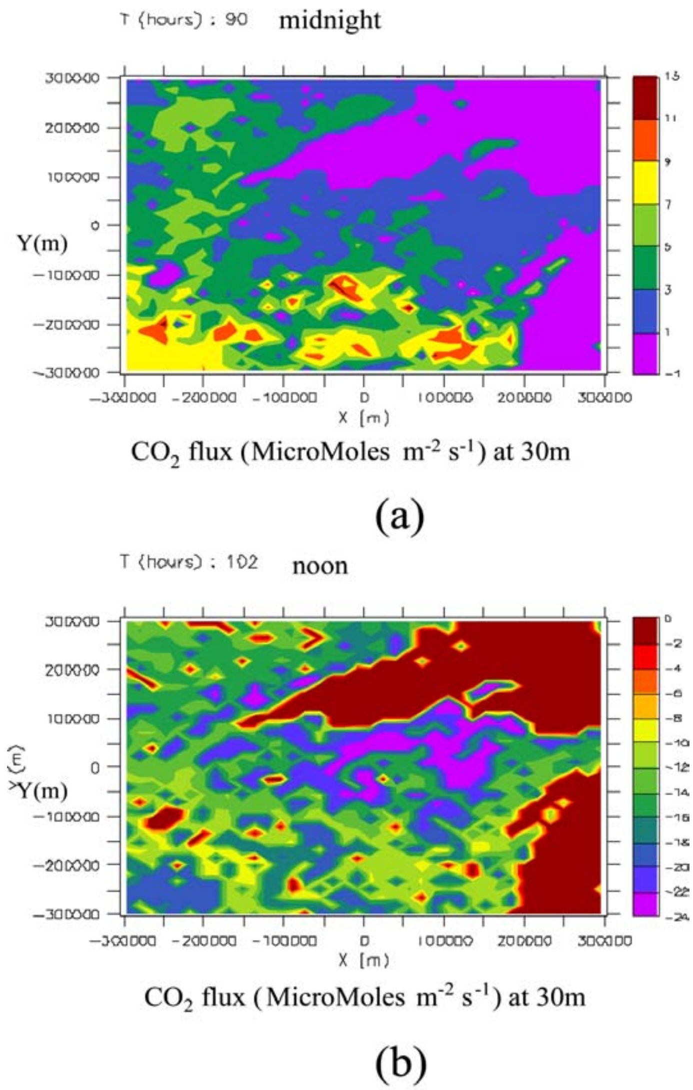


Figure 10: Simulated CO_2 fluxes for grid 1.

Figure 11 shows east-west and north-south vertical cross-sections of CO_2 concentrations at midnight and noon in grid 1 for the fourth day. The east-west section intersects Lake Michigan and the north-south section intersects Lake Superior. At midnight there are high concentrations in a shallow layer over land due to respiration. Above this is a deep residual layer of reduced CO_2 due to photosynthetic activity the previous day. Interestingly, very low values of CO_2 occur at midnight over Lake Superior and to a lesser extent over Lake Michigan. At noon low values of CO_2 are near the surface with relatively higher values over the lake. Despite the absence of CO_2 fluxes over the lake there was a very pronounced diurnal oscillation in CO_2 concentration, particularly over Lake Superior. It was found that katabatic winds, ambient winds, and the return flow of the lake sea breeze all played significant roles in causing this oscillation. This result indicates that there is a significant mass of CO_2 transferred off the lakes during the daytime and early on in the night, and onto the lakes later on in the night. It was also found that katabatic winds tended to cause pooling of CO_2 in valleys during the night. These results suggest that if regional scale CO_2 uptake is to be inferred from observations in this region, then account will need to be taken of these large-scale advective effects.

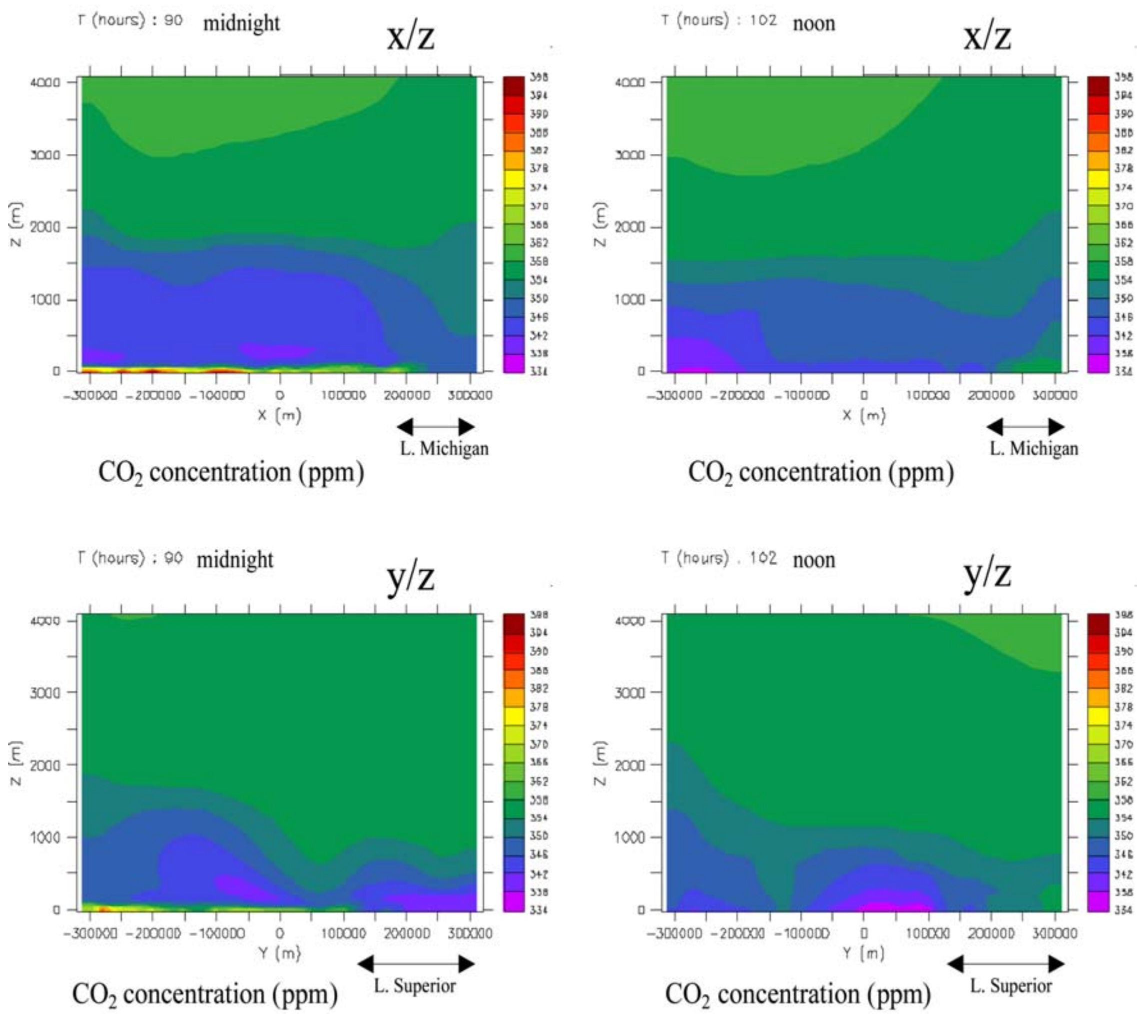
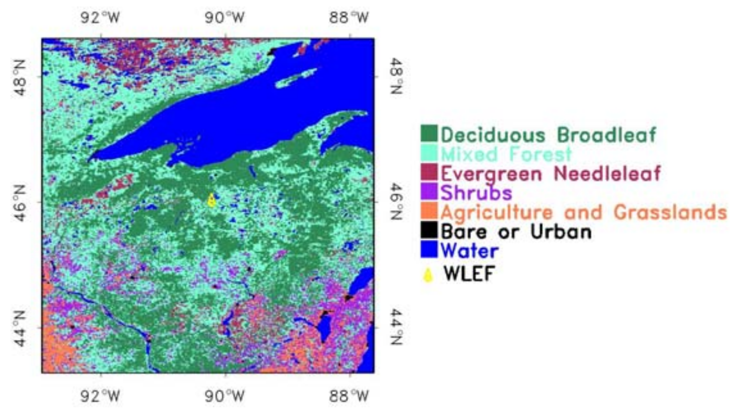


Figure 11: Vertical cross-sections of carbon dioxide for grid 1.

6) Sensitivity of Regional Fluxes simulated by SiB-RAMS to spatial resolution of land-surface heterogeneity



(a) **(b)**

Figure 12: The 640 x 640 km SiB-RAMS modeling domain vegetation class at **(a)** 1km and **(b)** 8km resolution.

The uncertainty in regional fluxes of carbon, water, and energy due to the resolution of spatial heterogeneity of the land surface was evaluated by specifying vegetation and soil parameters in SiB-RAMS from spatial data and imagery at different resolutions. 'Effective' 8km boundary conditions were created from the 1km data. Vegetation type was assigned by the dominant class in an 8 x 8km area (Figure 12). Soil percent sand and clay and monthly maximum NDVI were area averaged to 8km. Boundary conditions for the 8km simulations were calculated at 8km and then disaggregated to 1km. This was done because the resolution of the center grid of the SiB-RAMS simulation was kept 1km for intercomparability of results.

The SiB-RAMS simulations were set up with 3 nested grids: a 640 x 640km outer grid with 16km resolution, a 160 x 160km middle grid with 4 km resolution and a 38 x 38km fine grid with a resolution of 1km. The time steps for each grid are respectively 45,15 and 5 seconds. Twenty-three atmospheric levels were simulated and CO_2

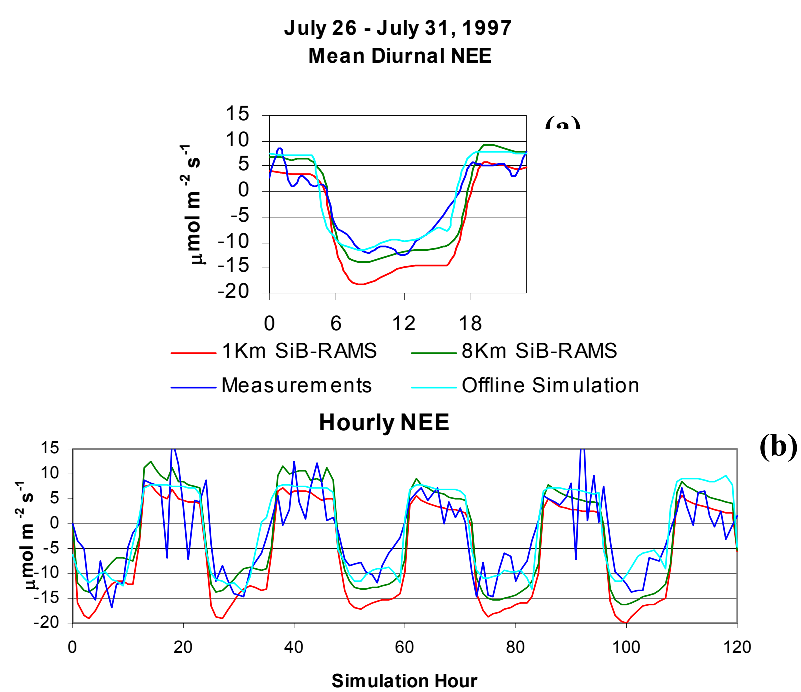


Figure 13: Measured and simulated Net Ecosystem Exchange at the WLEF tall tower site. **(a)** Mean diurnal NEE for July 26-31, 1997 **(b)** Hourly NEE for the 5 day simulation.

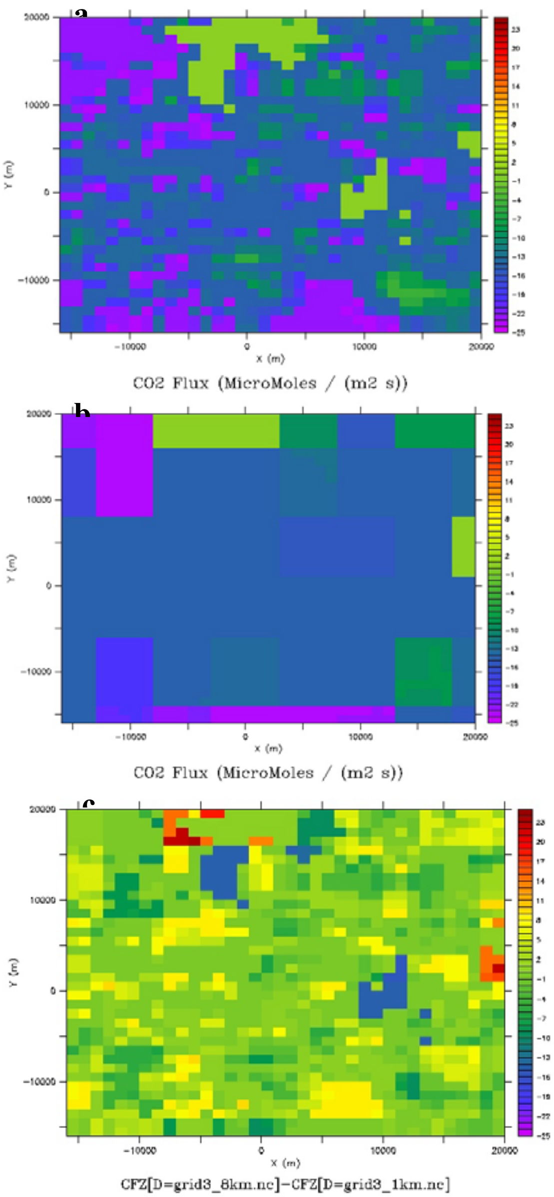


Figure 14: SiB2-RAMS simulation results for NEE at 12:00 noon, day 4 of the simulation for the fine grid (38 x 38km). (a) 1km simulations (b) 8km simulation (c) 8km – 1km difference.

concentration was initialized at 360ppm. The coupled model was forced with NCEP reanalysis data for July 26, 1997 through July 31, 1997 and hourly outputs of net ecosystem exchange (NEE), latent heat (LE) and sensible heat (H) were produced. Figure 13 shows measured and simulated NEE at the WLEF tall tower site extracted from the coupled simulations. Measured NEE is plotted together with the offline simulations of SiB2 reported above and modeled fluxes from the 1km and 8km Sib2-RAMS simulations. The offline and 8km simulations approximate measurements more closely than the 1km simulation. The tower flux measurements respond to an area of approximately 4-20 km^2 (M. Uliasz, personal communication) thus the offline (with boundary conditions corresponding to a 4 x 6km area and measured meteorology) and 8km calculated from the results of the 1km simulation more closely matches the observations for this same reason. Overall, the results show that the coupled simulations are able to simulate the exchange of CO_2 between the surface and atmosphere quite well. An example of the SiB2-RAMS simulations for the entire center grid is shown in Figure 14. The 1km data (Figure 14a) show much greater heterogeneity in NEE (shown), LE and H. Water features are poorly represented in the aggregated data (Figure 14b) and consequently the largest differences between the two simulations (8km – 1km, Figure 14c) result from edge effects around lakes, though smaller differences on the order of +/- 5μmol m^{-2} s^{-1} are present throughout the grid.

To better evaluate these differences, the grid mean (for the entire 38 x 38km fine grid) was calculated for NEE, LE and H for both the 1km and 8km simulations. The grid mean NEE shows more difference between the 1km and 8km simulations that the latent and sensible heat flux do (Figure 15a, c, e), through it is quite small. (~1μmol $m^{-2}s^{-1}$). However, over time these small differences (more persistent in nighttime respiration) begin to accumulate and lead to a larger divergence of the simulations over time (Figure 15b). Cumulative divergence in LE and

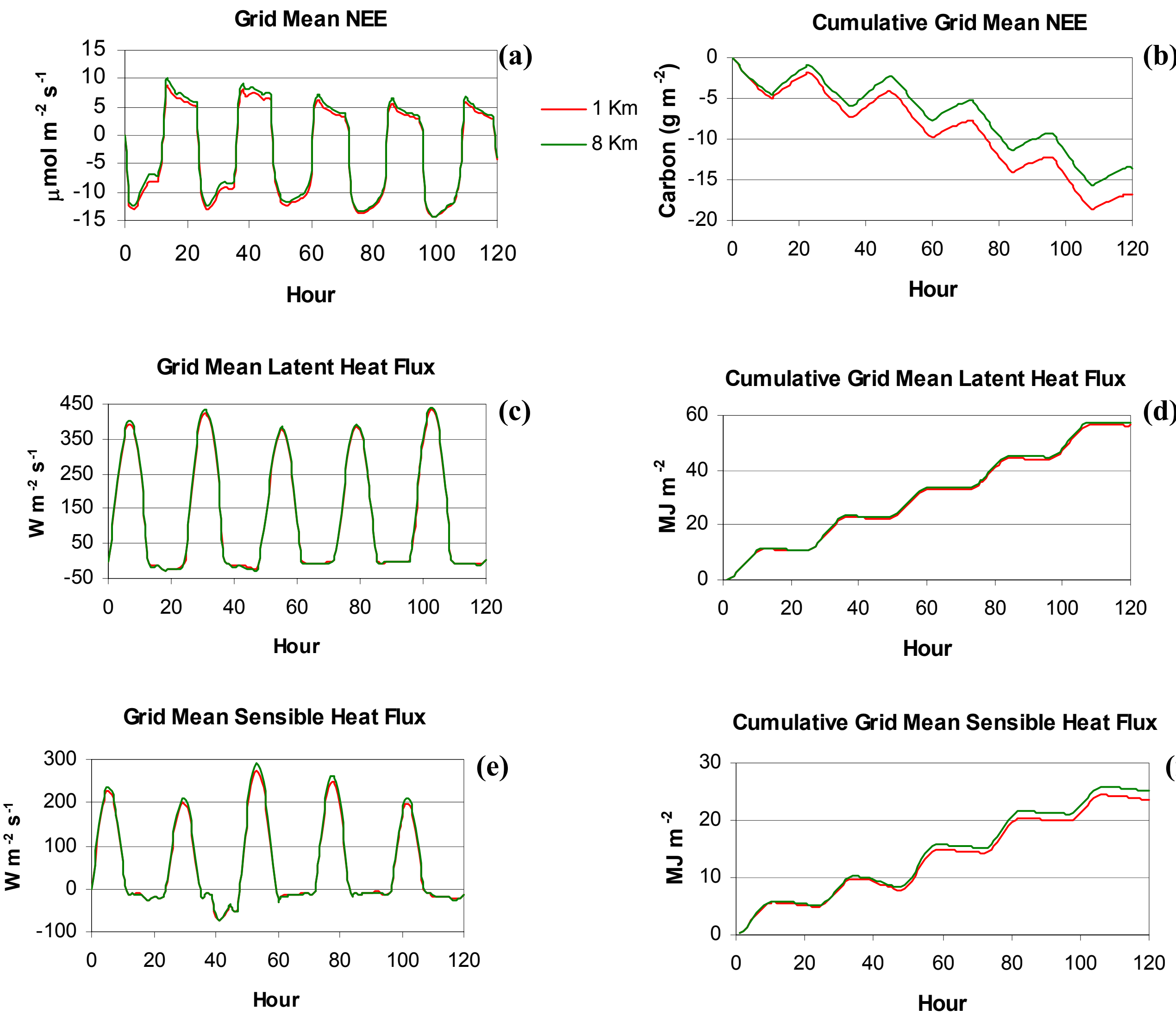


Figure 15: SiB2-RAMS simulation results for the entire fine grid (38 x 38km) for the 1km and 8km grids through time. (a,c,e) hourly grid means for NEE, LE and H and (b,d,f) cumulative grid means for NEE, LE and H.

H over time appears to be relatively smaller than NEE (Figure 15d, f), perhaps because of direct feedback between land surface temperature and moisture and the fluxes.

Because regional fluxes of quantities such as net ecosystem exchange, latent and sensible heat flux are largely unknown, it's not possible to say which result is correct. However, these results do suggest that although grid mean values of NEE over time are not significantly different between the fine and coarse resolution surfaces, cumulative sums of NEE on a regional basis may be sensitive to the level of representation of land surface heterogeneity. Therefore, when regional predictions of NEE are made, particularly if predictions of cumulative NEE are made over time, some accounting should be made for the representativeness of the surface.

The resolution sensitivity experiments were repeated for two other time periods, in April and October. Area-average differences in fluxes of heat, water, ad CO_2 were more pronounced in the shoulder season simulations. At specific grid points, there were large differences between predicted fluxes in space and time (Figure 16). The deviations in the fluxes resulting from representing a fine resolution land surface coarsely were compared to the uncertainty resulting from the parameterization of the model. In general, the uncertainty due to representing a fine resolution land surface coarsely was less than the uncertainty due to the parameterization of the model itself.

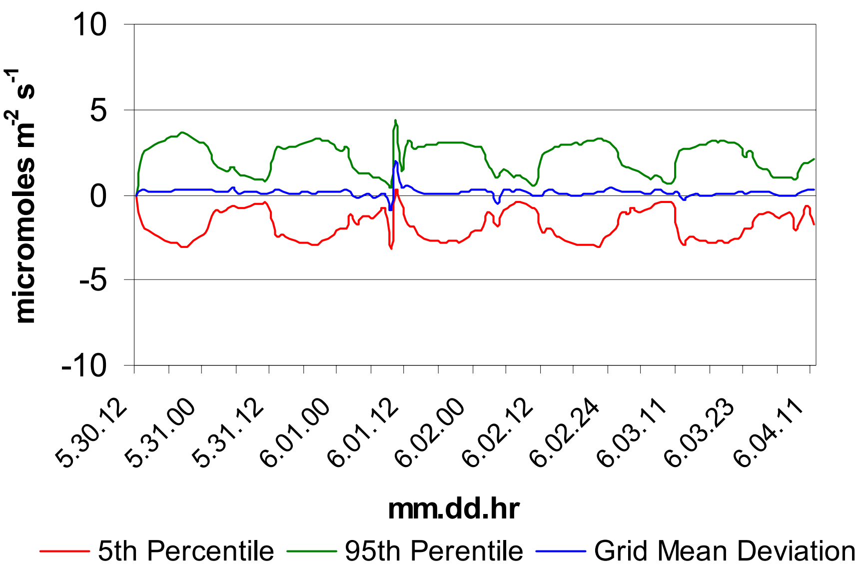


Figure 16. 5th and 95th percentile deviations from the mean difference (red and blue) and the grid mean deviation between simulations of net ecosystem exchange for two different representations of land surface heterogeneity (1km – 8km) for the time period surrounding leaf on of a mixed temperate forest.

•*What opportunities for training and development has the project helped provide?* **(also listed above under "education")**

1) several years of graduate study and research by Lara Prihodko, leading to a PhD in Ecology (Colorado State University) in 2004;
2) Contributed to a summer mini-course on Carbon Cycle Data Assimilation at the National Center for Atmospheric Research (NCAR), summer 2002; and
3) Contributed to a summer mini-course on Carbon Cycle Modeling and Data Assimilation at the Colorado State University (Program for Interdisciplinary Study of Mathematics, Ecology, and Statistics, summer 2003).

•*What outreach activities have you undertaken?*

None

3. Products: What has the project produced?

•*What have you published as a result of this work?*

•*Major Journal Publications*

Denning, A.S., M. Nicholls, L. Prihodko, I. Baker, P.-L. Vidale, K. Davis, and P. Bakwin, 2003. Simulated and observed variations in atmospheric CO_2 over a Wisconsin forest. *Global Change Biology*, **9**, 1241-1250.

Nicholls, M.E., A.S. Denning, L. Prihodko, P.-L. Vidale, K. Davis, P. Bakwin, 2004: A multiple-scale simulation of variations in atmospheric carbon dioxide using a coupled biosphere-atmospheric model. *Journal of Geophysical Research,* submitted.

Uliasz, M. and A. S. Denning, 2004. Deriving mesoscale surface fluxes of trace gases from concentration data. *Journal of Applied Meteorology*, submitted.

•*Books and other one-time publications*

L. Prihodko, 2004. "*Characterizing Uncertainty For Regional Carbon Cycle Modeling.*" PhD Dissertation, Graduate Degree Program in Ecology, Colorado State University.

•*What Web site(s) or other Internet site(s) reflect this project?*

http://biocycle.atmos.colostate.edu

•*What other specific products have you developed?*

1) Multiyear hourly continuous meteorological "forcing" data for WLEF tower site

2) 1km regional maps of ecophysiological parameters for a 1200x1200 km region in the upper Midwest USA surrounding the tower site for each month of the year 2000