MODEL-DATA COMPARISON OF MID-CONTINENTAL INTENSIVE FIELD
CAMPAIGN ATMOSPHERIC CO$_2$ MIXING RATIOS

A Thesis in
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by
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ABSTRACT

In-situ tower-based CO₂ observations from the Mid-Continental Intensive (MCI) field campaign are compared to Carbon Tracker simulated CO₂ concentrations. This study uses simulated CO₂ concentrations from the third level, which is the most representative of the convective boundary layer (CBL). Daily daytime average from both observed and simulated CO₂ concentrations are utilized in this study to ensure well-mixed, boundary conditions. This model-data comparison is applied using both time and spatial statistical analysis for two different periods: June through December 2007 and the 2007 growing season. The comparison shows that the model tends to predict 10 to 15 ppm higher mid-summer or growing season concentrations at three sites located in the “corn belt”. Carbon Tracker tends to be highly correlated to the observations for the period of June through December (≥ 0.8), but this correlation is lower for the growing season period (≤ 0.8). Residuals are not Gaussian, raising questions regarding the assumption of Gaussian residuals typically used in atmospheric inversions. The time scale for autocorrelation of the residuals is 30 to 80 days, the result of Carbon Tracker’s persistent overestimate of the growing season mixing ratio. Spatial correlations are largest between sites that are closer and share the same type of vegetation, but some other high spatial correlations diagnosed are not explained by these factors. The residuals do not show any clear correlations with synoptic weather. Overall, the model results for all sites are more inconsistent with the observations during the growing season, with the “corn belt” sites showing the least skill of all.
## TABLE OF CONTENTS

LIST OF FIGURES ............................................................................................................. v  
LIST OF TABLES ................................................................................................................ vi  
ACKNOWLEDGEMENTS ................................................................................................. viii  

Chapter 1 INTRODUCTION ......................................................................................... 1  

Chapter 2 METHODS ................................................................................................... 7  
  2.1 CO₂ Measurements ................................................................................................. 7  
  2.2 Model Description ................................................................................................. 10  
    2.2.1 Carbon Tracker (TM5-CASA) ......................................................................... 10  
  2.3 Data Selection ....................................................................................................... 12  
  2.4 Statistical Analysis ............................................................................................... 15  

Chapter 3 RESULTS & DISCUSSION .......................................................................... 17  
  3.1 Taylor Diagram ..................................................................................................... 19  
  3.2 Distribution of the Residuals ................................................................................ 22  
  3.3 Temporal and Spatial Correlations ....................................................................... 27  
  3.4 Meteorological Comparison .................................................................................. 31  

Chapter 4 CONCLUSION ............................................................................................... 34  

REFERENCES ............................................................................................................... 34
LIST OF FIGURES

Figure 1. Mid-Continent field campaign observation sites for 2007-2008 years from North American Carbon Program website.........................................................4

Figure 2. Map of the MCI field campaign-region, including NOAA tall tower and Ring2 tower locations overlaid upon estimates of 2007 corn net primary productivity (NPP) from Miles et al., in prep.................................................................8

Figure 3. Map of the seven tower locations measuring CO₂ concentrations in the mid-continental region of North America. This map includes both five Ring2 towers..........................................................................................................................9

Figure 4. Vertical profile of the CO₂ mixing ratio simulated by Carbon Tracker for the LEF tower, June 19, 2007 at 2200 UTC (1600 LST). This is the typical for a simulated daytime profile in the MCI region..............................................13

Figure 5. Carbon Tracker simulated CO₂ concentration differences between (a) levels 1 and 2 and (b) levels 2 and 3 for the LEF site, 2007. Each data point is one daily daytime average difference.................................................................14

Figure 6. Smoothed daily daytime average CO₂ mixing ratio (a) observed and (b) simulated by Carbon Tracker for each site in the MCI region. The smoothed daily daytime average CO₂ begins on 1 June and ends on 31 December, 2007...18

Figure 7. Residuals of the 31-day running mean of daily daytime average CO₂ mixing ratios for each of the sites in the MCI region.................................................................19

Figure 8. Taylor Diagram comparing observations vs. Carbon Tracker simulations of the daily daytime average CO₂ mixing ratio from June through December of 2007..............................................................................................................20

Figure 9. Taylor Diagram comparing observations vs. Carbon Tracker simulations of the daily daytime average CO₂ mixing ratio during the growing season (June through August) of 2007.................................................................20

Figure 10. Distribution of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of June through December 2007 at Galesville, WI. Red line is standard deviation and black line is the mean...........22

Figure 11. Distribution of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of June through December 2007 at Round Lake, MN. Red line is standard deviation and black line is the mean......22
Figure 12. Distribution of daily daytime average residuals for the period of growing season 2007 at Galesville, WI. Red line is standard deviation and black line is the mean.

Figure 13. Distribution of daily daytime average residuals for the period of growing season 2007 at Round Lake, MN. Red line is standard deviation and black line is the mean.

Figure 14. Gaussian fit of the distribution of residuals for (a) June through December 2007 and (b) the growing season of 2007 at Galesville, WI.

Figure 15. Autocorrelation from June through December of 2007 of the daily daytime average residuals from (a) Centerville, IA; (b) LEF, WI; (c) Round Lake, MN and (d) WBI, IA.

Figure 16. June through December power spectrum for Round Lake (a) and WBI (b). Red line indicates the period of 5 days.

Figure 17. Daily daytime average of the wind direction from Carbon Tracker versus CO₂ mixing ratio residuals for (a) Centerville and (c) Round Lake. Daily daytime average of the temperature from Carbon Tracker versus CO₂ mixing ratio residuals for (b) Centerville and (d) Round Lake. The data included in these figures are for the months of June through December 2007.

Figure 18. Daily daytime average of the wind direction from Carbon Tracker versus CO₂ mixing ratio residuals for (a) Centerville and (c) Round Lake. Daily daytime average of the temperature from Carbon Tracker versus CO₂ mixing ratio residuals for (b) Centerville and (d) Round Lake. The data included in these figures are for the months of Growing Season of 2007.
LIST OF TABLES

Table 1. Description of the sites used for this study. Sampling heights with * indicates the sampling height used for this comparison. ................................................................. 10

Table 2. Mean, standard deviation and skewness of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of June through December of 2007. N is the number of data points. Yellow shaded indicates the “corn belt” sites........................................................................................................ 23

Table 3. Mean, standard deviation and skewness of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of Growing Season 2007. N is the number of data points. Yellow shaded indicates the “corn belt” sites. ........................................................................................................ 24

Table 4. Chi Square values for June through December 2007 and the 2007 growing season. ....................................................................................................................... 27

Table 5. Spatial correlation coefficient of the residual (observed – modeled) of the daily daytime average CO₂ mixing ratio between sites for the period of June through December of 2007. Green shading indicates site-pairs where both sites are in the “corn belt”...................................................................................... 30

Table 6. Spatial correlation coefficient of the residual (observed –modeled) of the daily daytime average CO₂ mixing ratio between the seven sites for the period of growing season of 2007. Green shading indicates site-pairs where both sites are in the “corn belt”...................................................................................... 30
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Chapter 1

INTRODUCTION

Since the Industrial Revolution atmospheric CO$_2$ has increased significantly primarily due to fossil fuel combustion and land use change (IPCC, 2007, Houghton et al., 1999). Only half of the emitted CO$_2$ remains in the atmosphere, however, with the other half absorbed by the ocean and the terrestrial biosphere (Raupach et al., 2007). Several studies have concluded that a large net CO$_2$ sink exist in the temperate latitudes of the Northern Hemisphere and that a significant fraction is due to the net uptake by the terrestrial biosphere (Tans et al., 1990; Ciais et al., 1995; Fan et al., 1998). Nevertheless, the magnitude and causes of this terrestrial sink are still uncertain. Quantifying and understanding the mechanisms governing this sink are important steps toward successfully predicting and mitigating future atmospheric CO$_2$ growth (Sarmiento and Gruber, 2002).

One program that aims to understand sources and sinks of CO$_2$ is the North American Carbon Program (NACP) (Wofsy & Harris, 2002). The NACP’s strategy is to integrate models and observations used to estimate the continental carbon balance, to evaluate current modeling capability and to investigate discrepancies between the different models (Denning, 2005). The carbon balance can be estimated using “bottom-up” or “top-down” methods. “Bottom-up” methods are based on a combination of direct modeling of the processes involved over the continent, and direct evaluation of the carbon stock from crop and forest inventories (e.g. SOCCR, 2007). The “top-down” or
atmospheric inverse method uses atmospheric concentrations to constrain the carbon balance at the surface (e.g. Baker et al., 2006; Peters et al., 2007). The Carbon Tracker model, for example, is an inverse system that produces carbon fluxes estimates over the globe from year 2000 to present (Peters et al., 2007). This system assimilates surface observations around the world (flask, continuous measurements) over continents and oceans to produce CO$_2$ fluxes estimates at a global spatial domain and up to one degree spatial resolution across the United States. Carbon Tracker and other atmospheric inversions, however, tend to disagree with “bottom-up” methods (e.g. Fan et al, 1998) and amongst themselves (Gurney et al., 2002). In addition, when flux estimates do overlap between the two methods, (e.g. Pacala et al., 2001; Janssens et al., 2003) uncertainties remain large.

Causes of large uncertainty in atmospheric inversions include a lack of data, quality of the prior fluxes, and uncertainty in atmospheric transport. Atmospheric transport models contribute to the biases on the fluxes inferred by inverse systems. There are different causes of these biases such as the horizontal resolution of the model (Law et al., 2008, Patra et al., 2008), issues with capturing synoptic events (Wang et al., 2007), PBL schemes (Gerbig et al., 2008), and convection schemes (Stephens et al., 2007). It is known that transport models need to improve to reduce the uncertainty of the inverse systems, on the other hand, the limited network of atmospheric measurements also presents a challenge. Several studies have shown how difficult it is to estimate fluxes with a high degrees of confidence due to sparse atmospheric observations (Fan et al., 1998; Patra et al., 2003; Gurney et al, 2002). This issue becomes more significant as the
resolution of the model improves, and a dense network of measurements is needed to 
maximize the constraint of the atmospheric inversion results (Schuh et al., 2010).

A small number of investigations have attempted to conduct high resolution 
inversion at a regional scale. Some of these inverse studies have previously evaluated 
spatial and temporal correlations of transport errors using different approaches (Gerbig et 
al., 2003a; Lauvaux et al., 2009). In Gerbig et al., (2003a) aircraft data from the CO₂ 
Budget and Rectification Airborne (COBRA) campaign were used to investigate spatial 
correlations in the model data residuals, whereas Lauvaux et al., (2009) used an ensemble 
of perturbed simulations to investigate temporal and spatial correlations. Although 
transport error correlations are an essential component of the inverse system, most studies 
omit them.

Based on the need to quantify the skill of current inversion models, we perform a 
model-data comparison using Carbon Tracker and observations from the Mid-Continental 
(MCI) campaign developed by the North American Carbon Program (NACP). Some of 
the results mentioned from past studies, for example, the sparse measurements, lack of 
convergence among flux estimates, and the large uncertainty bound of the atmospheric 
inversion, motivate this MCI campaign (Ogle et al., 2006). The main goal of the MCI is 
to reach a convergence between the “top-down” atmospheric budgets and “bottom-up” 
ecosystem approaches, by studying each method in a specific time period and spatial 
region of North America to maximize the credibility of each method (Tans, 2003).

The selected region for the MCI is the Midwest agricultural belt in the north-
central U.S. This region includes eastern South Dakota, eastern Kansas, northern 
Missouri, Iowa, southern Minnesota, southern Wisconsin and Illinois (Figure 1). This
region is ideal for such an analysis because (1) Detailed records of the agricultural production exist for this area, which helps to provide accurate information of the carbon flux for the inventories (Ogle et al., 2006) (2) Difficulties of interpreting atmospheric measurements with transport models are minimized over the flat terrain characteristic of the U.S. Great Plains and (3) National Oceanic and Atmospheric Administration (NOAA) wind profilers cover the area, improving our ability to characterize atmospheric transport. This region is one of the most intensively farmed regions of the continent, with relatively low population density, but several concentrated metropolitans centers.

![Map of Mid-Continent field campaign observation sites for 2007-2008 years from North American Carbon Program website.](image)

The key additional element needed for the MCI was a dense network of well-calibrated atmospheric CO$_2$ observations, in order to reduce the issue of sparse in-situ
measurements established by different studies (Gurney et al., 2002). One source of data in this region is NOAA’s tall towers and aircraft profiling network. This network continues to grow, increasing the density of measurements within the continent. Another network called Ring2 was deployed within this region, and was composed of five CO₂ measurements towers that form a ring of roughly 500 km centered in Iowa (Miles et al., in prep.). This data density addresses the lack of measurements from previous forward (Wang et al., 2007) and inverse (Lauvaux et al., 2009) regional studies. Also, these studies have been performed for a time resolution of few days or weeks, but this study will work with data for about a year. Thus, this study is unique not only because of the measurement density, but the longevity as well.

In our study we will evaluate the performance of the Carbon Tracker global model within the U.S. mid-continent region for the periods of June through December, 2007 and growing season 2007 (June through August 2007). This is achieved by a comparison between the observed and simulated CO₂ mixing ratios in space and time. The density of data available from the MCI provides a combination of spatial and temporal resolution that is unparalleled, and thus should provide unique insights into both the seasonal and synoptic scale structure of the model-data residuals. Thus, a variety of spatial and statistical analyses are applied to the residuals. Our main focuses are the elements of the observation covariance matrix that includes the standard deviation of the residuals and the temporal and spatial correlations of the residuals. This statistical information is used in combination with the prior flux error covariance matrix to adjust surface fluxes and minimize the differences between the observed and simulated mixing ratios. The model-data residual mismatch is a product of contributions from transport,
representation, observational and flux errors. The model-data residual is a powerful tool for examining the cumulative influence of all of these errors. Since it is a cumulative measure, our ability to understand the causes of these statistical features is limited without additional controls on our comparison (e.g. an evaluation of residuals where only model transport differs). Our analysis moves toward an understanding of model-data errors that will enable us to build a more consistent inverse system.
Chapter 2

METHODS

2.1 CO$_2$ Measurements

We used continuous CO$_2$ mixing ratio observations from seven sites operating during the MCI campaign for this comparison. These sites sample CO$_2$ mixing ratio across the U.S. upper Midwest, with a distance between the sites ranging from 125 to 370 km (Miles et al., in prep.). All seven sites are located in the mid-continental region of North America (Figure 2), where agriculture dominates the land use. Three of these sites are located in what is called the “corn belt”, with corn being the dominant crop in a well-defined area stretching from the northwest to southeast across the center of the domain. Vegetation at the other sites is dominated by C3 crops/grasses and forests, although corn and soybean are common as well (Miles et al., in prep.). All sites reported data at two second or half hour resolution, but for this study we only used daily daytime average (DDA) CO$_2$ mixing ratios. This will be explained in section 2.3.
Five of these sites form a network of towers called “Ring2” managed by the Pennsylvania State University (PSU) and described by Miles et al., (in prep.). The Ring2 network consists of five communication towers fitted with cavity ring-down spectroscopy instruments used to measure atmospheric CO$_2$ (Picarro, Inc; Crosson, 2008; Richardson et al., (in prep)). This network was deployed between April and June 2007 and operated through November 2009. The sample heights at each tower are 30 m AGL (above ground level) and between 110 and 140 m AGL (Table 1).
Figure 3. Map of the seven tower locations measuring CO₂ concentrations in the mid-continental region of North America. This map includes both five Ring2 towers and NOAA tall towers.

The other two towers are part of the Earth System Research Laboratory/Global Monitoring Division (ESRL/GMD) tall tower network (Bakwin et al., 1998) managed by NOAA. The NOAA ESRL/GMD tall tower network uses existing television, radio and cell phone towers as sampling platforms for in-situ infrared-based (Licor, Inc) CO₂ measurements. The precision of the calibration and the accuracy of the CO₂ mixing ratio are better than 0.2 ppm (Zhao et al., 1997). This network started sampling CO₂ from tall towers in the 1990s (Bakwin et al., 1998) and has slowly grown in density. Only two sites from this network, the WLEF-TV transmitter tower in northern Wisconsin and the KWKB-TV tower in West Branch, IA, are in this study region, thus used in this investigation. Sampling heights on these towers are between 11 m AGL and 396 m AGL (Table 1). These two sites report data at a half-hour resolution.
<table>
<thead>
<tr>
<th>Site</th>
<th>Location</th>
<th>Operator</th>
<th>Latitude (°N)</th>
<th>Longitude (°W)</th>
<th>Starting Date</th>
<th>Sampling Height</th>
<th>CO₂ mixing ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>RCE</td>
<td>Centerville, IA</td>
<td>PSU</td>
<td>40.79</td>
<td>-92.88</td>
<td>April 2007</td>
<td>30, *110m AGL</td>
<td></td>
</tr>
<tr>
<td>RGV</td>
<td>Galesville, WI</td>
<td>PSU</td>
<td>44.10</td>
<td>-91.34</td>
<td>June 2007</td>
<td>30, *140m AGL</td>
<td></td>
</tr>
<tr>
<td>RKW</td>
<td>Kewanee, IL</td>
<td>PSU</td>
<td>41.28</td>
<td>-89.97</td>
<td>April 2007</td>
<td>30, *140m AGL</td>
<td></td>
</tr>
<tr>
<td>RMM</td>
<td>Mead, NE</td>
<td>PSU</td>
<td>41.14</td>
<td>-96.46</td>
<td>April 2007</td>
<td>30, *120m AGL</td>
<td></td>
</tr>
<tr>
<td>RRL</td>
<td>Round Lake, MN</td>
<td>PSU</td>
<td>43.53</td>
<td>-95.41</td>
<td>April 2007</td>
<td>30, *110m AGL</td>
<td></td>
</tr>
<tr>
<td>WBI</td>
<td>West Branch, IA</td>
<td>NOAA</td>
<td>41.72</td>
<td>-91.35</td>
<td>June 2007</td>
<td>31, *99, 379 m AGL</td>
<td></td>
</tr>
<tr>
<td>LEF</td>
<td>WLEF, WI</td>
<td>NOAA</td>
<td>45.95</td>
<td>-90.27</td>
<td>October 1994</td>
<td>11, 30, 76, *122, 244, 396 m AGL</td>
<td></td>
</tr>
</tbody>
</table>

Table 1. Description of the sites used for this study. Sampling heights with * indicates the sampling height used for this comparison.

### 2.2 Model Description

#### 2.2.1 Carbon Tracker (TM5-CASA)

To estimate surface CO₂ exchange NOAA’s Earth System Research Laboratory (ESRL) developed a data assimilation system called Carbon Tracker (Peters et al., 2007). This system is used to calculate biogenic CO₂ fluxes by integrating daily daytime averaged CO₂ concentrations from continuous observations with an atmospheric transport model and a first guess of the biogenic fluxes. The biogenic surface fluxes are optimized by minimizing the difference between observed and modeled atmospheric CO₂ mixing ratios.

The atmospheric transport model used in Carbon Tracker is a two-way nested global model called the Transport Model, version 5 (TM5, Krol et al., 2005). TM5 is an off-line model in which the meteorological data is provided by the model of the European Centre for Medium Range Weather Forecast (ECMWF) operational forecast model. The meteorological parameters taken from the ECMWF are supplied at time intervals of 6 hours but meteorological parameters related to the boundary layer mixing and surface
processes are provided every 3 hours (Krol et al., 2005). For this study TM5 is run at a horizontal global spatial resolution of 6º×4º (longitude × latitude), with nested regions over North America (3º×2º) and the United States (1º×1º) (Peters et al., 2007). The vertical resolution of TM5 used in Carbon Tracker is 25 hybrid sigma-pressure levels, with more levels near the surface. There is more vertical resolution in the boundary layer and the free troposphere because the main interest of this model version is within the troposphere (Krol et al., 2005).

Carbon Tracker uses the Carnegie-Ames Stanford Approach (CASA) global biogeochemical model as a biosphere model (van der Werf et al., 2006; Giglio et al., 2006). The CASA biosphere model produces Net Primary Production (NPP) fluxes at monthly time resolution and global 1×1 degree spatial resolution. To calculate the global fluxes, this model uses input from weather models and satellite observed Normalized Difference Vegetation Index (NDVI, De Fries & Townshend, 1994). CASA uses the vegetation classification of Dorman and Sellers (1989) that defines 12 plant functional types, later modified by Seller et al., (1993). This classification is chosen because the numbers of vegetation types are manageable and the classification is based on plant energy balance and life form which is more convenient for coupling the land surface with atmospheric chemistry (Potter et al., 1993). CASA calculates the monthly NPP as a product of intercepted photosynthetically active radiation (IPAR) and spatially varying light use efficiency (Field et al., 1995, De Fries et al., 1999). The IPAR is estimated by using solar radiance and the fraction of photosynthetically active radiation intercepted by the canopy (FPAR), which is calculated from the monthly NDVI (De Fries et al., 1999).
After the surface fluxes are optimized, a higher vertical resolution version is run only one time with the final inverse fluxes. This higher vertical resolution run forecasts new CO$_2$ concentrations at 34 different levels from the surface to 61km. These “posterior” mixing ratios are used for this comparison. The third level from the ground is used for the model-data comparison, for reasons described in section 2.3. Data from the LEF tall tower are used in Carbon Tracker to optimize the fluxes. In our study we will use this tower to evaluate the impact of the optimization scheme, compared to the other towers that were not used in the assimilation process.

2.3 Data Selection

Chemical transport models have difficulty simulating the strong vertical gradients in the stable nocturnal boundary layer but can better simulate the well-mixed boundary layer conditions that are often observed during daytime (Parazoo et al., 2008). We thus compare only mid-day CO$_2$ observations and simulations. The CO$_2$ concentrations are averaged from 1800-2200 UTC (12:00-16:00 LST), a time period when the boundary layer should be convective and well-mixed (e.g. Davis et al., 2003; Yi et al., 2001; Bakwin et al., 2008; Stull, 1988). All the sampling levels used for this comparison are around or above 100m AGL (Table 1), chosen because the Ring2 sites’ highest levels are between 110 and 140 m (AGL). This data should be representative of convective boundary layer (CBL) mixing ratios (Wang et al., 2007). The model level chosen for the comparison also needs to be in the CBL. We search for the model CBL by finding levels
close to the ground during the day, where the difference in CO₂ mixing ratios between levels is small (≤ 2ppm).

![Graph](image-url)

Figure 4. Vertical profile of the CO₂ mixing ratio simulated by Carbon Tracker for the LEF tower, June 19, 2007 at 2200 UTC (1600 LST). This is the typical for a simulated daytime profile in the MCI region.

Carbon Tracker has 34 levels. The first level has a constant geopotential height, which is between 200 and 400 m. AGL. Although this altitude should represent the well-mixed portion of the CBL, the concentrations at this height are more representative of the surface layer, very close to the earth’s surface (Figure 4). Gradients as strong as shown in Figure 4, in fact are not found within the surface layer at LEF down to 11 m AGL (Bakwin et al., 1998). To identify a level that is more representative of the CBL, we computed the differences of the daily daytime average between levels. Differences between levels 1 and 2 are 10 ppm or greater for most of the sites during the growing season (Figure 5.a). Daily daytime average differences between levels 2 and 3 are typically less than 2 ppm during the growing season (Figure 5.b). This suggests that
levels 2 and 3 are behaving more like the CBL. While level 2 is closer to the level of the observations, this level might be influenced by level 1 at times. To avoid any influence caused by the first level, we choose the third level to compare to the observations. This is also the level that is used in the Carbon Tracker data assimilation system (Peters et al., 2007).

![Graph](image)

*Figure 5. Carbon Tracker simulated CO₂ concentration differences between (a) levels 1 and 2 and (b) levels 2 and 3 for the LEF site, 2007. Each data point is one daily daytime average difference.*

The model-data mismatch will be evaluated in space and time at different sites by comparing the DDA posterior CO₂ mixing ratio estimates from Carbon Tracker to the measured the DDA CO₂ mixing ratio data from the network shown in Figure 3 and described above. Each of the sites will be compared for two time periods: June through December 2007 and the growing season of 2007. An assessment of these two time periods will let us study the model performance for both the seasonal cycle (June through December) and the synoptic variability or day-to-day variability (growing season). We are interested in the growing season because this is a period that shows larger variations that are harder to simulate but extremely important to constrain the carbon balance of the continent.
2.4 Statistical Analysis

A series of statistical analyses are performed to provide a complete description of the model-data mismatch. These analyses are performed for the two periods mentioned in section 2.3 to segregate the behavior of the model-data residual within the growing season, where synoptic weather dominates variability from the characteristics of the residual when including the seasonal cycle. The evaluation of the model performance provides a general idea of the accuracy with which the model simulates the observations. These statistical analyses will be used to describe model performance in time and space, which is required in the observation covariance matrix.

One way to represent the performance of the model is through a Taylor Diagram. The Taylor Diagram shows the correlation coefficient of the observation and the model, the centered root-mean-squared difference (CRMSD) and the ratio of the standard deviation (between the observation and the model) to show the degree of correspondence between simulated and observed fields (Taylor, 2001). Both the correlation coefficient and the CRMSD are measures of the degree to which the model represents the pattern for both periods (the growing season, and June through December 2007). The correlation and CRMSD would be 1 and 0, respectively, for a model which perfectly describes the data. The ratio of the standard deviations determines if both observation and model patterns have the same amplitude of variation.

The distribution of the residuals is evaluated for both June through December, 2007 and the growing season of 2007. Both the standard deviation and mean of the residuals are estimated for each site and period. For each site and period the degree to
which a Gaussian describes the residuals will be evaluated by performing a chi-squared ($\chi^2$) test. The mean of the distributions are one measure of the model-data mismatch, due to errors in the fluxes but also in the atmospheric transport model. The magnitude of the variability in the residual will be quantified by the standard deviation of the residual distribution.

The structure of the residuals in space and time will be evaluated. The temporal structure is evaluated by calculating the temporal auto-correlation. This analysis shows the degree to which the model-data errors persist over time. The spatial structure of the residuals is analyzed by computing the correlations of the residuals between the sites.

These components (standard deviation, time and spatial correlation) in theory represent the atmospheric transport errors in the observation error covariance matrix only, whereas the flux errors are described by a second error covariance matrix. Although in our case the fluxes are optimized and potential flux errors could still be affecting the results, most of the remaining structures in the residuals due to the fluxes should be minimized. Despite our approach described above, it remains difficult to determine the principal contributor of the model-data mismatch.

We finally explored whether or not there is a clear relationship between the data-model residuals and synoptic weather. We did this by searching for a correlation between the residuals and two different meteorological variables (wind direction and temperature). For this analysis we use the meteorological data provided by Carbon Tracker. This data is averaged also for the same hours as the mixing ratio (see section 2.3). We use scatter plots for temperature and wind versus the residuals at each of the sites to investigate this correlation.
Chapter 3

RESULTS & DISCUSSION

To provide an overall view of the observed seasonal patterns, CO₂ mixing ratio daily daytime averages were smoothed using a 31-day running mean for each of the seven sites (Figure 6.a). The same method was applied to the concentrations simulated by Carbon Tracker (Figure 6.b). Figure 6.a shows the influence of the local vegetation type during the growing season. The three sites with the highest drawdown in the CO₂ concentration through this period (Kewanee, Round Lake and WBI) are located in the “corn belt” (Figure 2). The other four sites (Centerville, Galesville, Mead, and LEF) have less seasonal drawdown compare to the sites within the “corn belt”. The dominant vegetation type around Centerville, Galesville and Mead is wheat/grasses, and LEF is in a mixed forest region (Miles et al., to be submitted). The “corn belt” sites show large seasonal amplitudes of CO₂ mixing ratio that reaches 40 ppm, whereas the other four sites have seasonal amplitudes of 24-29 ppm (Miles et al., to be submitted). This difference in seasonal draw down is not surprising given the intense photosynthesis of corn versus other vegetation types in similar light and temperature conditions (Lokupitiya et al., 2009; Davis et al., 2003).
Figure 6. Smoothed daily daytime average CO$_2$ mixing ratio (a) observed and (b) simulated by Carbon Tracker for each site in the MCI region. The smoothed daily daytime average CO$_2$ begins on 1 June and ends on 31 December, 2007.

Figure 6.b suggests that Carbon Tracker model does not simulate the intense drawdown of these three “corn belt” sites. Carbon Tracker tends to underestimate CO$_2$ (CO$_2$ mixing ratios higher than observed) through the growing season (Figure 7). Two possible explanations for this model-data difference are the following: first, the uptake is underestimated in the “corn belt”, or second, the vertical mixing in the model is wrong, affecting the simulated concentrations. In order to distinguish between these possibilities, the fluxes and transport model should be compared to flux measurements and meteorological data, respectively, to diagnose the exact causes of the mismatch. If we consider the inverse system and the fact that the three “corn belt” sites do not show lower concentrations than the others during the growing season (Figure 6.b), this suggests that despite the optimization of the fluxes, the system was not able to identify the spatial structure of the “corn belt”. Possible explanations for this behavior include the lack of concentration data in the original system to constrain the fluxes (only the LEF tower was used, Peters et al., 2007) and suggest a possible absence of a well-defined “corn belt” region in the CASA prior fluxes.
3.1 Taylor Diagram

Taylor Diagrams are used to illustrate the performance of the model compared to the observations. We use both observed and simulated daily daytime average CO₂ mixing ratios (unsmoothed) in order to quantify the model’s ability to reproduce day-to-day variability. The model is evaluated for the period of June through December 2007 (Figure 8) and for the 2007 growing season (Figure 9). The correlation coefficient has a range of \(-1.0 \leq R \leq 1.0\) and is used to quantify the pattern similarity. To determine the difference in variability between two patterns, a normalized standard deviation is applied:

\[
\sigma_n = \frac{\sigma_m}{\sigma_o} \tag{1}
\]

Where \(\sigma_m\) indicates the standard deviation of the model CO₂ mixing ratio and \(\sigma_o\) indicates the standard deviation of the observed CO₂ mixing ratio. If the normalized standard deviation is larger (lesser) than 1, it means that the model over (under) estimated...
the day-to-day variability. The other statistical value illustrated in the Taylor Diagram is the centered root mean square difference, which indicates the difference between the two patterns.

For the period of June through December, Figure 8 shows that the model is highly correlated to the observations, with a correlation greater than 0.8. For the growing season, however, the correlation is lower than 0.8 for most of the sites except for Centerville (Figure 9). This indicates the seasonal cycle is better represented by the model than the synoptic variability that dominates the growing season. This diagram also shows that LEF is the site with the highest correlation for the June through December period. One possible reason is that LEF data was included in the optimization algorithm. The Taylor plots show that the model tends to underestimate the amplitude of variability in CO₂ mixing ratio with the exception of Centerville, which shows an overestimation of the amplitude during the growing season. The CRMSD for the period of June through
December are lower (0.4 > CRMSD < 0.6) than those, for the growing season (0.6 > CRMSD < 0.9).

The fluxes during the growing season (June through August) are stronger than winter fluxes, which suggest that large fluxes amplify the difference between the observation and the model. During winter, the daytime boundary layer is more shallow and stable than during the growing season (Yi et al., 2001). As mentioned in section 2.2, nighttime CO$_2$ mixing ratios are not used because the models have a difficulty simulating the strong vertical gradient near the surface. When the winter season however is added to the Taylor Diagram (see Figure 8) the differences between model and observations are reduced, which indicates that simulated CO$_2$ is not so different from the observations. From this we can conclude that simulated growing season model-data mismatch have a significant impact from both fluxes and vertical transport, but for winter the transport alone might have a higher impact in the differences between model and observations.
3.2 Distribution of the Residuals

![Figure 10](image1.png)  ![Figure 11](image2.png)

Figure 10. Distribution of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of June through December 2007 at Galesville, WI. Red line is standard deviation and black line is the mean.

Figure 11. Distribution of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of June through December 2007 at Round Lake, MN. Red line is standard deviation and black line is the mean.

Because a smoothed difference of the daily daytime average CO₂ mixing ratio hides the day-to-day variability of the residuals, a distribution of the raw residuals is also analyzed. Figure 10 and Figure 11 show the distribution of the residuals for the period of June through December. The “corn belt” sites have a broader distribution than sites that are not located in this type of vegetation (Table 2). The mean of the residuals for this period is negative for all sites except Centerville, with a maximum offset magnitude of 4.42 ppm for Kewanee (Table 2). The skewnesses for the corn belt sites are all negative, while the skewnesses of the other sites appear to be random.
Table 2. Mean, standard deviation and skewness of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of June through December of 2007. N is the number of data points. Yellow shaded indicates the “corn belt” sites.

For the growing season the distributions tend to have a bimodal behavior for many of the sites (e.g., Figure 12 and Figure 13) with the exception of Centerville. The residual means are far from zero and negative for all the sites during the growing season. The “corn belt” sites have the highest residual mean and standard deviation in the growing season (Table 3). The distribution for the growing season shows that Carbon Tracker has larger error during the growing season; this is noticeable in the smoothed residuals time series as well (Figure 7). The growing season skewnesses appear to be randomly distributed about zero.
Table 3. Mean, standard deviation and skewness of the daily daytime average residuals (observed – Carbon Tracker CO₂) for the period of Growing Season 2007. N is the number of data points. Yellow shaded indicates the “corn belt” sites.

<table>
<thead>
<tr>
<th>Sites</th>
<th>Mean (ppm)</th>
<th>Standard Deviation (ppm)</th>
<th>Skewness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centerville (N= 90)</td>
<td>-2.85</td>
<td>5.11</td>
<td>0.22</td>
</tr>
<tr>
<td>Galesville (N = 62)</td>
<td>-2.71</td>
<td>7.22</td>
<td>0.16</td>
</tr>
<tr>
<td>Kewanee (N = 77)</td>
<td>-8.49</td>
<td>7.08</td>
<td>-0.36</td>
</tr>
<tr>
<td>Mead (N = 80)</td>
<td>-4.31</td>
<td>5.6</td>
<td>-0.95</td>
</tr>
<tr>
<td>Round Lake (N = 84)</td>
<td>-5.86</td>
<td>7.43</td>
<td>-0.42</td>
</tr>
<tr>
<td>WBI (N = 56)</td>
<td>-6.38</td>
<td>7.28</td>
<td>0.66</td>
</tr>
<tr>
<td>LEF (N = 92)</td>
<td>-3.85</td>
<td>4.35</td>
<td>-0.22</td>
</tr>
</tbody>
</table>

The atmospheric inversion used in Carbon Tracker is a Bayesian inversion (Tarantola, 2005). This method assumes that transport errors are unbiased (the mean of the errors are zero). Using this assumption in the inverse system considers not only flux errors to be Gaussian, but also fluxes are Gaussian as well. We are describing the model-data residual that combines both sources of errors (flux and transport). Combining two random variables that follow a Gaussian distribution (both are univariate) will recreate a Gaussian distribution if both variables are independent (normal multivariate; Tarantola, 2005). In our case it suggests that a linear relationship exists between both the fluxes and the transport error. This means that the transport model TM5 can be represented by a combination of scalars. Even though TM5 can not be represented in such a way, this assumption is made in most of the inversions, including Carbon Tracker. If TM5 follows this relationship our residual distributions will be Gaussian, however, our results show distributions that are bimodal and skew due to the non-linearity in the transport model. A second reason for a non Gaussian distribution of the residual could be that transport errors are biased (non Gaussian or not centered at zero). This leads to biased inverse
fluxes in practice, which were illustrated in several studies (Stephen et al., 2007; Gerbig et al., 2008). Because our main focus is the model-data mismatch we only suggest potential weakness in the transport, but the diagnosis of transport errors or non linearity will require further analysis that will not be attempted in this study.

We apply a fit to the distribution for both periods (Figure 14) to test the degree to which the residuals follow a Gaussian. The Gaussian distribution is defined as:

\[
f(y) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(y-\mu)^2}{2\sigma^2}} \tag{2}
\]

The density function \( f(y) \) gives the height of the curve, \( y \) is the random variable, \( \sigma \) indicates the standard deviation and \( \mu \) is the mean. Because the bin width of the residuals is 3ppm, in order to get the best fit the density function was multiplied by the number of data points \( N \) (see Table 2 and Table 3) and the width of the bins.

![Figure 14. Gaussian fit of the distribution of residuals for (a) June through December 2007 and (b) the growing season of 2007 at Galesville, WI.](image)

To determine the goodness of this fit to the distribution a Chi Squared (\( \chi^2 \)) test was applied. The \( \chi^2 \) test is evaluated using the following equation:

\[
\chi^2 = \sum \frac{(O - E)^2}{E} \tag{3}
\]
In this equation $O$ represents the observations and $E$ the expected values for each. If the fitted distribution is very close to the data the observed and the expected counts will be close for each class, and the $\chi^2$ values will be small. If the fit is poor, then large discrepancies might exist for some of the classes and this will lead to a large $\chi^2$.

The sites with the highest $\chi^2$ values for both periods are Centerville and LEF (Table 4). For the period of June through December both Kewanee and WBI have the lowest $\chi^2$ values. The sites with the lowest values for the growing season are WBI and Galesville. It is clear that $\chi^2$ values are much lower for the growing season than for June through December. Thus, while the distributions for both period of time are somewhat non-Gaussian, the non-Gaussian behavior is much more pronounced when the seasonal cycle is included in the analysis. Even though there are differences in $\chi^2$ values between each sites and time period, we observed a significant sensitivity of this test to the amount of data, especially for the growing season period. Both Centerville and LEF for example have more data available from June through August (growing season) and also have the highest chi squared values compared to the rest of the sites. WBI has less data available from June through August and the lowest chi square value. When we compare the shapes of these sites it suggests more of a Gaussian shape for Centerville and LEF rather than WBI. This shows that further studies are needed to identify more accurately if a Gaussian assumption should describe model-data residuals.
Table 4. Chi Square values for June through December 2007 and the 2007 growing season.

<table>
<thead>
<tr>
<th>Sites</th>
<th>June through December 2007 $\chi^2$</th>
<th>Growing Season $\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centerville</td>
<td>39.73</td>
<td>23.51</td>
</tr>
<tr>
<td>Galesville</td>
<td>26.46</td>
<td>8.11</td>
</tr>
<tr>
<td>Kewanee</td>
<td>16.1</td>
<td>14.59</td>
</tr>
<tr>
<td>Mead</td>
<td>33.78</td>
<td>18.67</td>
</tr>
<tr>
<td>Round Lake</td>
<td>27.83</td>
<td>13.48</td>
</tr>
<tr>
<td>WBI</td>
<td>18.19</td>
<td>7.12</td>
</tr>
<tr>
<td>LEF</td>
<td>31.99</td>
<td>60.65</td>
</tr>
</tbody>
</table>

3.3 Temporal and Spatial Correlations

Figure 15 shows the temporal auto correlation of the residuals. Centerville (Figure 15.a) and LEF (Figure 15.b) have relatively small auto correlation values. The rest of the sites have correlations that are 0.4 to 0.5 at all lag of one day and stay positive for 30 to 80 days. The two “corn belt” sites Round Lake (Figure 15.c) and WBI (Figure 15.d) illustrate this behavior. This period of correlation of the residuals is clearly related to the growing season length and Carbon Tracker’s difficulty in simulating the growing season draw-down (Figure 7). Auto correlation generally shows similar behavior for the sites located in the “corn belt”, illustrating that Carbon Tracker repeats the same errors for a period of 40 to 60 days in the “corn belt” sites. For the sites out of the “corn belt”, the correlation tends to be lower but lasts for a similar time period.
Figure 15. Autocorrelation from June through December of 2007 of the daily daytime average residuals from (a) Centerville, IA; (b) LEF, WI; (c) Round Lake, MN and (d) WBI, IA.

We also examined the spectral structure of the residuals. To evaluate this, we performed a power spectrum analysis. These power spectra show for all sites a weak peak at a period of 4 to 5 days (e.g. Figure 16a; b). This is the approximate periodicity of frontal passages. This suggests that the transport model may have difficulty simulating frontal passages. Wang et al., (2007), for example, showed how difficult it is for the RAMS model to capture the timing and location of a frontal passage. This information is important for the inverse system because this analysis suggests that boundary conditions for this model need to be adjusted every four to five days. The significance of this peak,
However, is not clear and further analysis is required to determine if there is truly a synoptic peak in the residual.

![Image of power spectrum graphs](image.png)

**Figure 16.** June through December power spectrum for Round Lake (a) and WBI (b). Red line indicates the period of 5 days.

The correlations of the residuals in space are shown for the periods of June through December, 2007 (Table 5) and the growing season of 2007 (Table 6). For both periods correlations of the residuals among the sites were estimated using daily daytime average CO₂ mixing ratios. The “corn belt” sites (Kewanee, Round Lake and WBI) have the highest spatial correlation for June through December. Mead, however, is highly correlated to the “corn belt” sites. Mead is not located in the “corn belt” but is surrounded by corn which might explain the spatial correlation with the “corn belt” sites. The WBI site shows the highest residual correlation in space with other sites. Centerville is the least correlated in space with the rest of the sites for this period.
Table 5. Spatial correlation coefficient of the residual (observed – modeled) of the daily daytime average CO$_2$ mixing ratio between sites for the period of June through December of 2007. Green shading indicates site-pairs where both sites are in the “corn belt”.

<table>
<thead>
<tr>
<th>Annual</th>
<th>Centerville</th>
<th>Galesville</th>
<th>Kewanee</th>
<th>Mead</th>
<th>Round Lake</th>
<th>WBI</th>
<th>LEF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centerville</td>
<td>1</td>
<td>0.231</td>
<td>0.420</td>
<td>0.362</td>
<td>0.156</td>
<td>0.429</td>
<td>0.178</td>
</tr>
<tr>
<td>Galesville</td>
<td>1</td>
<td>0.573</td>
<td>0.380</td>
<td>0.436</td>
<td>0.486</td>
<td>0.411</td>
<td></td>
</tr>
<tr>
<td>Kewanee</td>
<td>1</td>
<td>0.513</td>
<td>0.497</td>
<td>0.767</td>
<td>0.399</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mead</td>
<td>1</td>
<td>0.552</td>
<td>0.611</td>
<td>0.374</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Round Lake</td>
<td></td>
<td>1</td>
<td>0.525</td>
<td>0.529</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WBI</td>
<td></td>
<td></td>
<td>1</td>
<td>0.447</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LEF</td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Growing season residuals are less correlated in space for most of the sites as compared to the June through December period. WBI and Kewanee are the sites more correlated in space for the growing season compared to the rest of the sites which are less correlated. LEF and Centerville residuals are the least correlated in space.

Table 6. Spatial correlation coefficient of the residual (observed – modeled) of the daily daytime average CO$_2$ mixing ratio between the seven sites for the period of growing season of 2007. Green shading indicates site-pairs where both sites are in the “corn belt”.

<table>
<thead>
<tr>
<th>Growing Season</th>
<th>Centerville</th>
<th>Galesville</th>
<th>Kewanee</th>
<th>Mead</th>
<th>Round Lake</th>
<th>WBI</th>
<th>LEF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Centerville</td>
<td>1</td>
<td>0.135</td>
<td>0.258</td>
<td>0.255</td>
<td>-0.022</td>
<td>0.081</td>
<td>0.014</td>
</tr>
<tr>
<td>Galesville</td>
<td>1</td>
<td>0.444</td>
<td>0.157</td>
<td>0.266</td>
<td>0.378</td>
<td>0.133</td>
<td></td>
</tr>
<tr>
<td>Kewanee</td>
<td>1</td>
<td>0.213</td>
<td>0.249</td>
<td>0.626</td>
<td>0.128</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mead</td>
<td>1</td>
<td>0.283</td>
<td>0.367</td>
<td>0.156</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Round Lake</td>
<td></td>
<td>1</td>
<td>0.266</td>
<td>0.403</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>WBI</td>
<td></td>
<td></td>
<td>1</td>
<td>0.206</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LEF</td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Spatial correlations are highest when sites are nearby in space and have the same type of vegetation. For example, WBI and Kewanee have the highest spatial correlation for both time periods, are separated by a distance of 125 km (see Figure 3), and are located in the same type of vegetation (corn). This relationship is contradicted by Mead, however, which is a mixed vegetation site highly correlated to the “corn belt” sites and
relatively far from these sites. It is not clear why this site is correlated to the “corn belt” sites.

3.4 Meteorological Comparison

Meteorological variables (wind direction and temperature) are evaluated to determine if there is any relationship with the residuals. To evaluate the wind direction we used the wind components provided by Carbon Tracker at the third vertical level and estimated the wind direction from those components. The temperature data is provided by Carbon Tracker and was converted from Kelvin to Celsius. Both temperature and wind were averaged for the afternoon hours 1800-2200 UTC (12:00-4:00pm). Scatter plots of these two variables versus the residuals for the June through December period are performed for this analysis (e.g. Figure 17).
Figure 17 shows the correlation of the data-model residuals with weather related variables, temperature and wind direction. The CO$_2$ residuals are sometimes large and negative when the wind is coming from the north at the Round Lake site (Figure 17.c) but in Centerville there is no clear correlation (Figure 17.a). Other sites show behavior similar to Round Lake. Figure 17.d and 17.b show that residuals are higher with increasing temperature. This high residual is likely caused by the persistent data-model residual during the growing season (Figure 7) and is not necessarily evidence of a weather-related residual.
If this analysis is applied to the growing season (Figure 18) we observe that there is no relationship between residuals and temperature (Figure 18.b,d). Centerville residuals do not show any correlation with wind directions (Figure 18.a). Round Lake, however, still shows a weak relation between large negative residuals and wind coming from the North. Overall these results show that there is not a persistent evidence of the correlation between this meteorological data and the residuals.

Figure 18. Daily daytime average of the wind direction from Carbon Tracker versus CO₂ mixing ratio residuals for (a) Centerville and (c) Round Lake. Daily daytime average of the temperature from Carbon Tracker versus CO₂ mixing ratio residuals for (b) Centerville and (d) Round Lake. The data included in these figures are for the months of Growing Season of 2007.
Chapter 4

CONCLUSION

Using CO₂ mixing ratios simulated by the atmospheric inverse model Carbon Tracker and observations from seven different towers in the MCI field campaign, we have performed an analysis of the data-model residual in order to evaluate the performance of a global atmospheric inversion in the MCI region. These analyses were performed for two different periods, June through December, 2007 and the 2007 growing season. The model-data difference shows the difficulties that Carbon Tracker has in simulating the growing season, showing significant differences in the magnitude of the seasonal draw-down, especially for sites in the “corn belt” region. These differences could be caused by transport errors or underestimation of the fluxes in this region.

We show that LEF, which is the only site used for Carbon Tracker optimization, has the highest correlation of the model to the observations. All the sites tend to underestimate the day-to-day variability for both periods, with the exception of Centerville in the growing season. In general, Carbon Tracker better simulates the seasonal cycle than it does the day-to-day variability.

The distributions of the residuals show that both the mean and standard deviations are higher for the “corn belt” sites. Also, we illustrate that the residuals were non-Gaussian. This study cannot determine the cause of the non-Gaussian distributions, nevertheless, considering that the Gaussian assumption might be violated, future study will need to test what effect that this could cause on atmospheric inversions.
We studied the correlation of residual in space and time to guide the construction of future atmospheric inversions. Sites located in the “corn belt” have residuals that are correlated in time for a period of 40 to 60 days, reflecting the persistent offset during the growing season. For two sites (Centerville, LEF) the amplitude of the autocorrelation is much lower than the other sites. Also, we found that spectral analyses might show a peak in the residuals at a periodicity of 4 to 5 days, possibly the result of difficulty simulating frontal passages. These analyses suggest that high spatial correlations require sites to be close to each other and share the same type of vegetation (e.g. WBI and Kewanee). Many exceptions to these rules were found, however, questioning whether distance and vegetation type were most important in determining the spatial correlation.

We did not find a clear relationship between temperature or wind direction and the residuals. Growing season analyses did suggest a relationship between northerly winds and large negative residuals at the corn belt sites. In the past case studies have been used to examine the relationship between modeled vs. observed CO$_2$ concentrations and wind associated with frontal events (Wang et al., 2007). A similar approach might be beneficial with these data.

Both transport and flux errors influence our model-data mismatch analysis. Further studies focusing specifically on the comparison between the optimized and observed fluxes will help to understand the importance of flux errors in the data-model residuals. Also, comparison of meteorological data and high resolution transport models to the TM5 transport model will help to assess how well the current system simulates the atmospheric transport. It will be worthwhile to repeat this analysis, but using a
mesoscale transport model to find how much a high spatial model will improve the simulation.


Krol, M., S. Houweling, B. Bregman, M. van den Brock, A. Segers, P. van Velthoven, W. Peters, F. Dentener, and P. Bergamaschi, 2005: The two-way nested global


