The Pennsylvania State University
The Graduate School
College of Earth and Mineral Sciences

SPATIAL STRUCTURE IN NORTH AMERICAN TERRESTRIAL
BIOLOGICAL CARBON FLUXES AND FLUX MODEL ERRORS
EVALUATED WITH A SIMPLE LAND SURFACE MODEL

A dissertation in
Meteorology
by
Timothy William Hilton

© 2011 Timothy William Hilton

Submitted in Partial Fulfillment
of the Requirements
for the Degree of

Doctor of Philosophy

December 2011
The dissertation of Timothy William Hilton was reviewed and approved* by the following:

Kenneth J. Davis  
Professor of Meteorology  
Dissertation Advisor, Chair of Committee

Klaus Keller  
Associate Professor of Geosciences

Raymond G. Najjar  
Professor of Meteorology and Geosciences

Erica Smithwick  
Assistant Professor of Geography

William S. Brune  
Professor of Meteorology  
Head of the Department of Meteorology

*Signatures are on file in the Graduate School.
Abstract

Of the roughly 7 pG of carbon released annually to Earth’s atmosphere within anthropogenic carbon dioxide (CO₂), terrestrial ecosystems remove roughly 25% via gross primary production in excess of ecosystem respiration. Ecosystem–atmosphere exchange (net ecosystem exchange, NEE) of carbon dioxide is well-constrained at the global scale and, at field observation locations, at scales on the order of 1 km², but is poorly constrained at spatial scales in between. This makes it difficult to assess the ecological and atmospheric processes that interact to drive NEE, which in turn results in considerable uncertainty around future ecosystem CO₂ uptake, and therefore future concentrations of atmospheric CO₂, a primary driver of global climate change.

This dissertation seeks to constrain estimates of North American NEE by analyzing data from nearly 100 eddy covariance NEE measurement sites spanning the continent in conjunction with satellite observations of ecosystem behavior and a simple land surface model (vegetation photosynthesis and respiration model, VPRM).

VPRM is optimized to the eddy covariance observations. A spatial covariance function for VPRM NEE error is then estimated. This results in a characteristic length scale of roughly 400 km for VPRM NEE error spatial covariance and defines an error spatial covariance matrix for VPRM in North America. This new piece of information empirically constrains atmospheric inversions of CO₂ concentration measurements, thereby reducing their uncertainty.

A statistical regression model is then fit to annually integrated VPRM NEE error spread as a function of VPRM NEE magnitude, air temperature, and precipitation. The regression model is cross-validated at 27 eddy covariance sites not used for model fitting and shown to provide a reasonable fit at these sites. This provides a method to estimate errors for annually integrated VPRM NEE, allowing consideration of VPRM NEE interannual variability in the context of VPRM errors.
## Table of Contents

### Preface
- Preface ix

### Acknowledgments
- Acknowledgments x

### Chapter 1
- Introduction 1

### Chapter 2
- Improving terrestrial CO₂ flux diagnosis using spatial structure in land surface model residuals 3
  - 2.1 Introduction 3
  - 2.2 Methods 7
    - 2.2.1 Land surface model 7
    - 2.2.2 Data 8
    - 2.2.3 VPRM parameter estimation 9
    - 2.2.4 Quantifying spatial structure 11
  - 2.3 Results 14
    - 2.3.1 VPRM parametrization 14
    - 2.3.2 VPRM NEE residual spatial structure 15
  - 2.4 Discussion 19
    - 2.4.1 Caveats 19
    - 2.4.2 Implications 20
  - 2.5 Conclusions 22
  - 2.6 Figures and tables 24
Chapter 3
Evaluating terrestrial CO$_2$ flux diagnoses from a simple land surface model and its residuals

3.1 Introduction ................................................................. 34
3.2 Methods ................................................................. 37
  3.2.1 Land surface model .................................................. 37
  3.2.2 Land surface model parameterization ............................ 38
  3.2.3 Data ..................................................................... 39
  3.2.4 Ecosystem-atmosphere carbon dioxide flux calculation .... 40
  3.2.5 NEE residual spread estimation ................................. 40
3.3 Results and discussion ......................................................... 42
  3.3.1 Land surface model parameter set ranking ...................... 42
  3.3.2 VPRM NEE residual evaluation ................................... 43
  3.3.3 VPRM fluxes .......................................................... 44
  3.3.4 Estimated spread of VPRM fluxes ............................... 46
  3.3.5 NEE error covariance nugget ..................................... 48
  3.3.6 VPRM parameterization and NEE spatial behavior ........ 49
  3.3.7 Considering NEE error spatial covariance in NEE diagnosis 50
  3.3.8 Caveats .................................................................. 51
3.4 Conclusions .................................................................. 52
3.5 Figures and tables ............................................................. 53

Chapter 4
Conclusions and Future Work ................................................. 82

Bibliography .................................................................. 85
## List of Figures

2.1 Map of flux observation locations ........................................... 24
2.2 Parametric variogram model examples ..................................... 27
2.3 VPRM parameter boxplots ...................................................... 28
2.4 June-July-August mean VPRM flux residual variograms ................. 29
2.5 estimated covariance range values cumulative density functions, 1000 GRFs vs. observed VPRM residuals ........................................ 31
2.6 Best-fit range values (km) for cumulative annual anomalies of observed NEE, VPRM NEE, and VPRM NEE residuals. Best-fit values were determined by AIC as described in section 2.2.4. The number $y$ plotted denotes the year 200$y$. Years where the pure nugget covariance function fit more optimally than the exponential are shown in the shaded box. Anomalies were calculated as the departure from the mean value of 2000 to 2006 annual mean cumulative observed values. ........................................ 32
2.7 As Figure 2.6, but displaying semivariogram sill values. ................. 33
3.1 Map of cross-validation site locations. .................................... 53
3.2 SSE vs. number of VPRM parameters ...................................... 54
3.3 histogram, VPRM NEE residuals .......................................... 56
3.4 histogram, VPRM annual integrated NEE residuals ...................... 57
3.5 histograms, annual NEE, observed and VPRM .......................... 58
3.6 2002 VPRM integrated GEE ............................................... 59
3.6 2002 VPRM integrated R ................................................... 60
3.6 2003 VPRM integrated NEE ............................................... 61
3.7 2002 VPRM GEE anomalies ............................................... 62
3.7 2003 VPRM GEE anomalies ............................................... 63
3.7 2004 VPRM GEE anomalies ............................................... 64
3.7 2005 VPRM GEE anomalies ............................................... 65
3.7 2006 VPRM GEE anomalies ............................................... 66
3.8 2002 VPRM R anomalies ................................................... 67
3.8 2003 VPRM R anomalies ................................................... 68
3.8 2004 VPRM R anomalies ................................................... 69
3.8 2005 VPRM R anomalies ................................................... 70
3.8 2006 VPRM R anomalies ................................. 71
3.9 2002 VPRM NEE anomalies ............................... 72
3.9 2003 VPRM NEE anomalies ............................... 73
3.9 2004 VPRM NEE anomalies ............................... 74
3.9 2005 VPRM NEE anomalies ............................... 75
3.9 2006 VPRM NEE anomalies ............................... 76
3.10 2004 VPRM June-July-August integrated NEE. Units are gC m$^{-2}$ yr$^{-1}$. ........................................ 77
3.10 2004 VPRM June-July-August integrated NEE. Units are gC m$^{-2}$ yr$^{-1}$. ........................................ 78
3.11 Estimated square root of NEE residual squared difference, 2002 .......................... 79
3.12 Results from an empirical regression model (eq. 3.5) for VPRM NEE residual spread. Units are (gC m$^{-2}$ yr$^{-1}$)$^2$. Top panel shows observed values vs. predicted values at 27 cross-validation sites (Table 3.1). Observed values are outside of the 95% prediction interval where the solid line falls outside of the dashed lines. One of 56 predicted values (2%) is outside the 95% prediction interval. The bottom panel shows histograms for observed values and model-predicted values. ........................................ 80
3.13 Difference in total sum of squared errors (SSE): covariance-“adjusted” SSE at 27 cross-validation sites (fig 3.1, Table 3.1). Filled plotting makers show values greater than zero (i.e. the adjustment lowered the SSE). There is no adjusted SSE at US-FR2 and CA-TP2 because there are no data points within the 400-km kriging neighborhood. ........................................ 81
## List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>65 North American eddy covariance sites used to parameterize VPRM and calculate VPRM flux errors. PFTs are taken from the International Geosphere-Biosphere Programme (IGBP) land cover classification scheme (Loveland and Belward, 1997). The PFT classifications are taken from literature citations or investigator descriptions where available, and otherwise derived from MODIS 1-km land surface classifications. Data are from the 2007 Fluxnet Synthesis Dataset.</td>
<td>25</td>
</tr>
<tr>
<td>2.2</td>
<td>VPRM parameter sets and total number of parameters.</td>
<td>27</td>
</tr>
<tr>
<td>2.3</td>
<td>best-fit variogram ranges by year and season</td>
<td>30</td>
</tr>
<tr>
<td>3.1</td>
<td>27 North American eddy covariance cross-validation sites.</td>
<td>55</td>
</tr>
</tbody>
</table>
Preface

Chapters 2 and 3 of this dissertation consist of text prepared as two manuscripts to be submitted to Journal of Geophysical Research Biogeosciences. Timothy W. Hilton developed the scientific hypotheses, planned and conducted the scientific analyses, and wrote the text of both articles. Kenneth J. Davis, Klaus Keller, and Nathan M. Urban provided advice in formulating the hypotheses and choosing the data and analyses presented here and provided editorial suggestions for the text.

Chapter 2 will be submitted with title “Improving terrestrial CO$_2$ flux diagnosis using spatial structure in land surface model residuals” and authors Timothy W. Hilton, Kenneth J. Davis, Klaus Keller, and Nathan M. Urban.

Chapter 3 will be submitted with title “Evaluating terrestrial CO$_2$ flux diagnoses from a simple land surface model and its residuals” and authors Timothy W. Hilton, Kenneth J. Davis, and Klaus Keller.
Acknowledgments

This dissertation would not exist without the help and support of numerous people across many years.

My advisor, Dr. Kenneth J. Davis, has been more than generous in sharing his time, expertise, friendship, and patience throughout this undertaking. My committee members Dr. Klaus Keller, Dr. Raymond G. Najjar, and Dr. Erica Smithwick have similarly supported my efforts. In addition, all four were understanding beyond the call of duty in allowing me to complete this dissertation remotely from Penn State in order to live with my wife.

My parents, Dr. Ronald W. Hilton and Margaret J. Hilton, and my brother Bradley R. Hilton have been unwaveringly supportive for years.

Most importantly, my wife Dr. Kerry N. Makin-Byrd is the unseen pillar of love and support upon which all of this work rests.

The work presented here reflects the inspiration I received across almost three decades from teachers too numerous to list at Caroline Elementary School, Dewitt Middle School, and Ithaca High School in Ithaca, New York; Princeton University; and, most recently, the Pennsylvania State University. They instilled in me a desire to learn about how the world works and the skills and capability to go about learning.

A great many scientists contributed either data or advice to this effort.

M. Haran of the Penn State Department of Statistics provided advice on the geostatistical methods. M.O. Roman of NASA and F.A. Heinsch of the U.S. Forest Service provided helpful advice in selecting MODIS surface reflectance data products.

Data were processed using the R language and platform for statistical computing (R Development Core Team, 2007), using the gstat (Pebesma, 2004), geoR (Ribeiro Jr. and Diggle, 2001), and DEoptim (Ardia and Mullen, 2009) packages. Continental data processing in chapter 3 was performed using Scipy (Jones et al., 2001–) and matplotlib (Hunter, 2007).

Funding for this research was provided by the NOAA Office of Global Programs and the U.S. Department of Energy Terrestrial Carbon Processes Program. We wish to thank the many agencies that provided support for eddy covariance tower construction and maintenance.
The Metolius AmeriFlux research was supported by the Office of Science (BER), U.S. Department of Energy, Grant No. DE-FG02-06ER64318. The Metolius old-aged ponderosa pine study was supported by NASA (grant # NAG5-7531), and the Office of Science (BER), U.S. Department of Energy (grant # FG0300ER63014). Data collection for the US-ARM site was supported by the Office of Biological and Environmental Research of the U.S. Department of Energy under contract DE-AC02-05CH11231 as part of the Atmospheric Radiation Measurement Program. Research at the Morgan Monroe State Forest site was supported by the Office of Science (BER), U.S. Department of Energy, Grant No. DE-FG02-07ER64371.

This work used eddy covariance data acquired by the FLUXNET community and in particular by the following networks: AmeriFlux (U.S. Department of Energy, Biological and Environmental Research, Terrestrial Carbon Program (DE-FG02-04ER63917 and DE-FG02-04ER63911)), AfriFlux, AsiaFlux, CarboAfrica, CarboEuropeIP, CarboItaly, CarboMont, ChinaFlux, Fluxnet-Canada (supported by CFCAS, NSERC, BIOCAP, Environment Canada, and NRCan), GreenGrass, KoFlux, LBA, NECC, OzFlux, TCOS-Siberia, USCCC. We acknowledge the financial support to the eddy covariance data harmonization provided by CarboEuropeIP, FAO-GTOS-TCO, iLEAPS, Max Planck Institute for Biogeochemistry, National Science Foundation, University of Tuscia, Universit Laval and Environment Canada and US Department of Energy and the database development and technical support from Berkshire Water Center, Lawrence Berkeley National Laboratory, Microsoft Research eScience, Oak Ridge National Laboratory, University of California - Berkeley, University of Virginia.

This work used global temperature, precipitation, and downward surface radiation data from Princeton University, Department of Civil and Environmental Engineering, 2006: Global Meteorological Forcing Dataset for Land Surface Modeling. Dataset ds314.0 published by the CISL Data Support Section at the National Center for Atmospheric Research, Boulder, CO, available online at http://dss.ucar.edu/datasets/ds314.0/.

MODIS data are distributed by the Land Processes Distributed Active Archive Center (LP DAAC), located at the U.S. Geological Survey (USGS) Earth Resources Observation and Science (EROS) Center (lpdaac.usgs.gov).


I would like also to acknowledge the proprietors and workers of Saints Coffee, State College, Pennsylvania; Muddy Waters, San Francisco, California; and The Grind, Redwood City, California. Their workspace and their coffee boosted both my spirits and this work.

I offer my heartfelt thanks. Without all of these contributions this dissertation would not have been possible.
Dedication

To my true love Kerry, and to Mom, Dad, and Brad.
Introduction

The atmospheric mixing ratio of carbon dioxide (CO₂) has increased consistently and precipitously since the Industrial Revolution from 280 parts per million (ppm) to 388 ppm as of 2008 (Conway et al., 2009; Monnin et al., 2001). Emissions from human fossil fuel combustion, cement production, and deforestation caused the increase (Denman et al., 2007). Considering this in conjunction with fossil fuel burning statistics, however, proves that the measured annual increase in atmospheric CO₂ amounts to only 43 percent of human emissions to the atmosphere (Le Quéré et al., 2009).

Radiative forcing from carbon dioxide and other greenhouse gasses drives anthropogenic climate change (Denman et al., 2007). Thus, understanding the fate of the 57 percent of anthropogenic carbon dioxide emissions that does not remain in the atmosphere is crucial to predicting the behavior of the climate in the coming decades and centuries. Broadly, we know that this carbon is removed from the atmosphere by oceans and terrestrial plants in roughly equal proportions (e.g., Tans et al., 1990; Keeling and Shertz, 1992). The distribution across the world’s land masses of the terrestrial carbon sink is not well constrained, however (e.g., Jacobson et al., 2007a). Likewise, climatic drivers such as temperature and precipitation, ecological processes such as ecosystem recovery from disturbances (e.g., fires and logging) combine to determine the pace of terrestrial carbon uptake, but their relative contributions are poorly known (Pacala et al., 2001; Joos et al., 2002).

Because of the uncertainties surrounding terrestrial carbon sink locations
and their drivers, we cannot predict with confidence the strength of the terrestrial sink 100 years from now, or even whether the terrestrial sink might become a source as the climate changes (Friedlingstein et al., 2006). This adds considerable uncertainty to efforts to forecast climate change itself because of the significant role that terrestrial ecosystems presently play in removing anthropogenic carbon dioxide from the atmosphere: if the terrestrial sink were to disappear, carbon dioxide would accumulate in the atmosphere even more rapidly.

This dissertation seeks to reduce these crucial uncertainties by making several new contributions. The studies presented here use field observations of ecosystem-to-atmosphere carbon dioxide fluxes to inform a model of terrestrial carbon fluxes in an effort to shed light upon the drivers of terrestrial carbon uptake. They also present a method to analyze spatial correlations in flux model errors to extract more information from the observed fluxes with the goal of better constraining the spatial pattern of global fluxes. Flux observations are undertaken with the assumption that the small spatial area (order 10 km $^2$) than can be directly observed by field instruments will be characteristic of a much larger area of similar ecological characteristics. The work presented here quantifies the length scale (approximately 400 km) in which that assumption is correct.

Chapter 3 integrates these methods into diagnoses of North American terrestrial carbon fluxes for the years 2000 to 2006 at 1 km resolution, and develops a methodology to quantitatively estimate uncertainties surrounding these diagnoses. This uncertainty estimate is derived directly from eddy covariance flux observation–model residuals, and therefore comprehensively integrates a wide range of error sources from both the modeling and field observation sides of flux diagnosis. Such a comprehensive and quantitative error estimation is presently unique.
Improving terrestrial CO$_2$ flux diagnosis using spatial structure in land surface model residuals

2.1 Introduction

The rapid carbon dioxide (CO$_2$) accumulation in Earth’s atmosphere in the second half of the 20th Century (Conway et al., 2009) has been partially offset by natural biogeochemical processes. Without these buffers, atmospheric CO$_2$ could accumulate twice as fast: of the roughly 7 Pg of carbon humans release each year by burning fossil fuels, only roughly half remains in the atmosphere as carbon dioxide (Denman et al., 2007). The rest is absorbed by oceans through air-sea gas exchange or by terrestrial and marine flora through net primary production (NPP; Denman et al., 2007). Terrestrial biological fluxes of CO$_2$ through photosynthesis and respiration constituted a net sink from the atmosphere of two to three Pg C per year during the 1990s (Le Quéré et al., 2009), and they exhibit higher interannual variability than oceanic fluxes (Bousquet et al., 2000; Le Quéré et al., 2009). Understanding terrestrial fluxes is crucial to understanding and predicting the increase in atmospheric CO$_2$ caused by anthropogenic emissions.

Though the net global flux of CO$_2$ to the atmosphere is well-constrained
(Tans and Conway, 2005), continental biological CO₂ fluxes are not well characterized, and their drivers are, so far, poorly understood. Diagnostic skill at interannual timescales is poor: land surface models consistently fail to capture observed CO₂ flux interannual variability (e.g., Friend et al., 2007; Ricciuto et al., 2008; Prentice et al., 2000). Predictive skill is also poor: a sampling of terrestrial flux models project terrestrial sink strengths for the year 2100 that vary widely in magnitude and sign (Friedlingstein et al., 2006).

There are a number of sources of information available to constrain terrestrial fluxes. These include direct eddy covariance flux observations, observed atmospheric CO₂ concentrations coupled with atmospheric transport models, and land surface models.

Land surface models integrate ecological and meteorological drivers into a quantitative biological carbon flux estimate for some land region. They are useful because they can be used to extrapolate over large scales. Direct observation footprints of even the most spatially dense CO₂ flux observation networks cover only a tiny fraction of the land areas they span. For example, even with seven eddy covariance (EC) towers in a roughly 50 km by 75 km area, Goulden et al. (2006) estimate that they directly observe less than 0.01% of that space. Land surface models estimate fluxes where direct observations do not exist. Improving model diagnoses of the magnitudes and drivers of terrestrial fluxes is a necessary step toward improving overall predictive skill.

Atmospheric inversion calculations (e.g., Rayner et al., 1999; Gurney et al., 2002; Rödenbeck et al., 2003; Peters et al., 2005, 2007) offer one approach to use observed atmospheric CO₂ concentrations coupled to an atmospheric transport model to further constrain terrestrial CO₂ flux diagnoses. This approach usually divides the planet into regions, and within each region typically solves for a correction to a prior flux estimate from a land surface model (e.g. Gurney et al., 2002). In regions of the world where CO₂ concentration observations are scarce there is little information with which to correct the prior flux, and the resulting flux estimations are therefore heavily dependent on the prior. Rödenbeck et al. (2003) introduced a prescribed isotropic spatial covariance to the prior, choosing a spatial correlation scale of 1275 km based on the average scale of autocorrelation among four different land surface models examined by McGuire
et al. (2001). Peters et al. (2005, 2007) propagate inferred surface fluxes forward through time instead of using a prior flux estimate calculated offline for each time step before beginning the inversion calculations. They also use an ensemble Kalman filter to estimate a surface flux spatial covariance matrix. This relies on the assumption that flux errors are independent at weekly time scales and at spatial regions of 25% to 50% of each continent (Peters et al., 2005), an assumption that is conventional, though most likely not strictly accurate (Peters et al., 2005).

Jacobson et al. (2007a,b) describe an inversion approach that does not rely on prior fluxes on the grounds that modeled regional prior fluxes must either be assumed to be independent or treated as spatially correlated with an explicit spatial structure. In reality they are often correlated, though the quantitative correlations are unknown (Jacobson et al., 2007b, auxiliary materials). Jacobson et al. (2007b) show that this assumption of independence results in overconfident flux estimates. By eschewing prior flux estimates the Jacobson et al. (2007a,b) study avoids this pitfall, but at the cost of ignoring the knowledge of ecosystem behavior encapsulated in the flux model: the resulting posterior flux uncertainties are much larger than when modeled prior fluxes are included. That is, removing the information provided by a land surface model removes a significant constraint from the estimation.

Ideally, a flux diagnosis method would integrate all available sources of information. Here we focus on extracting information from a land surface model, while minimizing the overconfidence-producing assumptions demonstrated by Jacobson et al. (2007a,b). Model–data residuals are the combined effects of flux observation errors, model structural error, and natural variability uncaptured by the flux model. The spatial behavior of model residuals sheds light on the processes that drive fluxes. In the following analyses we will use that information to produce a data-derived quantification of the model-data residuals and their spatial structure that may be used to constrain the fluxes.

Terrestrial flux drivers (meteorological and ecological) do not appreciably vary at scales of, say, one centimeter; therefore model residuals should be correlated within some distance, however small. That distance is an upper bound on the area that a model result for a single spatial point can illuminate. Without
a quantitative method for determining a correlation structure for model residuals, it is convenient to assume model residuals are independent and identically distributed (i.i.d.) in space and time. For example, Pacala et al. (2001), Peylin et al. (2002), Gurney et al. (2002), and Peters et al. (2005) adopt this assumption in their inversions. In fact, inversions that solve for corrections to regional prior fluxes intrinsically assume that prior flux residuals are correlated within the time scale and spatial scale of the inversion (Rödenbeck et al., 2003; Michalak et al., 2004). If they are not, the inversion applies a uniform correction to a group of uncorrelated residuals, creating a source of error (Chevallier et al., 2006). As noted, Rödenbeck et al. (2003) impose a prior flux uncertainty spatial correlation length scale of 1275 km. They base that distance on the autocorrelation length scales of the four models used by McGuire et al. (2001). This depends on the assumption that the NEE range among those four models is representative of flux model uncertainty (Rödenbeck et al., 2003). Furthermore, Michalak et al. (2004) point out that spatial structure, if existent, contains information that constrains fluxes and suggests weights for fluxes to identify and remove redundant information.

We can improve on existing flux diagnoses by deriving a residual covariance matrix to characterize the spatial behavior of flux model residual correlation. A necessary (and independently useful) prerequisite for estimating a model’s residual covariance matrix is an estimation of the spatial scale at which the model’s residuals are correlated. Here we present an analysis of the residual covariance matrix of VPRM (Mahadevan et al., 2008), a simple land surface model.

We test the hypothesis that VPRM model residuals are spatially correlated at length scales smaller than the North American continent but larger than an individual EC tower footprint. Analyzing the spatial scale of VPRM residual correlation will provide that length scale. The Ameriflux and Fluxnet Canada networks of EC towers provide observations that allow us to directly analyze the spatial behavior of VPRM residuals. If that correlation length scale proves larger than the tower footprints, it will prove that the network of EC flux towers in North America has sufficient spatial span and density and has collected enough data across time to empirically define a flux model residual covariance
2.2 Methods

2.2.1 Land surface model

The Vegetation Photosynthesis and Respiration Model (VPRM) of Mahadevan et al. (2008) is a simple diagnostic terrestrial flux model. In spite of its simplicity, VPRM captures daily and annual cycles in CO$_2$ fluxes reasonably well (Mahadevan et al., 2008). VPRM structure and skill are described in great detail by Mahadevan et al. (2008). Here we provide a brief overview of the model structure.

VPRM models net ecosystem exchange (NEE) as the sum of a photosynthetic component (gross ecosystem exchange, GEE) and an ecosystem respiration component. GEE is modeled via the equation:

$$GEE = \lambda \times T_{\text{scale}} \times P_{\text{scale}} \times W_{\text{scale}} \times EVI \times \frac{1}{1 + PAR/PAR_0} \times PAR.$$  \hspace{1cm} (2.1)

$PAR$ is observed photosynthetically active radiation and $EV I$ is the satellite-derived enhanced vegetation index (Huete et al., 2002). $P_{\text{scale}}$ and $W_{\text{scale}}$ are satellite-derived dimensionless scaling terms describing phenology and canopy moisture. The value of the third dimensionless scaling term $T_{\text{scale}}$ is taken from literature and describes the relationship between photosynthesis and temperature. $P_{\text{scale}}, W_{\text{scale}},$ and $T_{\text{scale}}$ may vary in both time and space. $PAR_0$ and $\lambda$ are model parameters.

Respiration ($R$) is modeled as a linear function of observed air temperature ($T$):

$$R = \alpha \times T + \beta,$$ \hspace{1cm} (2.2)

with parameters $\alpha$ and $\beta$.

NEE is the difference between the photosynthetic flux and the respiration flux:

$$NEE = R - GEE.$$ \hspace{1cm} (2.3)
Within equations (2.1), (2.2), and (2.3), $\lambda$ governs the slope of the light-response curve (the relationship between photosynthetic CO$_2$ flux and PAR). $\alpha$ defines the slope of the respiration response to temperature. $PAR_0$ defines a half-saturation value for photosynthesis. That is, it specifies a PAR value at which further increases in PAR no longer enhance photosynthesis, as other limiting factors become dominant. VPRM places a PFT-specific floor $T_{low}, 1^\circ C \leq T_{low} \leq 5^\circ C$, on surface temperatures. Temperatures below $T_{low}$ are raised to $T_{low}$ when calculating respiration. $\beta$ thus specifies a minimal level of respiration that occurs regardless of air temperature.

In its simplicity, VPRM offers two important advantages over more complex models. First, it has only four user-defined parameters and is computationally inexpensive. This makes parameter estimation via data assimilation methods that do not require parametric assumptions computationally tractable. Second, as inputs, VPRM requires only air temperature, photosynthetically active radiation (PAR), and satellite-derived vegetation and moisture indices. It can thus be run globally, with no need to compile temporally-filled meteorological driver data. These advantages make VPRM a useful tool both for producing diagnostic regional flux maps, and also for evaluating spatial scales of model residuals in the manner of Chevallier et al. (2006).

### 2.2.2 Data

To constrain VPRM parameter values and examine NEE residuals we use data from 65 North American eddy covariance flux towers. Figure 2.1 shows the sites on a map, and Table 2.1 lists the sites and dominant plant functional type (PFT). These data are part of the 2007 Fluxnet Synthesis Dataset (http://www.fluxdata.org). For each site, this dataset contains CO$_2$ flux, air temperature, and PAR observations at 30-minute intervals, as well as many other quantities not needed for VPRM.

The Fluxnet dataset contains gap-filled NEE, as well as non-filled NEE. Structurally, VPRM does not consider driver data or flux results from previous time steps (equation (2.3)). VPRM simply does not report an NEE at timesteps where the required driver data are not available. In light of this, and to reduce potential
residuals due to gap filling, we use the non-filled data.

The 65 observation sites cover nine of the 17 PFTs of the International Geosphere-Biosphere Programme (IGBP) land cover classification scheme (Loveland and Belward, 1997): evergreen needleleaf forest (27 sites), deciduous broadleaf forest (8 sites), mixed forest (3 sites), closed shrublands (7 sites), open shrublands (2 sites), woody savannas (1 site), grasslands (7 sites), permanent wetlands (4 sites), and croplands (6 sites). The eight PFTs not represented are: deciduous needleleaf forest, evergreen broadleaf forest, savannas, water, cropland/natural vegetation mosaic, urban and built-up, snow and ice, and barren or sparsely vegetated.

Site phenology, land surface water, enhanced vegetation index (Huete et al., 2002), and land surface cover type are calculated from reflectances measured by the NOAA MODIS instrument, orbiting with the NASA Terra satellite since 2000 and the NASA Aqua satellite since 2002. Oak Ridge National Laboratory extracts MODIS data for many Fluxnet tower sites and makes them available on the world wide web (ORNL DAAC, 2009). For the present study, we use MODIS Collection 5 data (ORNL DAAC, 2010). Collection 5 data offer improved processing algorithms from Collection 4 (Friedl et al., 2010; Didan and Huete, 2006). Site phenology is from dataset M*D12Q2 (Strahler et al., 1999a), reflectances are from dataset M*D43A4 (Strahler et al., 1999b), vegetation indices are from dataset M*D13A2 (Huete et al., 2002, 1999), and IGBP land surface cover types are from dataset M*D12Q1 (Loveland and Belward, 1997; Strahler et al., 1999a). The ‘*’ in M*D is either ‘O’, representing the data from the Terra satellite, or ‘Y’ representing the data from the Aqua satellite. We considered only MODIS data of “best” quality, as indicated by each MODIS product’s associated quality QA flags.

We examine the time period 2000 to 2006, bounded in 2000 by the MODIS instrument launch and in 2006 by eddy covariance flux availability.

2.2.3 VPRM parameter estimation

VPRM has four user-estimated parameters that may depend on the location being simulated: $\lambda$, $\text{PAR}_0$, $\alpha$, and $\beta$. In this section we describe how we estimated
these parameter values.

We seek the parameter values that cause VPRM NEE to match observed NEE as closely as possible. We chose to minimize the sum of squared errors (SSE; we define VPRM residuals as $\text{NEE}_{\text{VPRM}}$ minus $\text{NEE}_{\text{observed}}$). If the residuals are normally distributed with a constant standard deviation (i.e., homoskedastic), minimizing SSE is equivalent to a maximum likelihood estimate (Hilborn and Mangel, 1997).

In reality, flux model residuals are neither independent nor identically distributed. A double exponential distribution describes EC observation error better than the normal distribution (Richardson et al., 2006). EC observation error is also proportional to NEE magnitude and wind speed (Richardson et al., 2006). Thus the strong daily and seasonal cycles of NEE cause EC observation errors to be temporally autocorrelated as well as heteroskedastic. The combined impact of land surface model structural error, incorrect parameter values, and natural variability—microscale variations in climate, ecosystem behavior, etc.—may also exhibit statistically significant autocorrelation (Ricciuto et al., 2008). We can approximate distributions for each of those error sources from published literature; therefore the full likelihood function may be written out as the integrated product of likelihood functions for several different statistical distributions. Reducing that integral to an analytical solution, however, is beyond the scope of this study.

NEE varies on a number of different time scales (e.g. daily, annual) and space scales (e.g. local land-use and PFT heterogeneity, larger regions that experience similar climate patterns). An ideal land surface model parameter estimation method would allow parameter values to vary at space and time scales matching the ecological variations in NEE. Optimizing parameter values in short time intervals and small spatial windows would run the risk of overfitting as well as incur unnecessary computational cost. We chose to examine three temporal and three spatial windows for SSE minimization—in time: monthly, annual, and all available data; and, in space: individual sites, sites grouped by PFT, and all sites together. This approach yields nine different parameter sets, ranging from four to more than 21000 parameter values. Table 2.2 summarizes the nine parameter sets.
To search for parameter values that minimize SSE we used differential evolution (DE) (Price et al., 2006). DE is a genetic optimization algorithm that is both fast and more reliable in identifying a global optimum compared to gradient-based minimization algorithms. We used the DEoptim package (Ardia and Mullen, 2009) for the R language and platform for statistical computing (R Development Core Team, 2007).

2.2.4 Quantifying spatial structure

The spatial covariance structure quantifies the spatial structure (or lack thereof) for an arbitrary function of space. The semivariogram offers a concise visual summary of the covariance structure. The spatial functions of interest here are VPRM NEE residuals, VPRM NEE, and observed NEE. This section defines the semivariogram and describes its typical behavior for geophysical quantities.

The semivariogram ($\gamma$) is generically defined (Cressie, 1993) as:

$$\gamma(h) = \frac{1}{2} \text{var}(Z(s_i) - Z(s_j)),$$  \hspace{1cm} (2.4)

where $s_i$ and $s_j$ are two locations in space, $h$ is the distance between $s_i$ and $s_j$, $\text{var}$ denotes variance, and $Z$ is some function of location—air temperature, VPRM NEE residual, etc. If $s_i$ and $s_j$ are near one another, one might expect $Z(s_i)$ and $Z(s_j)$ to have similar values, causing $\gamma$ to be correspondingly small. As $h$ increases, $Z(s_i)$ and $Z(s_j)$ typically diverge, and the value of $\gamma$ increases. At some sufficiently large $h$, $Z(s_i)$ and $Z(s_j)$ can become independent, causing $\gamma$ to level off. The value of $h$ where the leveling-off occurs is known as the range, and the value of $\gamma$ at this leveling-off is known as the sill. The range estimates the length scale of spatial correlation in $Z$. These easily-visualized semivariogram features are formal parameters (range, $\phi$; sill or variance, $\sigma^2$) of the covariance function.

In the same way that the population mean provides a statistical estimator for a population’s expected value, there is a statistical estimator to calculate an
empirical semivariogram (\(\hat{\gamma}\)) from a set of observed data (Cressie, 1993):

\[
\hat{\gamma}(h) \equiv \frac{1}{2|N(h)|} \sum_{N(h)} \left( Z(s_i) - Z(s_j) \right)^2,
\]

(2.5)

where \(N(h)\) is the number of location pairs separated by distance \(h\) and the \(\hat{\gamma}\) notation distinguishes the estimated semivariogram from the theoretical definition of equation (2.4); other terms are defined above. The separation distance \(h\) may be a precise distance for a single pair of locations, or may be an aggregated separation distance for a number of pairs of locations.

In this study we use the “robust” semivariogram estimator of Cressie and Hawkins (1980). This estimator includes a correction term for non-normally distributed data, and also reduces the impact of outlying data:

\[
\bar{\gamma}(h) \equiv \frac{\left( \frac{1}{|N(h)|} \sum_{N(h)} |Z(s_i) - Z(s_j)|^{0.5} \right)^4}{2 \left( 0.457 + \frac{0.494}{|N(h)|} \right)}.
\]

(2.6)

Purely mathematically, equation (2.4) requires the semivariogram to equal zero at \(h = 0\), because \(Z(s_i) - Z(s_i) = 0\). In practice, measurement errors cause repeated measurements at a single location to differ. Moreover, measurements are not made at infinitesimally small separation distances. There is no information about \(\gamma(h)\) at distances below the minimum separation distance \(h\) present in the data. This unknown behavior at small \(h\) is sometimes called microscale variation. When microscale variation or measurement error are present, \(\hat{\gamma}(h)\) does not approach zero as \(h\) approaches zero. The value of \(\hat{\gamma}(h = 0)\) is known as the semivariogram nugget, denoted by \(\tau^2\). Together, the sill, range, and nugget characterize the semivariogram and yield much information about the spatial structure of \(Z\).

In addition to providing the length scale of spatial correlation for \(Z\), the semivariogram also specifies the spatial covariance of \(Z\). Specifically,

\[
\text{cov} \left( Z(s_1), Z(s_2) \right) = \frac{1}{2} \text{var} \left( Z(s_1) \right) + \frac{1}{2} \text{var} \left( Z(s_2) \right) - \frac{1}{2} \text{var} \left( Z(s_1) - Z(s_2) \right),
\]

(2.7)

with \(\text{cov}\) denoting covariance, expresses the spatial covariance of VPRM resid-
uals in terms of available quantities: the first two terms on the right side of equation (2.7) are the variance within individual sites and the last term is the semivariogram.

Covariance parameters $\phi$, $\sigma^2$, and $\tau^2$ may be estimated directly from spatial data via maximum likelihood estimation (MLE) by maximizing the log-likelihood function (Diggle and Ribeiro Jr., 2007):

$$L(\beta, \tau^2, \sigma^2, \phi) = -0.5 \left\{ n \log(2\pi) + \log \{ \sigma^2 R(\phi) + \tau^2 I \} \right\} + (y - D\beta)^T (\sigma^2 R(\phi) + \tau^2 I)^{-1} (y - D\beta),$$

with the covariance matrix $\sigma^2 R(\phi) + \tau^2 I$ expressed in terms of $\phi$ (range), $\sigma^2$ (sill), and $\tau^2$ (nugget). The residual matrix $(y - D\beta)$ is the difference between observations $y$ and a model structure given by $D\beta$ with model explanatory variables $D$ and model parameters $\beta$. MLE is the preferred approach for formal covariance parameter estimation (Diggle and Ribeiro Jr., 2007) in large part because it considers the full set of available data rather than relying on the summary provided by an empirical semivariogram.

Fitting a parametric covariance function to observed VPRM residuals provides three key outcomes: (i) the range for VPRM NEE residuals; (ii) covariance of VPRM NEE residuals at arbitrary separation distances—that is, a residual covariance matrix; and (iii), via kriging, a VPRM NEE map that explicitly considers VPRM NEE residuals (Cressie, 1993). Figure 2.2 shows semivariograms for two common parametric covariance functions. When a spatial field has no spatial correlation, its semivariogram looks like the pure nugget covariance function. The exponential covariance function is one example of a model describing a spatial field that is correlated in space to a certain distance and uncorrelated beyond that distance.

For the nine VPRM parameterizations of section 2.2.3 we calculated seasonal mean VPRM residuals. We defined seasons as December-January-February (DJF), March-April-May (MAM), June-July-August (JJA), and September-October-November (SON). Within each season we maximized the negative log likelihood (equation (2.8)) to estimate covariance parameters for both the pure nugget as well as exponential covariance functions (Figure 2.2). We then compared the pure nugget
and exponential fits using AIC (Akaike, 1976). This experiment determines whether the observed VPRM NEE residuals are better described as covarying in space at some length scale (the exponential covariance model) or as spatially independent even at minimal distances (the pure nugget model). We follow this experiment with two pseudodata experiments to assess the tendency of 65 observation locations spread across North America and our AIC test to choose the exponential covariance function when no spatial covariance is present, or to choose the pure nugget covariance model when the underlying field was generated from an exponential covariance model. The rest of this paper describes our parametrization of VPRM and our analysis of VPRM NEE residual spatial structure.

2.3 Results

2.3.1 VPRM parametrization

As described in section 2.2.3, we calculated VPRM parameter values for nine different groupings of those sites in space and time (table 2.2), conditioned on observations from 65 North American eddy covariance sites (table 2.1, Figure 2.1).

Figure 2.3 shows the distribution of VPRM parameter values when estimated monthly within each PFT. Parameter distributions across PFTs for the other eight parameter sets in Table 2.2 are nearly identical to Figure 2.3. The parameter distributions are similar to those of Mahadevan et al. (2008). Most striking in Figure 2.3 is the failure of the parameterization to distinguish among plant functional types.

It is perhaps unexpected that VPRM parameters do not cluster by plant functional type. For example, one might expect that the model parameter estimates of a boreal needleleaf forest should be different from a cropland, for example. There is evidence that light-use efficiency (LUE) is not consistent within PFTs (Ruimy et al., 1994; Schwalm et al., 2006), particularly at daily timescales (Schwalm et al., 2006). Another recent study assumes that maximum LUE is constant across PFTs (Yuan et al., 2007). Schwalm et al. (2006) also suggest intra-
PFT LUE varies less at annual time-scales than at daily scales. The values of \( \lambda \) (the VPRM LUE parameter) in Figure 2.3, relatively invariant across different PFTs, differ from the results of Schwalm et al. (2006). VPRM respiration parameters \( \alpha \) and \( \beta \) also do not vary much across PFTs; this is consistent with previous studies indicating that PFTs are not predictive of soil respiration (Raich and Tufekciogul, 2000; Bond-Lamberty et al., 2004).

The similar parameter values in Figure 2.3 could be a consequence of VPRM’s simplicity; perhaps a two-equation model which takes climatology and phenology from satellite observations is only able to separate landscapes into “green—photosynthesizing” and “brown—not photosynthesizing.” These results offer hints; investigating the question rigorously would require parameter PDFs to ascertain whether the differences in Figure 2.3 are significant. That investigation should also compare model fluxes across different parameterizations. It is possible, for example, that the remote sensing data that drive VPRM are sufficient to separate the NEE of different plant functional types without large parameter differences. The question is intriguing, however. If PFTs truly are not important for NEE diagnosis and prediction, the task of estimating model parameters becomes much simpler: land surfaces may then be simply classified as “green” and “not-green.”

2.3.2 VPRM NEE residual spatial structure

Qualitatively inspecting the shape of an empirical semivariogram gives an intuitive sense for a function’s spatial covariance. Figure 2.4 plots binned semivariograms for June-July-August (JJA) mean VPRM NEE residuals. There is one curve for each of the nine VPRM parameter sets considered (Table 2.2); each point shows the mean semivariance within a 300 km bin.

The nugget is small for the site-specific parameter sets (black curves), and varies from 1 to 3 \((\mu \text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1})^2\), for the other six parameter sets. In units of standard deviation, these six nuggets equal roughly 2.0 \(\mu \text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1}\). The nugget represents the combined influence of variations at spatial scales smaller than the minimum separation distance as well the contributors to VPRM residuals (EC observation error, VPRM structural error, natural variability; see
In general, the semivariances for each parameter set increase from separation distances of 0 km to roughly 800 km, and level off or decrease thereafter. This suggests that VPRM NEE residuals are correlated at distances up to 800 km. We quantify this in the following results.

We are interested primarily in the parameters (range, sill, nugget) of the covariance function that best describes the VPRM residuals. To estimate these parameters, we employ maximum likelihood estimation (MLE, described by equation (2.8)).

We fit both pure nugget and exponential covariance functions (whose characteristic semivariograms are shown in Figure 2.2) to each of the nine sets of VPRM residuals summarized by the binned semivariograms in Figure 2.4. Within each VPRM parameter set we selected either the best-fit pure nugget covariance function or the best-fit exponential covariance function using Akaike’s Information Criterion (Akaike, 1974). AIC balances goodness of fit (more parameters) against parsimony (fewer parameters). Table 2.3 shows seasonal range values for the covariance function that optimally fit the observed VPRM NEE residuals. Blank entries show instances where the pure nugget function optimally fit the observed residuals; this indicates that no spatial correlation is present in the VPRM residuals. Among the 2000 to 2006 observed residuals, 92 of 252 (7 years × 4 seasons × 9 PFTs) were best described by the exponential covariance function. Of those, the median range is 402 km.

To interpret this result, we must test the adequacy of 65 observation locations across North America (Figure 2.1) to detect spatial correlations across hundreds of kilometers. The maximum distance between towers in this group of 65 is 6557 km (US-Atq – US-KS1). To quantitatively test the detection capacity of the data set we generated 1000 Gaussian Random Fields (GRFs) on a 6500 by 6500 grid. Each GRF had an imposed exponential covariance structure with a specified range of 402 km (equal to the median VPRM NEE error seasonal covariance range reported in Table 2.3.) We sampled each GRF at 65 randomly-generated locations and estimated exponential and pure nugget covariance function parameters for each sample set using MLE in the same manner that we estimated range values for the VPRM NEE residuals (Table 2.3). Of the 1000 GRFs, AIC
chose the exponential covariance function for only 74. Of those 74, the median estimated covariance range is 936 km; the median estimated covariance range across all 1000 GRFs is 313 km. This distribution of estimated range values is similar to the distribution estimated from the real VPRM NEE residual observations; Figure 2.5 plots the two distributions side by side. These results suggest that the estimated range values for VPRM NEE residuals (Table 2.3) are consistent with a scenario where VPRM NEE residuals have an exponential covariance structure with a range of roughly 400 km, and that 65 observation locations in the United States and Canada are minimally adequate for detecting that structure.

We also must consider the possibility of spurious MLE results: that the observed VPRM NEE residual realization may occasionally be better fit by an exponential covariance structure when the complete spatial field has no true structure. We generated another set of 1000 GRFs, each containing 65 points within a 6500 by 6500 grid, and each specified to have a pure nugget covariance structure. We calculated MLE covariance function parameters for these 1000 fields. AIC chose the exponential function over the pure nugget for only 25 of the 1000 fields, suggesting that we might expect a data set like our VPRM NEE residuals to produce a spurious exponential covariance structure in only a small minority of realizations considered.

These results suggest quantitatively that JJA mean VPRM NEE residuals are spatially correlated at a length scale on the order of 400 km.

Anomalies from the 2000 to 2006 means for annual cumulative VPRM NEE, annual cumulative observed NEE, and annual cumulative VPRM NEE residuals displayed similar spatial scales (Figure 2.6). This analysis tests the hypothesis that while NEE itself varies significantly at spatial scales on the order of 10 km (e.g., Desai et al., 2008), NEE interannual variability (IAV) is driven by phenomena that operate at much larger scales. If so, then we should see spatial correlation in annual cumulative NEE$_{\text{obs}}$ anomalies. If VPRM is able to capture that large-scale variation, then annual cumulative NEE$_{\text{VPRM}}$ anomalies will show similar spatial correlation. Any spatial structure that exists in NEE$_{\text{obs}}$ anomalies that VPRM fails to capture should appear in VPRM NEE residual anomalies.

As with the VPRM NEE residual semivariograms, we chose optimal anomaly
covariance structures by AIC. Of the seven years examined, NEE$_{obs}$ anomalies show correlation at scales of roughly 1000 km only for 2006 (Figure 2.6). This rate of detection is consistent with that of the pseudodata experiment (Figure 2.5), in which we were able to detect a known exponential covariance structure in only 62 of 1000 attempts. This could indicate that large-scale structure does not consistently exist. It could also suggest that NEE interannual variability could be shaped by larger-scale drivers than is NEE itself, and that our flux tower spatial density is insufficient to consistently detect it in a noisy NEE signal. This seems reasonable; land use, which influences NEE, is markedly diverse throughout the study area. Also, disturbance events that heavily influence NEE (e.g. fire, insects, tree harvest) usually do not impact 500-km stretches of land surface. VPRM is strongly driven by climate variables (Eqns (2.1), (2.2)), so spatial structure in VPRM NEE interannual variability could simply reflect large-scale spatial structure in climatic interannual variability. Though VPRM no doubt contains structural error, it is an attempt to combine climatic terms as ecological research suggests they influence NEE. Therefore, we believe it makes sense to investigate this combined effect of several climate terms (that is, VPRM NEE) rather than attempt to explain NEE interannual variability by searching for spatial coherence in a number of climate variables individually.

Because VPRM NEE residuals are simply the difference between NEE$_{obs}$ and NEE$_{VPRM}$, the spatial behaviors of these three quantities are interrelated. Where spatial structure exists in observations, we expect it to be partitioned among NEE$_{VPRM}$ and VPRM NEE residuals. Results in Figure 2.6 from all nine VPRM parameter sets show strong spatial structure in VPRM NEE residuals. This structure occurs at length scales similar to the length scale exhibited by NEE$_{obs}$. Sill and nugget values for NEE$_{VPRM}$ and VPRM NEE residuals are also of similar magnitude to the sill and nugget for NEE$_{obs}$. VPRM NEE residuals are the combination of NEE observation error, VPRM structural error, and natural variability. Because of its correlation to NEE magnitude (Richardson et al., 2006), we expect the NEE observation error component of VPRM residuals to reflect whatever spatial structure is present in NEE itself. It therefore makes sense that the spatial structure present in NEE$_{obs}$ is not partitioned exclusively into NEE$_{VPRM}$ or VPRM NEE residuals, but appears in both.
The covariance sill value provides an estimate of variance. The sill values (Figure 2.7) for the annual anomalies of annual cumulative VPRM NEE, annual cumulative observed NEE, and annual cumulative VPRM NEE residuals display standard deviations (Figure 2.7, right-side axis) on the order of the annual cumulative NEE typically observed by an eddy covariance site. This suggests that annual VPRM errors at a single location in space are on the order of the flux at that point. If annual VPRM errors are indeed spatially correlated at length scales of 500 km to 1000 km, as suggested by Figure 2.6, then spatially aggregating VPRM NEE at that length scale should provide a method to reduce the VPRM error variance.

2.4 Discussion

Our findings are relevant to both land surface model upscaling as well as atmospheric inversion studies, though several important uncertainties should guide consideration of our results.

2.4.1 Caveats

Several caveats accompany these implications. The structural simplicity of VPRM allows us to conduct parameter estimations that use many thousands of model evaluations. The designers of VPRM achieve that simplicity by abstracting the broadest drivers of NEE out of what is in reality a complex ecology and by considering only short-term drivers of NEE. Longer-term drivers, such as carbon pools (e.g., Curtis et al., 2002) and disturbance histories (e.g., Thornton et al., 2002), are known to be first-order drivers as well. These simplifications caution us against attempting detailed ecological interpretation of the VPRM NEE results and VPRM residuals.

In addition, the carbon cycle community’s understanding of the statistical properties of land surface model NEE residuals remains rudimentary. Several studies have explored the distribution of NEE observation error (e.g., Richardson et al., 2008, 2006). Richardson et al. (2006) find the observational error to exhibit a double exponential distribution Observation error, however, is but one
component of NEE model residuals. In the absence of a rigorous likelihood function that integrates all of the sources of uncertainty that contribute to NEE model residuals, we have used the mathematically simple sum of squared NEE residuals to estimate VPRM parameters. Implementing a statistically proper likelihood function is non-trivial and is the subject of ongoing research.

Our spatial analysis of VPRM residuals compared a pure nugget model with no spatial covariance to an isotropic exponential covariance function that treated all land surface classifications as equal. It is possible that VPRM residuals co-vary differently in the East-West direction than North-South, or that plant functional types, disturbance history, or some other land surface descriptor is important. The present spatial density of eddy covariance observations limits our ability to test these.

2.4.2 Implications

It is critically important to quantitatively tailor NEE model parameter estimates to the domain in which the model is to be run; generic parameter values can reproduce observed NEE poorly (Ricciuto, 2006). Good NEE simulation is crucial to calculating accurate model errors, which are in turn crucial to detecting model error spatial structure.

Our finding that VPRM does not resolve different PFTs through its parameter values can be viewed in at least two different lights. First, studies wishing to provide first-order regional NEE estimates via a low-complexity land surface model may not need to distinguish among PFTs for parameterization on pure statistical grounds. This could lead to considerable savings in computation time and CPU resources. Second, PFTs are commonly assumed to partition land into sections with functionally different participations in the carbon cycle. Our results suggest that PFTs may not be the most useful predictor of a land area’s carbon cycle dynamics, and that alternative partitioning schemes may be more skillful. Stand age and disturbance history are interesting “land surface NEE descriptor” alternatives to PFTs. Thornton et al. (2002) used the BiomeBGC model to explore the impacts of disturbance history, PFT, site climate, atmospheric CO₂ concentration, and nitrogen deposition on NEE variability among seven ever-
green sites spanning North America, and concluded that of those, disturbance history dominated. Goulden et al. (2006) examined seven eddy covariance sites within 50 km of each other that were recovering from burn disturbances that occurred 0, 5, 14, 22, 39, ~73, and ~153 years previously. They found that mid-growing season EVI and CO$_2$ fluxes took roughly 50 years following a burn disturbance to become approximately interannually constant. That 50-year period included transition from primarily deciduous species to primarily black spruce. These results and others suggest that disturbance history could be at least important as climate and plant functional type to understanding NEE for large areas.

The results of Goulden et al. (2006) suggest, at least for boreal evergreen forests, a satellite record on the order of 50 to 100 years or longer could be necessary before stand age and recovery from disturbance can be widely and directly described by remote sensing. Recent landsat products have begun to assemble landscape disturbance records beginning in the 1980s (Huang et al., 2010), offering an opportunity to assess these influences at larger scales.

The spatial length scale of land surface model NEE residual covariance bears directly on atmospheric inversion calculations. Inversions seek to use observed atmospheric CO$_2$ concentrations to refine estimated biological CO$_2$ fluxes within a region of defined boundaries, with the estimated fluxes typically coming from models. Intrinsic to the method is the assumption that prior flux errors are correlated within each region treated as a separate unknown (Rödenbeck et al., 2003; Michalak et al., 2004). Moreover, this correlation must be assumed to exist at both the time scale of the inversion as well as the spatial scale of the inversion regions. Our results indicate strongly that this implicit assumption is valid at seasonal time scales (Table 2.3) and, for annual anomalies, for annual time scales. The relevant spatial scale is approximately 400 km. This length scale is smaller than the scale of 1275 km estimated by Rödenbeck et al. (2003), and is based on eddy covariance flux measurements rather than land surface model comparison. Our length scale also contrasts starkly with the conclusion of minimal spatial covariance presented by Chevallier et al. (2006). Potentially incorrect prior flux error covariance assumptions are but one source of error that an inversion must consider. Scarcity of well-calibrated CO$_2$ concentration
observations, for example, pushes inversion calculations toward regions larger than 1000 km (e.g., Butler et al., 2010). The North American Carbon Program’s Mid-Continental Intensive (MCI) region is a notable exception to this scarcity of \( \text{CO}_2 \) concentration observations (Lauvaux et al., 2011), and presents an opportunity to investigate the impacts of prior flux error covariance assumptions more deeply. Solving for too many regions in an inversion (that is, too many unknowns) risks overfitting the data, and solving for too few risks oversimplifying the inversion and producing over-confident results. We suggest that inversion calculations should optimally use regions with spatial scales on the order of 400 km.

2.5 Conclusions

Using observed NEE from 65 North American eddy covariance sites for the years 2000 through 2006, we make point estimates of parameter values for VPRM, a simple land surface model. We then estimate and analyze covariance structures of VPRM NEE residuals in the interest of quantifying spatial structure in the residuals.

PFTs demonstrate little skill as land surface classifications for model parameter estimation. This may allow large-region model studies to partition land surfaces into a “photosynthetically active or not” dichotomy, thereby simplifying model parameterization.

The semivariogram analyses presented here demonstrate that VPRM NEE residuals are spatially correlated at length scales well beyond individual tower footprints but well short of continental scales. Depending on the model parameterization, that length scale lies somewhere between 100 km and 900 km, with a median value of roughly 400 km. This result is consistent at both seasonal and interannual time scales, and demonstrates that the North American EC tower network is minimally sufficient to define a VPRM residual covariance matrix. This information will allow us to construct a map of VPRM North American \( \text{CO}_2 \) fluxes, optimized to eddy covariance observations.

Our estimated covariance functions for model NEE residuals prove that the North American flux tower observation network is adequate for determining a
land surface model residual covariance matrix.
2.6 Figures and tables

Figure 2.1: The 65 eddy covariance flux tower sites from the Fluxnet network (http://www.fluxdata.org) that provide observations for VPRM parametrization and VPRM flux residual calculation. ENF: evergreen needleleaf forest, DBF: deciduous broadleaf forest, MF: mixed forest, CS: closed shrubland, OS: open shrubland, WS: woody savanna, Gr: grassland, Wet: permanent wetland, Crop: cropland.
Table 2.1: 65 North American eddy covariance sites used to parameterize VPRM and calculate VPRM flux errors. PFTs are taken from the International Geosphere-Biosphere Programme (IGBP) land cover classification scheme (Loveland and Belward, 1997). The PFT classifications are taken from literature citations or investigator descriptions where available, and otherwise derived from MODIS 1-km land surface classifications. Data are from the 2007 Fluxnet Synthesis Dataset.

<table>
<thead>
<tr>
<th>Site Code</th>
<th>Site Name</th>
<th>Latitude</th>
<th>Longitude</th>
<th>Land Cover</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA-Ca1</td>
<td>British Columbia- Campbell River - Mature Forest Site</td>
<td>49.870</td>
<td>−125.340</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Humphreys et al. (2006)</td>
</tr>
<tr>
<td>CA-Ca2</td>
<td>British Columbia- Campbell River - Clearcut Site</td>
<td>49.870</td>
<td>−125.290</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Humphreys et al. (2006)</td>
</tr>
<tr>
<td>CA-Ca3</td>
<td>British Columbia- Campbell River - Young Plantation Site</td>
<td>49.520</td>
<td>−124.900</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Humphreys et al. (2006)</td>
</tr>
<tr>
<td>CA-Long</td>
<td>Lethbridge</td>
<td>49.710</td>
<td>−112.940</td>
<td>10 - Grasslands</td>
<td>Flanagan et al. (2002)</td>
</tr>
<tr>
<td>CA-Mer</td>
<td>Eastern Peatland- Mer Bleue</td>
<td>45.410</td>
<td>−75.520</td>
<td>11 - Permanent Wetlands</td>
<td>Lafleur et al. (2003)</td>
</tr>
<tr>
<td>CA-NS2</td>
<td>UCI-1930 burn site</td>
<td>55.910</td>
<td>−98.520</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Goulden et al. (2006)</td>
</tr>
<tr>
<td>CA-NS3</td>
<td>UCI-1964 burn site</td>
<td>55.910</td>
<td>−98.380</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Goulden et al. (2006)</td>
</tr>
<tr>
<td>CA-NS4</td>
<td>UCI-1964 burn site wet</td>
<td>55.910</td>
<td>−98.380</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Goulden et al. (2006)</td>
</tr>
<tr>
<td>CA-NS5</td>
<td>UCI-1981 burn site</td>
<td>55.860</td>
<td>−98.490</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Goulden et al. (2006)</td>
</tr>
<tr>
<td>CA-NS6</td>
<td>UCI-1989 burn site</td>
<td>55.920</td>
<td>−98.960</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Goulden et al. (2006)</td>
</tr>
<tr>
<td>CA-Oas</td>
<td>Sask- SSA Old Aspen</td>
<td>53.630</td>
<td>−106.200</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Black et al. (2000)</td>
</tr>
<tr>
<td>CA-Obs</td>
<td>Sask- SSA Old Black Spruce</td>
<td>53.990</td>
<td>−105.120</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Bergeron et al. (2007)</td>
</tr>
<tr>
<td>CA-Ojp</td>
<td>Sask- SSA Old Jack Pine</td>
<td>53.920</td>
<td>−104.690</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Howard et al. (2004)</td>
</tr>
<tr>
<td>CA-Qcu</td>
<td>Quebec Boreal Cutover Site</td>
<td>49.270</td>
<td>−74.040</td>
<td>7 - Open Shrublands</td>
<td>Giasson et al. (2006)</td>
</tr>
<tr>
<td>CA-Qfo</td>
<td>Quebec Mature Boreal Forest Site</td>
<td>49.660</td>
<td>−74.340</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Bergeron et al. (2007)</td>
</tr>
<tr>
<td>CA-SF2</td>
<td>Sask- Fire 1989</td>
<td>54.250</td>
<td>−105.880</td>
<td>6 - Closed Shrublands</td>
<td>Mkhabela et al. (2009)</td>
</tr>
<tr>
<td>CA-SF3</td>
<td>Sask- Fire 1998</td>
<td>54.090</td>
<td>−106.010</td>
<td>6 - Closed Shrublands</td>
<td>Mkhabela et al. (2009)</td>
</tr>
<tr>
<td>CA-SFJ2</td>
<td>Sask- 2002 Harvested Jack Pine</td>
<td>53.950</td>
<td>−104.650</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>(Zha et al., 2009)</td>
</tr>
<tr>
<td>CA-WP1</td>
<td>Western Peatland- LaBiche-Black Spruce/Larch Fen</td>
<td>54.960</td>
<td>−112.460</td>
<td>11 - Permanent Wetlands</td>
<td>Syed et al. (2006)</td>
</tr>
<tr>
<td>US-Bn1</td>
<td>Delta Junction 1920 Control site</td>
<td>63.920</td>
<td>−145.370</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Liu et al. (2005)</td>
</tr>
<tr>
<td>US-Bn2</td>
<td>Delta Junction 1987 Burn site</td>
<td>63.920</td>
<td>−145.370</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Liu et al. (2005)</td>
</tr>
<tr>
<td>US-Bn3</td>
<td>Delta Junction 1999 Burn site</td>
<td>63.920</td>
<td>−145.740</td>
<td>7 - Open Shrublands</td>
<td>Liu et al. (2005)</td>
</tr>
<tr>
<td>US-Dk2</td>
<td>Duke Forest-hardwoods- North Carolina</td>
<td>35.970</td>
<td>−79.100</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Stoy et al. (2006)</td>
</tr>
<tr>
<td>US-Goo</td>
<td>Goodwin Creek- Mississippi</td>
<td>34.250</td>
<td>−89.970</td>
<td>10 - Grasslands</td>
<td>Wilson and Meyers (2007)</td>
</tr>
<tr>
<td>Site Code</td>
<td>Site Name</td>
<td>Latitude</td>
<td>Longitude</td>
<td>Land Cover</td>
<td>Reference</td>
</tr>
<tr>
<td>-----------</td>
<td>-----------</td>
<td>----------</td>
<td>-----------</td>
<td>------------</td>
<td>-----------</td>
</tr>
<tr>
<td>US-Ha1</td>
<td>Harvard Forest EMS Tower- Massachusetts (HFR1)</td>
<td>42.54</td>
<td>-72.17</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Urbanski et al. (2007)</td>
</tr>
<tr>
<td>US-Ha2</td>
<td>Harvard Forest Hemlock Site- Massachusetts</td>
<td>42.54</td>
<td>-72.17</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Hadley and Schedlbauer (2002)</td>
</tr>
<tr>
<td>US-Ho1</td>
<td>Howland Forest (main tower)- Maine</td>
<td>45.20</td>
<td>-68.74</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Hollinger et al. (1999)</td>
</tr>
<tr>
<td>US-Ho2</td>
<td>Howland Forest (west tower)- Maine</td>
<td>45.21</td>
<td>-68.75</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Hollinger et al. (2004)</td>
</tr>
<tr>
<td>US-KS2</td>
<td>Florida-Kenedy Space Center (scrub oak)</td>
<td>28.61</td>
<td>-80.67</td>
<td>6 - Closed Shrublands</td>
<td>Powell et al. (2006)</td>
</tr>
<tr>
<td>US-Los</td>
<td>Lost Creek- Wisconsin</td>
<td>46.08</td>
<td>-89.98</td>
<td>6 - Closed Shrublands</td>
<td>Sulfman et al. (2009)</td>
</tr>
<tr>
<td>US-Me2</td>
<td>Metolius-intermediate aged ponderosa pine- Oregon</td>
<td>44.45</td>
<td>-121.56</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Thomas et al. (2009)</td>
</tr>
<tr>
<td>US-Me4</td>
<td>Metolius-old aged ponderosa pine- Oregon</td>
<td>44.50</td>
<td>-121.62</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Anthoni et al. (2002)</td>
</tr>
<tr>
<td>US-MMS</td>
<td>Morgan Monroe State Forest- Indiana</td>
<td>39.32</td>
<td>-86.41</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Schmid et al. (2000)</td>
</tr>
<tr>
<td>US-MOz</td>
<td>Missouri Ozark Site</td>
<td>38.74</td>
<td>-92.20</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Gu et al. (2006)</td>
</tr>
<tr>
<td>US-Ne1</td>
<td>Mead - irrigated continuous maize site- Nebraska</td>
<td>41.10</td>
<td>-96.29</td>
<td>12 - Croplands</td>
<td>Verma et al. (2005)</td>
</tr>
<tr>
<td>US-Ne2</td>
<td>Mead - irrigated maize-soybean rotation site- Nebraska</td>
<td>41.10</td>
<td>-96.28</td>
<td>12 - Croplands</td>
<td>Verma et al. (2005)</td>
</tr>
<tr>
<td>US-Ne3</td>
<td>Mead - rainfed maize-soybean rotation site- Nebraska</td>
<td>41.18</td>
<td>-96.44</td>
<td>12 - Croplands</td>
<td>Verma et al. (2005)</td>
</tr>
<tr>
<td>US-NR1</td>
<td>Niwot Ridge Forest- Colorado (LTER NWT1)</td>
<td>40.03</td>
<td>-105.55</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Monson et al. (2002)</td>
</tr>
<tr>
<td>US-PFa</td>
<td>Park Falls/WLEF- Wisconsin</td>
<td>45.95</td>
<td>-90.27</td>
<td>5 - Mixed Forest</td>
<td>Davis et al. (2003)</td>
</tr>
<tr>
<td>US-SP1</td>
<td>Slashpine-Austin Cary- 65yrs nat regen-FL</td>
<td>29.74</td>
<td>-82.22</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Clark et al. (1999)</td>
</tr>
<tr>
<td>US-SP2</td>
<td>Slashpine-Mize-clearcut-3yr-regen-FL</td>
<td>29.76</td>
<td>-82.24</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Clark et al. (1999)</td>
</tr>
<tr>
<td>US-SP3</td>
<td>Slashpine-Donaldson-mid-rot-12yrs-FL</td>
<td>29.75</td>
<td>-82.16</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Clark et al. (1999)</td>
</tr>
<tr>
<td>US-Syy</td>
<td>Sylvania Wilderness Area- Michigan</td>
<td>46.24</td>
<td>-89.35</td>
<td>5 - Mixed Forest</td>
<td>Desai et al. (2005)</td>
</tr>
<tr>
<td>US-Ton</td>
<td>Tonzi Ranch- California</td>
<td>38.43</td>
<td>-120.97</td>
<td>8 - Woody Savannas</td>
<td>Ma et al. (2007)</td>
</tr>
<tr>
<td>US-UMB</td>
<td>Univ. of Mich. Biological Station- Michigan</td>
<td>45.50</td>
<td>-84.71</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Gough et al. (2008)</td>
</tr>
<tr>
<td>US-Var</td>
<td>Vaira Ranch- Ione- California</td>
<td>38.41</td>
<td>-120.95</td>
<td>10 - Grasslands</td>
<td>Ma et al. (2007)</td>
</tr>
<tr>
<td>US-WCr</td>
<td>Willow Creek- Wisconsin</td>
<td>45.81</td>
<td>-90.08</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Cook et al. (2004)</td>
</tr>
</tbody>
</table>
Table 2.2: Total number of parameters resulting from the nine different schemes used to group observation sites for VPRM parameter estimation.

<table>
<thead>
<tr>
<th>site groupings in space</th>
<th>site groupings in time</th>
<th>monthly intervals</th>
<th>annual intervals</th>
<th>all available data, 2000 to 2006</th>
</tr>
</thead>
<tbody>
<tr>
<td>individual sites (65)</td>
<td></td>
<td>21840</td>
<td>1820</td>
<td>260</td>
</tr>
<tr>
<td>PFTs (9)</td>
<td></td>
<td>3360</td>
<td>280</td>
<td>40</td>
</tr>
<tr>
<td>all sites together</td>
<td></td>
<td>336</td>
<td>28</td>
<td>4</td>
</tr>
</tbody>
</table>

Figure 2.2: Two examples of generic parametric variogram models. The parameter symbols correspond to section 2.2.4 and equation (2.8). Because these are purely illustrative, units for semivariance and distance are irrelevant.
Figure 2.3: Box and whisker plots for values of VPRM parameters, estimated monthly by plant functional type (PFT). Whiskers show 1.5 times the interquartile range. Units for parameters are: $\lambda$: $\mu$mol CO$_2$ m$^{-2}$ s$^{-1}$ / $\mu$mol PAR m$^{-2}$ s$^{-1}$; $\alpha$: $\mu$mol CO$_2$ m$^{-2}$ s$^{-1}$ / $^\circ$C; $\beta$: $\mu$mol CO$_2$ m$^{-2}$ s$^{-1}$; $\text{PAR}_0$: $\mu$mol PAR m$^{-2}$ s$^{-1}$. 
Figure 2.4: June-July-August mean VPRM NEE residual empirical semivariograms. Each point represents the mean semivariance and mean separation distance from grouping pairs of towers into 300 km bins. VPRM parametrizations are described in Table 2.2. The left vertical axis shows units of semivariance ($\hat{\gamma}$), and the right vertical axis shows units of standard deviation ($\sigma$). $\sigma$ is related to $\hat{\gamma}$ by $\sigma = (2\hat{\gamma})^{1/2}$. 
Table 2.3: Range parameter values (km) for VPRM flux error best-fit parametric variogram models. VPRM parameterizations are described in table 2.2. Where a value is present, Akaike’s information criterion (AIC) analysis concludes the exponential variogram model fit more parsimoniously than the pure nugget model. Where the range is blank the pure nugget model fit most parsimoniously, indicating no spatial correlation is present.

<table>
<thead>
<tr>
<th>season</th>
<th>VPRM Parameterization</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>2000 2001 2002 2003 2004 2005 2006</td>
</tr>
<tr>
<td>space</td>
<td>time</td>
<td></td>
</tr>
<tr>
<td></td>
<td>DJF site monthly</td>
<td>1640 3051 4 1518 605</td>
</tr>
<tr>
<td></td>
<td>site annual</td>
<td>1299 368 772 3787</td>
</tr>
<tr>
<td></td>
<td>site all data</td>
<td>403 2382 115</td>
</tr>
<tr>
<td></td>
<td>PFT monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>PFT annual</td>
<td>249 301 48</td>
</tr>
<tr>
<td></td>
<td>PFT all data</td>
<td>258 460 76</td>
</tr>
<tr>
<td></td>
<td>all sites monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>all sites annual</td>
<td>1 450</td>
</tr>
<tr>
<td></td>
<td>all sites all data</td>
<td>1 461</td>
</tr>
<tr>
<td>MAM</td>
<td>site monthly</td>
<td>285</td>
</tr>
<tr>
<td></td>
<td>site annual</td>
<td>207</td>
</tr>
<tr>
<td></td>
<td>site all data</td>
<td></td>
</tr>
<tr>
<td></td>
<td>PFT monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>PFT annual</td>
<td>748</td>
</tr>
<tr>
<td></td>
<td>PFT all data</td>
<td>769</td>
</tr>
<tr>
<td></td>
<td>all sites monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>all sites annual</td>
<td>4</td>
</tr>
<tr>
<td></td>
<td>all sites all data</td>
<td>5</td>
</tr>
<tr>
<td></td>
<td>all sites all data</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td>JJA site monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>site annual</td>
<td>267 631 1354</td>
</tr>
<tr>
<td></td>
<td>site all data</td>
<td>34 405 1 368 316</td>
</tr>
<tr>
<td></td>
<td>PFT monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>PFT annual</td>
<td>30 461 323</td>
</tr>
<tr>
<td></td>
<td>PFT all data</td>
<td>734 407 287</td>
</tr>
<tr>
<td></td>
<td>all sites monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>all sites annual</td>
<td>401 537 289</td>
</tr>
<tr>
<td></td>
<td>all sites all data</td>
<td>401 534 292</td>
</tr>
<tr>
<td></td>
<td>all sites all data</td>
<td>404 534 296</td>
</tr>
<tr>
<td>SON</td>
<td>site monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>site annual</td>
<td>227 314 840 4600 129</td>
</tr>
<tr>
<td></td>
<td>site all data</td>
<td>1004 2</td>
</tr>
<tr>
<td></td>
<td>PFT monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>PFT annual</td>
<td>2689 710 56</td>
</tr>
<tr>
<td></td>
<td>PFT all data</td>
<td>406 1046 1466 70 77</td>
</tr>
<tr>
<td></td>
<td>all sites monthly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>all sites annual</td>
<td>406 1046 1466 70 77</td>
</tr>
<tr>
<td></td>
<td>all sites all data</td>
<td>649 1041 2086 0 19</td>
</tr>
</tbody>
</table>
Figure 2.5: Cumulative density functions for covariance range parameter, estimated by maximum likelihood estimation (MLE). Each panel shows range values for seasonal VPRM NEE residuals (values in Table 2.3) along with values from 1000 Gaussian random fields (GRFs) with similar (and known) covariance structure. The left panel shows the range distribution for only the pseudodata range estimations where the exponential covariance model fit more optimally than the pure nugget; the right panel shows the distribution for all 1000 GRFs.
Figure 2.6: Best-fit range values (km) for cumulative annual anomalies of observed NEE, VPRM NEE, and VPRM NEE residuals. Best-fit values were determined by AIC as described in section 2.2.4. The number \( y \) plotted denotes the year 200\( y \). Years where the pure nugget covariance function fit more optimally than the exponential are shown in the shaded box. Anomalies were calculated as the departure from the mean value of 2000 to 2006 annual mean cumulative observed values.
Figure 2.7: As Figure 2.6, but displaying semivariogram sill values.
Chapter 3

Evaluating terrestrial CO$_2$ flux diagnoses from a simple land surface model and its residuals

3.1 Introduction

Terrestrial ecosystems remove roughly 25 percent of annual anthropogenic fossil fuel carbon dioxide (CO$_2$) via gross primary production (GPP) in excess of respiration (Keeling et al., 1996). More completely, net ecosystem exchange (NEE) – the balance between photosynthesis and heterotrophic respiration – controls the magnitude of atmosphere to ecosystem CO$_2$ uptake. Diagnosing terrestrial biological carbon dioxide fluxes with confidence is a necessary step toward understanding biological and climatological drivers of these fluxes. Because these fluxes are first-order influences on the accumulation of carbon dioxide in the atmosphere (Denman et al., 2007), understanding their mechanics is necessary to forecast impacts of past and future fossil fuel emissions. In spite of this, atmosphere-based methods to estimate global NEE (e.g., Peters et al., 2007; Janssens et al., 2003) and ground-based approaches (e.g., Potter et al., 2007; Janssens et al., 2003) have produced conflicting estimates, demonstrating substantial uncertainty surrounding these efforts to describe terrestrial carbon cycle mechanics.
Several recent studies demonstrate the discrepancy in diagnosed NEE between “top-down” atmosphere-based approaches and ground-based “bottom-up” approaches rooted in eddy covariance (EC) flux measurements combined with ecosystem models. Janssens et al. (2003) assembled top-down and bottom-up estimates for late 20th Century annual cumulative European NEE and found that the top down estimates are larger by roughly 100 Tg CO$_2$ per year. This 100 Tg difference is between 30% and 100% of their best-estimate annual total of 100 to 300 Tg per year. Peters et al. (2007) estimated a North American uptake for 2001 to 2005 of roughly 700 Tg CO$_2$ per year using a top-down approach, while Potter et al. (2007) estimated uptake of 100 to 200 Pg CO$_2$ per year over the same period using a bottom-up method.

A number of studies have explored approaches to estimate regional NEE using some combination of land surface models and eddy covariance fluxes (bottom-up methods). Potter et al. (2007) chose a set of four North American EC towers to represent characteristic North American ecosystems and used them to evaluate the performance of the NASA-CASA ecosystem model run with a global set of previously published parameter values. They then used the NASA-CASA model to estimate North American annual cumulative NEE. This approach requires no computationally intensive data assimilation (e.g. parameter estimation), but achieves such savings at the cost of considering only a small portion of the NEE observations that are now available.

Xiao et al. (2008) used a modified regression tree to create a model suite to explain observed NEE as a function of a variety of satellite-derived ecological measures. A regression tree is a method to empirically derive a best-fit statistical model based on a set of linear models. They derived the models using data from 42 Ameriflux EC sites in the coterminous United States, producing a set of empirical models capable of upscaling the tower observations to the continental scale. The model that best explained the observed NEE used a combination of MODIS surface reflectances, enhanced vegetation index (EVI), land surface temperature, and normalized difference water index (NDWI). Though statistical, this model structure is quite similar to light-use efficiency (LUE) based models such as the Vegetation Photosynthesis Respiration Model (VPRM) of (Mahadevan et al., 2008).
Beer et al. (2010) compared five different diagnostic gross primary production (GPP) models with sharply contrasting structures, including two machine learning approaches, an NEE–biome region look-up table, and a LUE model. Each of these approaches was then used to estimate regional NEE values and uncertainties. The Beer et al. study explicitly considered many sources of uncertainty in the models considered. For the light-use efficiency model, the authors estimated site-specific parameter probability density functions (PDFs) at a number of Fluxnet eddy covariance sites around the globe. The Bayesian framework of the study allowed the authors to consider PDFs from multiple uncertainty sources: parameter value uncertainty as well as driver data uncertainty. By taking random draws from these parameter PDFs, Beer et al. (2010) constructed a population of global GPP estimates driven by their distribution of parameter values. This population then provided confidence intervals for their global GPP estimates.

Each study outlined above presents a framework to use ecosystem modeling to combine the information in eddy covariance flux tower observations with the information contained in an ecosystem model structure and allows estimation of regional biological CO$_2$ fluxes. These studies exhibit many ways to treat uncertainty sources, ranging in complexity from not including uncertainty to Bayesian consideration of multiple uncertainty sources. The set of available eddy covariance NEE observations has increased dramatically in recent years (http://www.fluxdata.org); none of the above studies, however, take advantage of the wide spatial coverage of these observations except to perform site-specific calibration of model parameters.

The work presented in chapter 2 uses North American eddy covariance NEE observations from 65 different locations from the Fluxnet project (http://www.fluxdata.org) to optimize parameter values for a simple ecosystem model (VPRM, Mahadevan et al., 2008). The 65 tower locations span North America in both space and plant functional type. We conducted extensive experiments varying the temporal and spatial periods for parameter estimation to determine an optimal strategy, producing nine different spatial and temporal resolutions. Chapter 2 also presented quantitative estimates of the spatial covariance structure for VPRM NEE errors.
Here we use VPRM and the assimilated data from this extensive tower network to diagnose annual integrated gross ecosystem exchange (GEE), ecosystem respiration (R), and NEE for the coterminous United States of America, Alaska, and Canada for the period 2002 to 2006. We use eddy covariance observations from a further 27 Fluxnet tower locations to quantitatively cross-validate the parameter optimizations. This rigorous cross-validation analysis is a crucial step in a model-based carbon flux upscaling; without such an exercise it is difficult to measure the spatial accuracy, or lack thereof, of estimating unobserved fluxes using a model and data assimilation. Cross validation would not be possible without the recent growth of eddy covariance observation networks: if only a handful of observation locations exist, as in the recent past, we cannot afford to withhold data from parameter estimation.

We also extend the analysis to derive empirical confidence intervals for NEE diagnoses based on observed NEE residuals and NEE drivers. Because this uncertainty is derived from eddy covariance-observation–model NEE residuals, it considers all of the uncertainty sources that are present in model-based upscaling: eddy covariance observation error, model structural error, model parameterization error, and random natural ecosystem variability. This comprehensive and quantitative uncertainty analysis is also, to our knowledge, unique.

We also explore the usefulness of the VPRM NEE residual spatial covariance structure presented in section 2.3.2 toward informing bottom-up NEE diagnosis. By explicitly considering this spatial covariance structure a diagnosis can include not only the highly local information provided by a flux tower site, but also the information contained in the spatial extent of the network of flux tower sites as a whole.

3.2 Methods

3.2.1 Land surface model

The Vegetation Photosynthesis and Respiration Model (VPRM, Mahadevan et al., 2008) is a light-use efficiency (LUE)-based land surface model. Ecosystem res-
piration is treated as a linear function of surface air temperature:

\[ R = \alpha T + \beta, \]  

(3.1)

with slope \( \alpha \) and intercept \( \beta \); \( \beta \) determines the basal rate of respiration that occurs at near-freezing temperatures. Gross Ecosystem Exchange (GEE) is modeled as

\[ GEE = \lambda \times T_{\text{scale}} \times P_{\text{scale}} \times W_{\text{scale}} \times EVI \times \frac{1}{1 + \frac{PAR}{PAR_0}} \times PAR, \]  

(3.2)

with \( PAR \) denoting photosynthetically active radiation and \( EVI \) the satellite-derived enhanced vegetation index (Huete et al., 2002). \( P_{\text{scale}} \) (satellite-derived), \( W_{\text{scale}} \) (satellite-derived), and \( T_{\text{scale}} \) (literature-derived) are scaling terms that take values between 0.0 and 1.0 and attenuate GEE according to phenology, moisture conditions, and temperature, respectively. Parameter \( \lambda \) encodes light use efficiency, and parameter \( PAR_0 \) encodes the LUE curve half-saturation value.

Mahadevan et al. (2008) provide detailed description of VPRM structure and performance. As described more fully in section 3.2, the relatively simple structure of VPRM and its small number of parameters make it computationally inexpensive. This makes relatively sophisticated parameter estimation methods possible (section 2.2.3) and makes VPRM a useful tool for diagnosing carbon fluxes, estimating flux uncertainty, and exploring the impacts of model parameterization and model error spatial covariance.

### 3.2.2 Land surface model parameterization

Section 2.3.1 presented estimated values for \( \lambda, PAR_0, \alpha, \) and \( \beta \) using data from 65 North American eddy covariance towers (Figure 2.1, Table 2.1). For parameter estimation, the eddy-covariance data were partitioned in three different ways in space (individual sites, plant functional types (PFTs), and all-sites-together), and three different ways in time (monthly, annual, and all-available-data). This produced nine unique VPRM parameter sets with differing spatial and temporal optimization “resolutions”: single sites–monthly, PFT–annual, etc. Upscaling tower measurements intrinsically requires model parameters that are applica-
ble in spatial locations without tower observations, making the single-site parameters not useful for the task. This leaves the six parameter sets from the PFT and all-sites-together spatial groupings available for upscaling. In addition to those six, PFT-ten-day parameters were calculated as well. The sum of squared errors (SSE) were computed for the seven VPRM parameter sets that are useful for upscaling, using observations from 27 “cross-validation” eddy covariance sites (Table 3.1; Figure 3.1; section 3.2.3) that were not used for parameter estimation.

3.2.3 Data

The 2007 Fluxnet Synthesis dataset (http://www.fluxdata.org) assembled eddy covariance observations from field sites around the world. The data were gap-filled and assigned quality scores using published methods (Papale et al., 2006; Moffat et al., 2007). The present study uses non-gapfilled NEE from 92 eddy covariance sites from the United States and Canada: the 65 flux towers used to estimate VPRM parameter and VPRM NEE error covariance structure (Table 2.1, Figure 2.1), plus 27 “cross-validation” sites (Table 3.1, Figure 3.1). The cross-validation sites were not used to estimate parameters or covariance structure; they are used in the present study to evaluate the performance of the optimized VPRM.

VPRM uses temperature and photosynthetically active radiation (PAR) to drive GEE and respiration. To run VPRM at the continental scale, air temperature and downward surface radiation values were obtained from the reanalysis products of Sheffield et al. (2006). The Sheffield et al. (2006) products attempt to correct known biases (Brotzge, 2004) to the NCEP-NCAR reanalysis products (Kalnay et al., 1996). VPRM was driven with the three-hourly, $1^\circ \times 1^\circ$ product for temperature and PAR.

VPRM is also driven by satellite-derived moisture and phenology. MODIS products MOD13A2 (enhanced vegetation index (EVI); Huete et al., 2002, 1999), MCD12Q1 (land cover; Friedl et al., 2002; Strahler et al., 1999a), MCD12Q2 (vegetation dynamics; Zhang et al., 2003), and MCD43B4 (Bidirectional Reflectance Distribution Function (BRDF) reflectances; Schaaf et al., 2002) provided these
drivers. EVI data reported with quality ratings of “lowest quality” and “not useful” (VI quality bits 2-3 equal to 11) were discarded. Gaps from discarded MODIS data were not filled; VPRM fluxes were not calculated in these instances. EVI and BRDF data are reported at one-kilometer, 16-day resolution; land cover and vegetation dynamics are reported at 500-meter, annual resolution and were processed from 500-meter resolution to 1000-meter resolution using software tools provided by the MODIS Land quality assessment group (Roy et al., 2002).

3.2.4 Ecosystem-atmosphere carbon dioxide flux calculation

VPRM gross ecosystem exchange (GEE), ecosystem respiration (R), and net ecosystem exchange (NEE) were calculated for the 48 coterminous United States, Alaska, and Canada at three hourly temporal resolution and one kilometer spatial resolution for 2002 to 2006. The MODIS products with 16-day temporal resolution were simply repeated at each three-hourly interval across the 16 days. Three-hourly diagnoses of GEE, R, and NEE were integrated to annual values and used to calculate annual anomalies (defined as the annual integrated value minus the 2002 to 2006 mean annual integrated value).

3.2.5 NEE residual spread estimation

This study seeks upscaled NEE diagnoses accompanied by uncertainty estimates. There are several methods of varying complexity available to quantify this uncertainty. A joint Bayesian inversion of VPRM parameters and VPRM NEE variance against eddy covariance NEE observations using a joint likelihood function would extract information from the available data with maximum mathematical rigor (though is still vulnerable to aggregation errors in grouping scheme (e.g. plant functional types), as well as errors in observations and driver data). Statistically rigorous likelihood functions for model NEE error, however, remain an ongoing research topic, and the calculation itself is computationally expensive.

The method employed here uses an empirically-derived statistical model to characterize VPRM NEE residual spread – a middle ground between the joint Bayesian inversion with MCMC and the simple interpolation.
It is known that eddy covariance observation error is proportional to NEE magnitude itself (Richardson et al., 2006). Typical magnitude for this random EC observation error is roughly 20 to 30 gC m\(^{-2}\) yr\(^{-1}\) (Richardson et al., 2006; Goulden et al., 1996), roughly an order of magnitude smaller than the VPRM annual NEE residuals. Random eddy covariance observation error is a component of VPRM NEE error, making it reasonable to posit that VPRM NEE residual magnitude is correlated to VPRM NEE magnitude. Furthermore, the structure of VPRM (eqs (3.1), (3.2)) assumes that temperature, water availability, and greenness (EVI) are primary drivers of NEE. It seems reasonable, then, that VPRM residuals would be affected by these influences as well.

Using non-gapfilled observations from the 65 eddy covariance sites used to estimate VPRM parameter values, annual integrated NEE residuals were calculated as the integrated sum of non-gapfilled NEE observations minus VPRM NEE, both at EC site-specific native reporting resolution (generally 30 minutes, 60 minutes at a few sites). Residuals were calculated only at time stamps where both quantities were available. With these integrated residuals squared differences were calculated for each site-year:

\[
\text{NEE}'_{\text{sq diff}} \equiv (\text{NEE}' - \overline{\text{NEE}'})^2.
\]

(3.3)

\(\text{NEE}'\) denotes annually integrated VPRM residual, and \(\overline{\text{NEE}'}\) denotes the mean of \(\text{NEE}'\) across all site-years. \(\text{NEE}'_{\text{sq diff}}\) is closely related to statistical variance \(\sigma^2\) \(\left(\sigma^2 \equiv \sum_{i=1}^{N} (x_i - \overline{x})^2/(N - 1)\right)\). Estimating \(\text{NEE}'_{\text{sq diff}}\) in terms of known quantities provides a method to estimate the spread of VPRM NEE errors that can be upscaled along with the flux diagnoses.

Regression models for \(\text{NEE}'_{\text{sq diff}}\) were derived from subsets of these candidate explanatory variables: VPRM annual integrated NEE, total annual precipitation, annual mean surface air temperature, annual mean EVI, PFT, and year. The set of models consisting of all combinations within the categorical variables, the linear numerical terms, and the quadratic numerical terms was searched exhaustively using the glmulti package (Calcagno, 2011) for R (R Development Core Team, 2007) and the results ranked by Akaike’s Information Criterion (AIC, Akaike, 1976). Annual mean EVI was calculated as the mean
of 16-day MODIS EVI values (see section 3.2.3). Annual total precipitation and annual mean temperature were calculated as the sum and mean, respectively, of the monthly mean $1^\circ \times 1^\circ$ Sheffield et al. (2006) reanalysis products.

### 3.3 Results and discussion

#### 3.3.1 Land surface model parameter set ranking

As described in section 3.2.2, we ranked the parameter sets that are useful for upscaling (this excludes the three individual-site-based parameter sets) by sum of squared errors (SSE). Figure 3.2 presents these SSE values, plotted against the number of unique parameter values. The solid curve plots the SSE for the 27 cross-validation sites not used for VPRM parameter estimation, and the dashed curve plots the penalized sum of squared errors (PSSE, e.g. Hilborn and Mangel, 1997) for all 92 sites (the 27 cross-validation sites and the 65 sites used to parameterize VPRM.) PSSE is given by

$$PSSE = \frac{SSE}{n_{obs} - 2n_{pars}},$$

with SSE the sum of squared errors, $n_{pars}$ the number of unique model parameter values, and $n_{obs}$ the number of data points available. Among cross-validation sites withheld from parameter estimation, we can detect overfitting when the SSE begins to increase with the number of parameters. Because model parameterization, by definition, fits the model to observed data, SSE among parameterization sites should only decrease with additional parameters. PSSE provides a method to detect overfitting among parameterization sites. Figure 3.2 suggests that the monthly and 10-day VPRM parameter sets overfit the data.

The PFT–all-data VPRM parameters achieved the lowest cross-validation SSE as well as a PSSE only slightly above the lowest PSSE; therefore, those parameters are used for most of the analyses presented here. The five lowest cross-validation SSE values in Figure 3.2 are not drastically different from one another, though the penalized SSE values for the two most parsimonious parameter sets (all–all and all–annual) are significantly higher. In combination with the param-
eter distributions presented in Figure 2.3, this result might suggest that order 100 parameters are optimal for flux upscaling. The two parameter sets considered in Figure 3.2 that use parameterization temporal windows shorter than annual (monthly and 10-day) produced notably higher cross-validation SSE values and higher penalized SSE values than the other five parameter sets, suggesting these parameterizations overfit the observations.

### 3.3.2 VPRM NEE residual evaluation

To evaluate the quality of VPRM NEE diagnoses, Figure 3.3 presents the histogram of VPRM NEE residuals calculated at eddy covariance site reporting intervals (30 minutes at most sites; 60 minutes at a few sites), calculated using PFT–all-data VPRM parameters. The mean residual of $4.66 \times 10^{-4} \, \mu\text{mol CO}_2 \, \text{m}^{-2} \, \text{s}^{-1}$ corresponds to an annually integrated flux of 0.18 gC m$^{-2}$ yr$^{-1}$, small compared to a typical observed EC annual NEE between 100 and 300 gC m$^{-2}$ yr$^{-1}$. This suggests that the parameter optimization (section 2.3.1) achieved its task of optimizing VPRM to observed fluxes at hourly time scales. A normal distribution with the same mean and standard deviation is overlaid; the observed residuals show a higher peak around their mean but otherwise correspond closely to the normal distribution.

Having demonstrated the parameter optimization performs well at hourly intervals we turn now to the annual time scale. Figure 3.4 examines the distribution at the annual timescale, showing the VPRM NEE residuals integrated by site-year. Because NEE gapfilling would introduce a new source of error to VPRM residuals, the annual integrated residuals in Figure 3.4 are calculated from non-gapfilled NEE observations. The mean integrated residual value of 1.6 gC m$^{-2}$ yr$^{-1}$ demonstrates that VPRM optimization also performed well at the annual scale. This observed residual distribution also follows a normal distribution (overlaid) reasonably well.

Satisfied now that VPRM residuals are small relative to EC-observed fluxes, we investigate whether 1 km VPRM diagnosed annual NEE for North America seems reasonable when compared to EC-observed annual NEE. Figure 3.5 compares the distribution of annually integrated VPRM NEE diagnoses for the mod-
eling domain (section 3.2.4) with the distribution of annually integrated NEE observations from the 2007 Fluxnet synthesis dataset for the sites in Table 2.1. To obtain a meaningful comparison to model diagnoses we use the Fluxnet synthesis dataset gapfilled NEE observations in this case. The gapfilling used the methods of Papale et al. (2006) and Moffat et al. (2007). VPRM reproduces well the mode of the observed distribution as well as the right-hand tail (sources of CO₂ to the atmosphere). The left tail of the observed NEE distribution contains more density than the VPRM diagnoses, suggesting that VPRM estimates lower sinks of atmospheric CO₂ than the gapfilled Fluxnet 2007 Synthesis dataset in some cases. The Fluxnet synthesis dataset contains a handful of site-years with sinks of atmospheric CO₂ approaching or even exceeding 1000 gC m⁻² yr⁻¹. VPRM was optimized to these data, and the left-side tail of the VPRM diagnosed NEE distributions does contain more mass than the right side.

In all, the VPRM performance summarized by Figures 3.3, 3.4, and 3.5 are encouraging for the ability of the parameter estimation process to optimize VPRM to eddy covariance observations at both hourly and annual timescales.

3.3.3 VPRM fluxes

Figure 3.6 shows annually integrated VPRM GEE (3.6a), R (3.6b), and NEE (3.6c) for 2002. The larger-scale (order >100 km) spatial patterns are representative of the integrated fluxes for 2003 to 2006 (not shown). NEE is the difference between GEE and R, both much larger in magnitude. This raises detectability issues for NEE: this difference between two larger and roughly equal quantities is easily polluted by errors from GEE and R estimation. Therefore, rather than focus on integrated annual NEE values or aggregated continental NEE, this study instead focuses on year-to-year NEE differences and NEE differences across different VPRM parameter sets.

The broad spatial patterns in these results largely agree with other analyses (e.g., Beer et al., 2010; Xiao et al., 2011; Running et al., 2004). As we would expect given the prominence of the vegetation index in VPRM structure (eq. (3.2)), the patterns of strong GPP reflect areas of relatively dense vegetation as measured by vegetation index (Huete et al., 2002) or biomass (Myneni et al., 2001).
The relatively large respiration diagnoses for the southeastern USA in Figure 3.6b is also present in the 2003 to 2006 diagnoses. This area, roughly covering the U.S. states of Louisiana, Mississippi, Alabama, Georgia, and South Carolina, is dominated by the mixed forest PFT in the MODIS land cover classification (section 3.2.3). The three mixed forest eddy covariance sites used for VPRM parameterization are in Wisconsin, USA and Ontario, Canada. Rather than conclude that the mixed forests of the U.S. Gulf Coast are much stronger sources of biological CO\textsubscript{2} than other classes of southern forests or more northerly mixed-forests, several alternative explanations seem more likely. First, perhaps the carbon cycle mechanics of northern mixed forests do not describe well the behavior of southerly mixed forests and diagnose erroneously strong respiration when applied in southerly regions. Second, three eddy covariance sites may provide insufficient data to characterize this (or any) PFT. Last, stand age is an important driver of NEE (Litvak et al., 2003), and is ignored by the modeling methods employed here.

Year to year flux differences are reported here as annual anomalies, calculated as (integrated annual flux) minus (mean integrated annual flux, 2002 to 2006). VPRM integrated annual flux anomalies for 2002 to 2006 are shown in Figures 3.7 (GEE), 3.8 (R), and 3.9 (NEE). Notable in these diagnoses is the much larger variability of GEE as compared to R. That GEE variability is reflected in NEE variability as well. This could be a consequence of VPRM’s structural treatment of respiration as a linear function of temperature (eq. 3.1). In contrast VPRM GEE (eq. 3.2) considers a number of other variables in addition to temperature. Increased interannual variability (IAV) in GEE may simply reflect that there are more constituent quantities to vary.

Much of the stronger GEE IAV (Figure 3.7) occurs in the upper Midwestern USA. 2006, for example, showed a particularly strong VPRM GEE diagnosis centered around the U.S. state of Indiana. This area is dominated by agriculture – the cropland PFT in the MODIS IGBP landcover classification. Within the cropland PFT different agricultural products are known to vary in the strength of their carbon uptake. Corn, for example, has particularly strong atmospheric CO\textsubscript{2} uptake (Lokupitiya et al., 2009). Without parameterizations specific to particular crops, model NEE diagnosis can be poor (Lokupitiya et al., 2009). There
are only five agricultural EC sites in the group used to parameterize VPRM (Table 2.1). This makes it possible that the model parameterization suffers from the same representativeness problem that may cause potentially spurious VPRM respiration spatial structure in the southeastern USA. Many farms rotate crops from one season to the next; for example, corn in year \( y \) followed by soybeans in year \( y + 1 \). If reflected in remotely sensed ecosystem variables (e.g. vegetation indices or moisture) this sort of rotation could itself cause the GEE interannual variation seen in the VPRM annual anomalies. Similarly, if the cropland VPRM parameter estimation EC sites (US-Ne1, US-Ne2, US-Ne3, US-Bo1, and US-Bo2) were consistently planted with a particular crop during the periods used for parameter estimation, VPRM should not be expected to perform well for different crops. Looking to other potential causes for large year to year changes in the upper Midwestern USA, VPRM R diagnoses in that region show little year to year variation, removing temperature anomalies as a driver of GEE IAV. From the structure of VPRM GEE (eq. 3.2) this leaves moisture availability, PAR, and vegetation index as primary candidates for driving GEE variability.

### 3.3.4 Estimated spread of VPRM fluxes

Determining whether these flux diagnoses are able to detect meaningful interannual variability (IAV) requires a measure of the variance of annual integrated NEE. Section 3.2.5 describes the empirical derivation of a statistical model to predict the squared difference between the annual integrated VPRM residual and its mean (\( \text{NEE}'_{\text{sq diff}} \), eq. (3.3)) across site years. Of the candidate models, the best-fitting model (lowest AIC) was

\[
\text{NEE}'_{\text{sq diff}} = 2.66 \times 10^{-1} \text{NEE}_{\text{VPRM}}^2 + \\
5.72 \text{NEE}_{\text{VPRM}} + 9.86 \times 10^2 \ T + \\
3.95 \times 10^{-2} \ pcp^2 + 2.05 \times 10^3.
\]  

(3.5)

\( \text{NEE}_{\text{VPRM}} \) is annual integrated VPRM NEE, \( T \) is annual mean temperature (°C), and \( \text{pcp} \) is annual total precipitation (mm). The fit achieved a multiple R-squared of 0.289, with the coefficients significant at \( p < 0.001 (\text{NEE}_{\text{VPRM}}^2), p < 0.05 \)
(pcp²), \( p < 0.1 \) (T), and no significance for NEE\textsubscript{VPRM} \( (p = 0.12) \).

The regression model in equation (3.5) was tested at the cross-validation EC sites (Table 3.1, fig. 3.1). Figure 3.12 (top panel) shows observed vs. predicted NEE\textsubscript{sq diff} with the 95% prediction interval. The prediction intervals at each point are calculated from the regression slope and intercept variances, which are estimated from the residuals of the regression fit. Of 56 site years in the cross-validation data set, one observation is outside of the 95% prediction interval. The bottom panel of Figure 3.12 shows histograms of the observed and predicted values. The distributions are similar, except for predicted values around zero. This highlights a shortcoming of the regression model approach: negative predicted NEE\textsubscript{sq diff} values are possible. This should emphasize that, as with any regression model, predictions are only valid when the explanatory variables take values within the ranges used to fit the model.

The regression model performs well, then, at the cross-validation eddy covariance sites. Figure 3.11 shows the square root of estimated NEE\textsubscript{sq diff} for the modeling area for 2002. The spatial patterns for 2003 to 2006 (not shown) are similar. The estimated VPRM errors are broadly of similar magnitude to the VPRM NEE differences between years (fig. 3.9) and the VPRM NEE differences between VPRM parameter sets (fig. 3.10a, 3.10b).

Though the regression model estimation methods developed here are applied to estimate VPRM NEE error magnitude, the approach is equally applicable to estimating errors in an ecosystem model diagnosis of GEE or R; this change would be subject only to quality of the partitioning of EC NEE observations into GEE and R.

As noted in section 3.1, several recent studies have attempted continent-scale carbon flux diagnoses; those diagnoses generally do not report uncertainty. Beer et al. (2010) reported spatial estimates of GPP accompanied by globally aggregated uncertainties. The work presented here reports spatial GPP, R, and NEE diagnoses, and further extends the literature by estimating annual continental NEE uncertainty in space.

Beer et al. (2010) estimate GPP uncertainty for their LUE model by randomly resampling from within their population of parameters optimized to eddy covariance observations at each observation site. Because the parameters are op-
timized to flux observations, these uncertainty estimates include observation errors and model parameterization errors. Driver data uncertainty is quantified by analyzing uncertainty separately for three different reanalysis products.

Because they are based on model-observation differences, the estimates presented here include eddy covariance observation error, model parameterization error, model structural error, and driver data error. This makes these estimates inclusive of a broader range of error sources relative to approaches that focus on propagating specific errors through a model calculation. This inclusiveness sacrifices the possibility of partitioning the estimated error into contributions from constituent sources.

As an empirical approach based upon observed model residuals the regression model approach to uncertainty estimation studies flux diagnosis uncertainty from a foundation independent of the method of Beer et al. (2010). Direct comparison is difficult because the uncertainty estimates presented here quantify NEE errors for North America, while Beer et al. estimate globally aggregated GPP uncertainty. It is simple in concept, however, to extend the methods shown here to GPP uncertainty and to the global scale.

### 3.3.5 NEE error covariance nugget

The estimated nugget values from the VPRM NEE error spatial covariance structure (section 2.3.2) quantify combined eddy covariance observation error and “microscale variation”, that is, the behavior of the difference in VPRM NEE error between two locations that are closer to one another than the closest pairs of towers among the 65 used for covariance parameter estimation. The median estimated seasonal nugget values range from $5.42 \times 10^{-5}$ (individual-site–monthly VPRM parameters) through 0.775 (PFT–all-data parameters) to 0.884 (all-sites–all-data parameters), with units of flux squared: $(\mu\text{mol CO}_2 \text{ m}^{-2} \text{ s}^{-1})^2$. Converted to standard deviation and integrated annually (gC m$^{-2}$ yr$^{-1}$) these nuggets are 21.0, 586, and 603.

In units of standard deviation the annual integrated NEE error nugget of 21.0 gC m$^{-2}$ yr$^{-1}$ from the individual-site–monthly VPRM parameters is essentially equal to the annual total eddy covariance random observation error of ±20 gC
m$^{-2}$ yr$^{-1}$ estimated by Richardson and Hollinger (2005). The 65 eddy covariance sites used for fitting include 26 pairs that are within 10 kilometers of each other, so there are many data points at small separation distances to quantify the nugget.

At coarser spatial and temporal parameter estimation resolutions (PFT–all-data, all-sites–all-data, etc.) the NEE error standard deviations of roughly 600 gC m$^{-2}$ yr$^{-1}$ calculated from the nuggets are of similar magnitude to the errors estimated from VPRM NEE and climate drivers (fig. 3.12) for high-productivity PFTs (e.g. forests, croplands).

These results suggest that when VPRM is optimized to NEE observations at short temporal scales (order one month) the VPRM NEE nugget is dominated by eddy covariance observation error – that is, under these conditions VPRM performs quite well in close proximity (order one kilometer) to an optimization location. Eddy covariance observation error is independent of VPRM optimization spatial and temporal windows, so its contribution to either nugget should remain constant across these windows. The much larger nugget when the temporal optimization window is all available observations therefore suggests that microscale VPRM NEE error increases dramatically from its value when VPRM is optimized monthly for individual sites. This means that VPRM can perform quite poorly even in close proximity to an optimization location in these cases.

Light use efficiency models such as VPRM make climate-driven diagnoses of NEE (eqs (3.1), (3.2)). Widespread VPRM annual NEE error magnitudes (fig. 3.11, this section) on the order of VPRM NEE interannual variability (fig. 3.9) imply that climate (or, at least, climate viewed through the prism of VPRM) cannot reliably explain NEE interannual variability.

### 3.3.6 VPRM parameterization and NEE spatial behavior

The PFT–all-data and all-sites–all-data VPRM parameter sets produce starkly different spatial patterns of growing season NEE in the southeastern USA (fig. 3.10a, 3.10b). This result highlights a question: what are the most appropriate parameterization time and space windows for a land surface model? In contrast, other results of the present study (e.g. Figure 2.3, fig. 3.2) might suggest deem-
phasizing this line of inquiry. For example, the total 30-minute cross-validation SSE values (fig. 3.2) across the five most optimally fitting VPRM parameter sets are nearly equal, suggesting that the choice of parameter optimization spatial and temporal windows is perhaps of secondary importance. In that case, the drastically lesser computational cost makes coarser spatial and temporal windows preferable.

The region of positive NEE in Figure 3.10a corresponds to the region of large diagnosed respiration discussed in section 3.3.3. Once again, instead of concluding that respiration is causing the mixed forests of the southeastern USA to release on the order of 150 gC m$^{-2}$ yr$^{-1}$ to the atmosphere, the explanations discussed in section 3.3.3 seem more plausible.

Considered in conjunction with the differing spatial behaviors in Figures 3.10a and 3.10b, the similar PSSE values among the better-performing parameter sets in Figure 3.2 suggest an instance of equifinality: PFT–all-data parameters and all-sites–all-data parameters produce comparable sums of 30-minute squared residuals via strongly divergent spatial outcomes.

### 3.3.7 Considering NEE error spatial covariance in NEE diagnosis

Chapter 2 fit parametric spatial covariance functions to observed VPRM NEE residuals, and found that the observations are consistent with an exponential covariance model with a range of roughly 400 km. This covariance function can be explicitly included when spatially interpolating NEE residuals to produce spatial estimates of VPRM NEE errors, a process known as kriging (Cressie, 1993). Figure 3.13 shows the change in the total sum of squared errors at 22 locations achieved by adding the kriged VPRM NEE errors to VPRM NEE diagnoses to produce an “adjusted” NEE diagnosis. The 22 locations are all in the set of cross-validation eddy covariance sites (Table 3.1, Figure 3.1); cross-validation sites were not used for VPRM parameter estimation or covariance parameter estimation. The spatial covariance-adjusted NEE produced a smaller SSE at 10 of the 22 cross-validation sites; it produced a larger SSE at the other 12. The adjustment lowered the total SSE among all 22 sites, but this result was only be-
cause of the extreme SSE reduction at US-DK1 (the outlier in Figure 3.13). The spatial covariance adjustment “success rate” at reducing SSE stayed roughly constant around 50% whether SSE was calculated across all data (shown in fig. 3.13), annually, seasonally, monthly, or only within seasons where structure was detected (Table 2.3).

### 3.3.8 Caveats

The results reported here were compiled using VPRM, a simple LUE-based ecosystem model, and are therefore most directly informative toward similar models. Questions of spatial and temporal resolution for model parameterization arise for more complicated mechanistic ecosystem models as well. Whether optimizing more complex model structures would result in similar total PSSE values for strongly contrasting spatial and temporal optimization windows (as reported here in fig. 3.2) is a question for further analysis. Regardless, this work suggests that applying model parameterizations outside of the climate and ecosystem conditions where the parameter values were optimized can produce suspicious spatial structures such as the widespread flux of CO$_2$ to the atmosphere across the southeastern USA in Figure 3.10a and Figure 3.6b.

The 27 cross-validation sites (fig. 3.1, table 3.1) generally have shorter observational records than the sites used for VPRM parameterization. Repeating the cross-validation experiment with different, perhaps randomly selected subsets might be a useful exercise.

In addition, forest stand age since disturbance is a first order determinant of NEE magnitude (Litvak et al., 2003). Structurally, VPRM does not consider stand age (eqs. 3.2, 3.1), and the work presented here does not attempt to assess disturbance history. For this reason, this work does not emphasize integrated NEE magnitudes or attempt regional NEE aggregation.

Likewise, the NEE residual magnitude statistical model derived here (section 3.2.5) was fit using observed NEE residuals and observed climatic drivers. While estimating uncertainty directly from observed residuals is a strength of the approach, as with any regression these results cannot produce meaningful estimates where the driver variables depart the range of values used for fitting.
3.4 Conclusions

This work presents high-resolution diagnoses of North American NEE and NEE interannual variability accompanied by NEE error estimates, all derived from a simple light use efficiency-based ecosystem model (VPRM). Several different model optimization spatial and temporal resolutions achieve similar fits when evaluated by total sum of squared errors at cross-validation sites and penalized sum of squared errors at the model parameterization sites. Cross validation is useful for identifying parameterizations that overfit assimilated data, however. Cross-validation SSE eliminated two of seven parameterizations we considered for upscaling. Penalized SSE from the parameterization sites eliminated another three. This sort of method to evaluate model parameter sets is computationally inexpensive and would make a welcome addition to future flux diagnoses.

Two of our model parameterizations achieved similar cross-validation SSE, but reached their NEE diagnoses through starkly contrasting spatial distributions of NEE. Modeling efforts that do not consider multiple spatial and temporal parameterization resolutions risk missing the structural uncertainty that this equifinality reveals, and that radically different fluxes across space may not be readily distinguishable when viewed through the lens of aggregated model errors.

The results here demonstrate that modeled annual integrated flux magnitude, annual mean surface temperature, and annual total precipitation provide reasonable (and computationally inexpensive) empirical predictors of NEE error magnitude. Estimated NEE errors are of equal magnitude to diagnosed NEE interannual variability. That a climate-driven ecosystem model cannot reliably separate year-to-year differences in model NEE from model error suggests that NEE interannual variability has important drivers outside of large-scale climate, or, alternatively, that the present network of North American eddy covariance NEE observation sites provide insufficient constraints on NEE and NEE error to reveal a strong climate–NEE interannual variability connection.
3.5 Figures and tables

Figure 3.1: 27 eddy covariance flux tower “cross-validation” sites from the 2007 Fluxnet synthesis dataset that were not used for VPRM parametrization or for VPRM NEE error covariance parameter estimation. Plant functional type abbreviations: ENF: evergreen needleleaf forest, DBF: deciduous broadleaf forest, MF: mixed forest, CS: closed shrubland, OS: open shrubland, WS: woody savanna, Gr: grassland, Wet: permanent wetland, Crop: cropland.
Figure 3.2: VPRM sum of squared errors vs. number of unique parameter values. Shown are the seven VPRM parameter sets available for upscaling. Parameter sets are labeled as [space grouping]-[time grouping] used for VPRM parameter estimation (Table 2.2). Left vertical axis shows sum of squared errors (SSE) for the 27 cross-validation sites not used to estimate VPRM parameters (figure 3.1, table 2.1); right vertical axis shows penalized sum of squared errors (PSSE) for the 27 cross-validation sites combined with the 65 sites used to parameterize VPRM (figure 2.1, table 2.1). Note the log scale on the horizontal axis.
Table 3.1: 27 North American eddy covariance cross-validation sites.

<table>
<thead>
<tr>
<th>Site Code</th>
<th>Site Name</th>
<th>Latitude (° W)</th>
<th>Longitude (° E)</th>
<th>Land Cover</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>CA-SJ3</td>
<td>Sask- SSA, 1975 Harv Yng Jack Pine</td>
<td>53.880</td>
<td>-104.650</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Zha et al. (2009)</td>
</tr>
<tr>
<td>US-SP4</td>
<td>Slashpine-Rayonier-mid-rot-12yrs-FL</td>
<td>29.800</td>
<td>-82.200</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Clark et al. (2004)</td>
</tr>
<tr>
<td>CA-SF1</td>
<td>Sask- Fire 1977</td>
<td>54.490</td>
<td>-105.830</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Amiro et al. (2006)</td>
</tr>
<tr>
<td>CA-TP2</td>
<td>Ontario- Turkey Point Young White Pine</td>
<td>42.770</td>
<td>-80.460</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Peichl and Arain (2006)</td>
</tr>
<tr>
<td>US-NC1</td>
<td>NC Clearcut</td>
<td>35.810</td>
<td>-76.710</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Sun et al. (2010)</td>
</tr>
<tr>
<td>US-NC2</td>
<td>NC Loblolly Plantation</td>
<td>35.800</td>
<td>-76.670</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Sun et al. (2010)</td>
</tr>
<tr>
<td>CA-TP3</td>
<td>Ontario- Turkey Point Middle-aged White Pine</td>
<td>42.710</td>
<td>-80.350</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Peichl and Arain (2006)</td>
</tr>
<tr>
<td>CA-TP4</td>
<td>Ontario- Turkey Point Mature White Pine</td>
<td>42.710</td>
<td>-80.360</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Peichl and Arain (2006)</td>
</tr>
<tr>
<td>CA-TP1</td>
<td>Ontario- Turkey Point Seedling White Pine</td>
<td>42.660</td>
<td>-80.560</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Peichl and Arain (2006)</td>
</tr>
<tr>
<td>US-WBW</td>
<td>Walker Branch Watershed- Tennessee</td>
<td>35.060</td>
<td>-84.290</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Hanson et al. (2005)</td>
</tr>
<tr>
<td>CA-Man</td>
<td>BOREAS NSA - Old Black Spruce</td>
<td>55.880</td>
<td>-98.480</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Dunn et al. (2007)</td>
</tr>
<tr>
<td>US-LPH</td>
<td>Little Prospect Hill- Massachusetts</td>
<td>42.540</td>
<td>-72.180</td>
<td>5 - Mixed Forest</td>
<td>Borken et al. (2006)</td>
</tr>
<tr>
<td>US-Bar</td>
<td>Bartlett Experimental Forest- New Hampshire</td>
<td>44.060</td>
<td>-71.290</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Smith et al. (2002)</td>
</tr>
<tr>
<td>US-Me3</td>
<td>Metolius-second young aged pine- Oregon</td>
<td>44.320</td>
<td>-121.610</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Hibbard et al. (2005)</td>
</tr>
<tr>
<td>US-Wi1</td>
<td>Intermediate hardwood (IHW)</td>
<td>46.730</td>
<td>-91.230</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Noormets et al. (2008)</td>
</tr>
<tr>
<td>US-Wi2</td>
<td>Intermediate red pine (IRP)</td>
<td>46.690</td>
<td>-91.150</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Noormets et al. (2008)</td>
</tr>
<tr>
<td>US-Wi4</td>
<td>Mature red pine (MRP)</td>
<td>46.740</td>
<td>-91.170</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Noormets et al. (2007)</td>
</tr>
<tr>
<td>US-Wi5</td>
<td>Mixed young jack pine (MYJP)</td>
<td>46.650</td>
<td>-91.090</td>
<td>1 - Evergreen Needleleaf Forest</td>
<td>Noormets et al. (2007)</td>
</tr>
<tr>
<td>US-Wi6</td>
<td>Pine barrens #1 (PB1)</td>
<td>46.620</td>
<td>-91.300</td>
<td>7 - Open Shrublands</td>
<td>Noormets et al. (2007)</td>
</tr>
<tr>
<td>US-Wi8</td>
<td>Young hardwood clearcut (YHWC)</td>
<td>46.720</td>
<td>-91.250</td>
<td>4 - Deciduous Broadleaf Forest</td>
<td>Noormets et al. (2007)</td>
</tr>
<tr>
<td>CA-WP2</td>
<td>Poor Fen</td>
<td>55.540</td>
<td>-112.330</td>
<td>11 - Permanent Wetlands</td>
<td>Glenn et al. (2006)</td>
</tr>
</tbody>
</table>
Figure 3.3: Histogram of VPRM NEE residuals at eddy covariance site reporting temporal resolution (30 minutes or 60 minutes), PFT–all-data VPRM parameters. NEE residuals are calculated as observed NEE (non-gapfilled) minus VPRM NEE. A normal distribution probability density function with the same mean and standard deviation is overlaid.
Figure 3.4: Histogram of VPRM annual integrated NEE residuals, PFT–all-data VPRM parameters. These are the residuals in Figure 3.3 integrated by site-year. The residuals are calculated as [(annual integrated observed NEE, non-gapfilled) minus (VPRM annual integrated NEE)].
Figure 3.5: Histograms of annually integrated NEE. Observations are the 2007 Fluxnet synthesis gapfilled annual NEE.
Figure 3.6: 2002 annual integrated VPRM GEE, gC m$^{-2}$ yr$^{-1}$. PFT–all-data VPRM parameters.
Figure 3.6: 2002 annual integrated VPRM respiration, gC m\(^{-2}\) yr\(^{-1}\). PFT–all-data VPRM parameters.
Figure 3.6: 2002 annual integrated VPRM NEE, gC m\(^{-2}\) yr\(^{-1}\). PFT–all-data VPRM parameters.
Figure 3.7: Annual anomaly, annual integrated VPRM GEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM GEE minus the 2002 to 2006 mean annual integrated VPRM GEE. Thus negative values denote lesser than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.7: Annual anomaly, annual integrated VPRM GEE, calculated using PFT–all-data VPRM parameters. Units are gC m\(^{-2}\) yr\(^{-1}\). Anomalies are calculated as annual integrated VPRM GEE minus the 2002 to 2006 mean annual integrated VPRM GEE. Thus negative values denote lesser than average atmosphere to ecosystem CO\(_2\) flux.
Figure 3.7: Annual anomaly, annual integrated VPRM GEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM GEE minus the 2002 to 2006 mean annual integrated VPRM GEE. Thus negative values denote lesser than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.7: Annual anomaly, annual integrated VPRM GEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM GEE minus the 2002 to 2006 mean annual integrated VPRM GEE. Thus negative values denote lesser than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.7: Annual anomaly, annual integrated VPRM GEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM GEE minus the 2002 to 2006 mean annual integrated VPRM GEE. Thus negative values denote lesser than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.8: Annual anomaly, annual integrated VPRM respiration, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM R minus the 2002 to 2006 mean annual integrated VPRM R. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.8: Annual anomaly, annual integrated VPRM respiration, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM R minus the 2002 to 2006 mean annual integrated VPRM R. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.8: Annual anomaly, annual integrated VPRM respiration, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM R minus the 2002 to 2006 mean annual integrated VPRM R. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.8: Annual anomaly, annual integrated VPRM respiration, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM R minus the 2002 to 2006 mean annual integrated VPRM R. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.8: Annual anomaly, annual integrated VPRM respiration, calculated using PFT–all-data VPRM parameters. Units are gC m\(^{-2}\) yr\(^{-1}\). Anomalies are calculated as annual integrated VPRM R minus the 2002 to 2006 mean annual integrated VPRM R. Thus negative values denote greater than average atmosphere to ecosystem CO\(_2\) flux.
Figure 3.9: Annual anomaly, annual integrated VPRM NEE, calculated using PFT–all-data VPRM parameters. Units are gC m\(^{-2}\) yr\(^{-1}\). Anomalies are calculated as annual integrated VPRM NEE minus the 2002 to 2006 mean annual integrated VPRM NEE. Thus negative values denote greater than average atmosphere to ecosystem CO\(_2\) flux.
Figure 3.9: Annual anomaly, annual integrated VPRM NEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM NEE minus the 2002 to 2006 mean annual integrated VPRM NEE. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.9: Annual anomaly, annual integrated VPRM NEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM NEE minus the 2002 to 2006 mean annual integrated VPRM NEE. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.9: Annual anomaly, annual integrated VPRM NEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM NEE minus the 2002 to 2006 mean annual integrated VPRM NEE. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.9: Annual anomaly, annual integrated VPRM NEE, calculated using PFT–all-data VPRM parameters. Units are gC m$^{-2}$ yr$^{-1}$. Anomalies are calculated as annual integrated VPRM NEE minus the 2002 to 2006 mean annual integrated VPRM NEE. Thus negative values denote greater than average atmosphere to ecosystem CO$_2$ flux.
Figure 3.10: 2004 VPRM June-July-August integrated NEE. Units are gC m$^{-2}$ yr$^{-1}$. 

(a) PFT-all-data VPRM parameters
Figure 3.10: 2004 VPRM June-July-August integrated NEE. Units are gC m\(^{-2}\) yr\(^{-1}\).
Figure 3.11: 2002 estimated square root of NEE residual squared difference (eq. 3.3), calculated using PFT–all-data VPRM parameters. Units are $\text{gC m}^{-2} \text{ yr}^{-1}$. Estimates are calculated by a statistical model (eq. 3.5, section 3.2.5) with explanatory variables annual integrated VPRM NEE, annual total precipitation, and annual mean surface temperature. 2003 to 2006 estimated annual errors (not shown) show similar spatial patterns.
Figure 3.12: Results from an empirical regression model (eq. 3.5) for VPRM NEE residual spread. Units are (gC m$^{-2}$ yr$^{-1}$)$^2$. Top panel shows observed values vs. predicted values at 27 cross-validation sites (Table 3.1). Observed values are outside of the 95% prediction interval where the solid line falls outside of the dashed lines. One of 56 predicted values (2%) is outside the 95% prediction interval. The bottom panel shows histograms for observed values and model-predicted values.
Figure 3.13: Difference in total sum of squared errors (SSE): covariance-"adjusted" SSE at 27 cross-validation sites (fig 3.1, Table 3.1). Filled plotting makers show values greater than zero (i.e. the adjustment lowered the SSE). There is no adjusted SSE at US-FR2 and CA-TP2 because there are no data points within the 400-km kriging neighborhood.
Chapter 4

Conclusions and Future Work

The studies presented in this dissertation assimilate eddy covariance net ecosystem exchange (NEE) observations from 92 field sites spanning North America into a simple light-use efficiency-based model (the Vegetation Photosynthesis Respiration Model, VPRM). We conclude that observed NEE–VPRM NEE residuals exhibit a correlation length scale of approximately 400 km. This length scale approximates the radius to which an eddy covariance site, coupled with a flux model, can provide information about NEE. The covariance structure derived here also suggests a quantitative error covariance matrix for atmospheric inversion analyses. To date, these analyses have typically used the mathematically convenient, though simplistic, assumption of independent and identically normally distributed errors.

We have also used the eddy covariance observation-informed VPRM to diagnose North American continental NEE for 2000 to 2006. In a unique contribution, we also quantitatively derive cross-validated, spatially-explicit and comprehensive uncertainty estimates for these fluxes at 1 km resolution.

The spatial structure and uncertainty estimates depend crucially on the vast spatial proliferation of North American eddy covariance NEE observations in the early 2000s. Without the numerous sites that came online between 2000 and 2005 there would not have been sufficient data to derive a spatial covariance structure or to cross-validate model parameter values for uncertainty estimation.

The uncertainties presented here are in most cases large, on the order of the
estimated NEE itself. This, on the surface, may seem a disquieting assessment of the information gained from 15 years of observations. However, the uncertainty estimates are the first of their kind. It should be considered a triumph to have collected sufficient data, in space and time, to characterize ecosystem behavior to this extent. Future work, informed by ever greater amounts of data, will reduce the uncertainties around flux diagnoses. Uncertainties must necessarily be larger before they can be made smaller.

To that end, the work shown here suggests several approaches for further refining NEE uncertainty estimates toward the goal of better understanding ecosystem carbon cycle dynamics. First, and crucially, existing eddy covariance observations should be maintained. We have demonstrated that the current observation spatial density is minimally sufficient for detecting model error spatial covariance some of the time. Cross-validation of model parameters is important for detecting overfitting, and as new data accumulate more data can be used for cross-validation without sacrificing data for parameter estimation.

As noted, the 400 km model error covariance length scale suggests a footprint within which a flux tower paired with an ecosystem model can characterize landscape-atmosphere interactions. While additional data are always attractive for characterizing an incompletely understood phenomenon such as the terrestrial biological carbon cycle, we must consider the optimal allocation of resources toward that goal. It is unrealistic to propose blanketing North America with eddy covariance towers in a 400 km grid, and, fortunately, unnecessary. Chapter 3 presents an approach to estimate modeled NEE uncertainty from model residuals. Eddy covariance “Pseudo-towers” could be created from modeled NEE at locations where eddy covariance sites do not presently exist. We could thus evaluate the contribution of additional flux tower locations toward reducing diagnosed flux uncertainty. We could locate, for example, the optimal site for a single flux tower in addition to the present set of towers. Performing this analysis recursively would then suggest sites for consecutive additional towers. We could identify a point of diminishing returns or conduct a cost-benefit study for additional flux towers.

Similarly, this work suggests that plant function types (PFTs) do not come close to completely specifying NEE for model parameterization. Stand age since
major disturbance (logging, fire, insect infestation, etc.) is an important determinant of NEE. Because such disturbances often operate at scales of order 1 km or less, compiling large-scale disturbance data is time-consuming. Several landscape-scale datasets have recently become available, however. Compiling detailed disturbance histories for existing eddy covariance locations could be a worthy use of terrestrial carbon cycle resources.
Bibliography


Hanson, P., S. Wullschleger, R. Norby, T. Tschaplinski, and C. Gunderson, 2005: Importance of changing CO$_2$, temperature, precipitation, and ozone on carbon


URL http://www.atmos-chem-phys-discuss.net/11/20855/2011/


URL http://www.biogeosciences.net/6/969/2009/


URL http://www.R-project.org


URL http://CRAN.R-project.org/doc/Rnews/


Vita

Timothy William Hilton

Timothy William Hilton was born and raised in Ithaca, New York, where his father Ronald Walter Hilton is a Professor of Accounting at Cornell University and his mother Margaret Johnstone Hilton is retired after teaching at the Ellis Hollow Nursery school. Tim graduated from Ithaca High School in 1997 and attended Princeton University, earning a Bachelor of Science in Engineering in Computer Science in June 2001. His independent research project at Princeton, supervised by Dr. Steven H. Kleinstein and Dr. Jaswinder Pal Singh, explored methods to use a computational immunobiology model to estimate hypermutation rates during immune and autoimmune responses.

Following his undergraduate studies Tim volunteered with the U.S. National Park Service’s Hawksbill Sea Turtle Protection Program in Hawai’i Volcanoes National Park, identifying backcountry hawksbill nesting sites and protecting hawksbill hatchlings.

From 2002 to 2003 Tim worked in the Energy and Infrastructure Analysis Group at Los Alamos National Laboratory. Under the supervision of Dr. Michael H. Brown he developed user interfaces for the QUICUrb/QUICPlume atmospheric dispersion model. He was a member of the LANL team that participated in the Joint Urban 2003 field experiment in Oklahoma City, Oklahoma, USA. The team placed instruments on several highrise buildings in downtown Oklahoma City to study atmospheric dispersion in an urban environment.

In August 2003 Tim undertook graduate study in the Department of Meteorology at Pennsylvania State University. With advisor Raymond G. Najjar, his masters thesis integrated 50 years of Chesapeake Bay salinity observations with flow volume observations from the Bay’s tributaries to test the hypothesis that after river discharge is controlled for, Chesapeake Bay salinity has risen since 1950. Tim earned his M.S. in meteorology in December 2005.

In 2006 Tim was admitted to PhD candidacy, working with advisor Kenneth J. Davis to develop methods to combine eddy covariance observations of net ecosystem exchange of carbon dioxide with land surface models to characterize the North American terrestrial biological carbon cycle.

Tim met Kerry Noel Makin-Byrd in 2004, and they were married in July of 2009.