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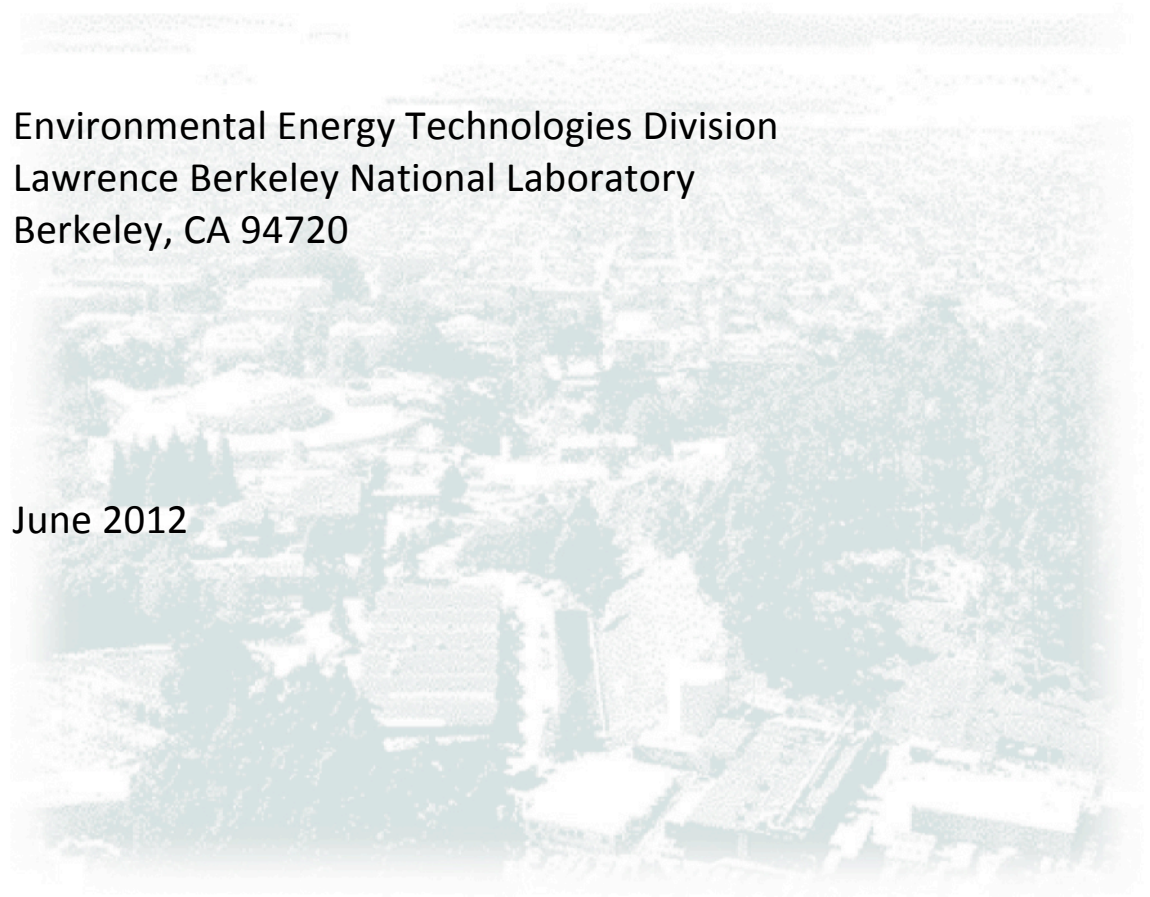
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1 **North American CO₂ exchange: Inter-comparison of modeled estimates with**
2 **results from a fine-scale atmospheric inversion**

3
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24
25
26 **Abstract**

27 Atmospheric inversion models have the potential to quantify CO₂ fluxes at regional, sub-
28 continental scales by taking advantage of near-surface CO₂ mixing ratio observations collected
29 in areas with high flux variability. This study presents results from a series of regional
30 geostatistical inverse models (GIM) over North America for 2004, and uses them as the basis for
31 an inter-comparison to other inversion studies and estimates from biospheric models collected
32 through the North American Carbon Program Regional and Continental Interim Synthesis.
33 Because the GIM approach does not require explicit prior flux estimates and resolves fluxes at
34 fine spatiotemporal scales (i.e. 1°x1°, 3-hourly in this study), it avoids temporal and spatial
35 aggregation errors and allows for the recovery of realistic spatial patterns from the atmospheric
36 data relative to previous inversion studies. Results from a GIM inversion using only available
37 atmospheric observations and a fine-scale fossil fuel inventory were used to confirm the quality
38 of the inventory and inversion setup. An inversion additionally including auxiliary variables
39 from the North American Regional Reanalysis found inferred relationships with flux consistent
40 with physiological understanding of the biospheric carbon cycle. Comparison of GIM results

1 with bottom-up biospheric models showed stronger agreement during the growing relative to
2 the dormant season, in part because most of the biospheric models do not fully represent
3 agricultural land-management practices and the fate of both residual biomass and harvested
4 products. Comparison to earlier inversion studies pointed to aggregation errors as a likely
5 source of bias in previous sub-continental scale flux estimates, particularly for inversions that
6 adjust fluxes at the coarsest scales and use atmospheric observations averaged over long
7 periods. Finally, whereas the continental CO₂ boundary conditions used in the GIM inversions
8 have a minor impact on spatial patterns, they have a substantial impact on the continental
9 carbon budget, with a difference of 0.8 PgC/yr in the total continental flux resulting from the
10 use of two plausible sets of boundary CO₂ mixing ratios. Overall, this inter-comparison study
11 helps to assess the state of the science in estimating regional-scale CO₂ fluxes, while pointing
12 towards the path forward for improvements in future top-down and bottom-up modeling
13 efforts.

14

15 **1. Introduction**

16 Carbon cycle scientists are increasingly called upon to provide information in support of
17 efforts to monitor anthropogenic CO₂ emissions, and to provide predictions of future changes
18 to the carbon cycle within the context of a changing climate and land-use choices (CCSP, 2007).
19 Atmospheric inverse models can contribute towards these goals by taking advantage of the
20 information contained in atmospheric CO₂ mixing ratio measurements regarding upwind
21 surface CO₂ exchange. Using these measurements, together with an atmospheric transport
22 model and within a robust statistical framework (e.g. Enting, 2002), inverse models are used to
23 infer the spatiotemporal distribution and magnitude of surface CO₂ fluxes. In addition, inverse-
24 modeling derived CO₂ flux estimates are potentially useful for evaluating the process-based
25 formulations of terrestrial ecosystem models. In fact, atmospheric measurements of CO₂
26 provide one of the key means of evaluating mechanistic models (e.g. Randerson et al., 2009;
27 Cadule et al., 2010), given the lack of direct flux observations at regional scales.

28 Inversions that can take advantage of spatial and temporal atmospheric CO₂ gradients
29 measured in areas with high flux variability provide the potential to resolve sub-continental
30 scale fluxes, thereby informing carbon management efforts and evaluations of mechanistic
31 models of the carbon cycle. An expanding *in situ* continuous measurement network across the
32 North American and European continents (e.g. NOAA-ESRL, 2011; CGGMN, 2011; CEAD, 2011) is

1 making this possible, but optimally extracting the flux signal from these data is complicated by
2 the combined influence on atmospheric CO₂ mixing ratios of the diurnal cycle of the terrestrial
3 biosphere, heterogeneous land cover, point source fossil fuel emissions, and complex
4 atmospheric transport (Bakwin et al., 1998). Therefore, simultaneous improvements in
5 inversion setups (e.g. Law et al., 2002; Schuh et al., 2009; Gourdji et al., 2010) and in the quality
6 of atmospheric transport models (e.g. Geels et al., 2007) have been necessary.

7 By limiting the domain size in regional inversions, fluxes can be estimated at relatively
8 fine spatial scales (e.g. 1°x1°), thereby reducing aggregation errors (e.g. Kaminski et al., 2001;
9 Engelen et al., 2002) associated with estimating coarse-scale fluxes using highly variable CO₂
10 measurement data, while simultaneously keeping the computational cost of inversions
11 manageable. In addition, with a limited domain, it is possible to take advantage of high-
12 resolution meteorological information and Lagrangian transport models that can better resolve
13 atmospheric dynamics in the near-field of measurement locations (e.g. Lin et al., 2003; Gerbig
14 et al., 2008). However, it has proven difficult to reconcile observed differences in estimates
15 across regional inverse modeling studies due to a number of potential factors: atmospheric
16 transport, flux spatial and temporal resolution, boundary conditions, errors in the bottom-up
17 models used as priors, treatment of fossil fuels, spatiotemporal flux covariance assumptions,
18 and the processing and filtering of observations, among other possible causes.

19 Similarly, large discrepancies have also been seen in inter-comparisons of mechanistic
20 models of biospheric CO₂ flux (Huntzinger et al., in review; Hayes et al., in press). Given that
21 atmospheric CO₂ mixing ratio observations are a key data constraint on biospheric CO₂ fluxes, a
22 reconciliation of top-down flux estimates across inversion studies could be especially useful for
23 evaluating biospheric model estimates and their process-based assumptions.

24 As a step towards reconciling CO₂ flux estimates from regional inversions and biospheric
25 models, this study presents a regional grid-scale geostatistical inversion (Michalak et al., 2004;
26 Mueller et al., 2008; Gourdji et al., 2008; Gourdji et al., 2010) for North America in 2004, using
27 the sampling network of 9 towers collecting continuous CO₂ measurements at that time, as well
28 as available surface flask and aircraft data. The geostatistical inverse modeling (GIM) approach
29 implemented here uses the optimized setup from Gourdji et al. (2010), which resolves fluxes at

1 finer spatial and temporal scales than other published inversion studies for the same domain
2 (e.g. Peters et al., 2007; Deng et al., 2007; Schuh et al., 2010; Butler et al., 2010), and relies
3 strongly on the atmospheric measurements and spatiotemporal flux covariance assumptions to
4 help constrain the problem. Also, by eliminating the requirement for explicit prior flux
5 estimates and optimizing covariance parameters directly with the atmospheric data, the
6 inversions presented here reduce potential biases associated with these setup choices. Four
7 sets of geostatistical results are presented, with and without process-based auxiliary datasets
8 that can help to explain biospheric fluxes, and using two plausible sets of continental boundary
9 conditions.

10 Geostatistical inversion results are compared at various spatial and temporal scales to
11 estimates from other inversion studies over North America to help illuminate potential causes
12 of their differences and associated strengths and weaknesses of the various approaches.
13 Geostatistical inversion estimates are also used to interpret the spread seen across a collection
14 of biospheric models participating in the North American Carbon Program (NACP) Regional and
15 Continental Interim Synthesis study (RCIS; Huntzinger et al., in review).

16

17 **2. Data and Methods**

18 The presented inversions use the setup described as part of a synthetic data study for
19 June 2004 (i.e. Gourdji et al., 2010) and further evaluated using synthetic data for a full year. A
20 brief overview of the setup and methods is provided below, with methodological details
21 available in Gourdji et al. (2010).

22 ***2.1 Flux domain and resolution***

23 Fluxes are estimated at a $1^{\circ} \times 1^{\circ}$, 3-hourly resolution for the North American continent in
24 2004. Positive values indicate a flux from the biosphere to the atmosphere, and conversely,
25 negative values refer to net uptake. The estimation domain spans from 10°N to 70°N and 50°W
26 to 170°W , yielding 2635 land grid-cells (Figure 1). Altogether, 8 million fluxes are estimated for
27 the year (2635 regions \times 366 days \times 8 flux periods per day). Resolving fluxes for a 4-day-
28 averaged diurnal cycle temporal resolution, as described in Gourdji et al. (2010), was also

1 explored to reduce computational expense, but the penalty in terms of the quality of the flux
2 estimates was found to be unacceptable.

3 Flux estimates are not well-constrained at this fine spatiotemporal estimation resolution
4 by the limited atmospheric network; however, biases due to estimating fluxes directly at large
5 scales, termed aggregation errors (Kaminski et al., 2001; Engelen et al., 2002), are minimized by
6 estimating fluxes first at fine scales and then aggregating to better-constrained resolutions *a*
7 *posteriori*. Spatial aggregation errors have been shown to be particularly problematic when
8 making use of continental, continuous CO₂ measurements in inversions (Gerbig et al., 2003b;
9 Schuh et al., 2009). Temporal aggregation errors are also a concern when the shape of the
10 diurnal cycle is fixed from biospheric models (Gourdji et al., 2010; Huntzinger et al., 2011) or
11 assumed flat, rather than estimated directly as in the current study.

12 **2.2 Geostatistical inversions**

13 GIM (e.g. Hoeksema & Kitanidis, 1984; Zimmerman et al., 1998) has been used to
14 identify atmospheric trace gas sources and sinks (e.g. Michalak et al., 2004; Mueller et al., 2008;
15 Gourdji et al., 2008; 2010; Miller et al., in review). Although GIM is Bayesian, it differs from
16 synthesis Bayesian inversions (e.g. Baker et al., 2006; Peters et al., 2007; Butler et al., 2010) in a
17 few key ways. GIM does not rely on a set of explicit prior flux estimates derived from
18 biospheric models, fossil fuel inventories, fire emissions estimates, and/or ocean flux estimates.
19 Traditional Bayesian inversion studies (e.g. Peters et al., 2007; Butler et al., 2010) typically use
20 such explicit priors both to define a first estimate of flux magnitudes and to fix the fine-scale
21 variability in the inversion, while the atmospheric data are used to adjust fluxes only at larger
22 scales. Instead, GIM estimates fluxes directly at fine scales, and relies on *a priori* information
23 on the spatiotemporal covariance between estimated fluxes to help constrain the problem.
24 The parameters describing this covariance structure are optimized directly using the
25 atmospheric measurements. Some recent synthesis Bayesian inversion studies also estimate
26 fluxes at relatively fine spatial scales and rely on spatial covariance assumptions (e.g.
27 Rödenbeck et al., 2003; Carouge et al., 2010a,b; Chevallier et al., 2010; Schuh et al., 2010), with
28 the covariance parameters based on analyses of variability in biospheric models, or sensitivity
29 testing to assess their impact on flux estimates. The GIM estimates presented here also

1 estimate, rather than prescribe the diurnal cycle based on results from Gourджи et al. (2010) and
2 Huntzinger et al. (2011). We are not aware of any other regional inversions that have taken this
3 step, which is aimed at minimizing temporal aggregation errors that can result from fluxes
4 being adjusted at coarser (e.g. weekly to monthly) scales (e.g. Peters et al., 2007; Butler et al.,
5 2010; Schuh et al., 2010).

6 The objective function $L_{s,\beta}$ for GIM is:

$$7 \quad L_{s,\beta} = \frac{1}{2}(\mathbf{z} - \mathbf{H}\mathbf{s})^T \mathbf{R}^{-1}(\mathbf{z} - \mathbf{H}\mathbf{s}) + \frac{1}{2}(\mathbf{s} - \mathbf{X}\boldsymbol{\beta})^T \mathbf{Q}^{-1}(\mathbf{s} - \mathbf{X}\boldsymbol{\beta}) \quad (1)$$

8 where \mathbf{z} represents the atmospheric CO₂ measurements [ppm], and \mathbf{s} are the unknown surface
9 CO₂ fluxes [$\mu\text{mol}/(\text{m}^2\text{s})$]. \mathbf{H} describes the sensitivity of CO₂ measurements to fluxes, as
10 quantified from an atmospheric transport model, with units of [ppm/($\mu\text{mol}/(\text{m}^2\text{s})$)]. \mathbf{X} contains
11 any pre-selected flux covariates or alternately, one or more columns of ones (see Section 2.4),
12 $\boldsymbol{\beta}$ are the associated drift coefficients, and $\mathbf{X}\boldsymbol{\beta}$ is the component of the flux variability that can
13 be explained by the covariates, a.k.a. the “trend.” Fluxes (\mathbf{s}) and regression coefficients ($\boldsymbol{\beta}$) are
14 optimized simultaneously by minimizing Eq. 1. \mathbf{R} is the model-data mismatch covariance
15 matrix, describing the expected magnitude of discrepancies between observed (\mathbf{z}) and modeled
16 ($\mathbf{H}\mathbf{s}$) CO₂ mixing ratios (due to measurement, transport, representation, and aggregation
17 errors). \mathbf{Q} is the *a priori* flux covariance matrix, characterizing how flux deviations from the
18 model of the trend (i.e. $\mathbf{s} - \mathbf{X}\boldsymbol{\beta}$) are correlated in time and space.

19 The structure of \mathbf{Q} and \mathbf{R} remain the same as in Gourджи et al. (2010), with a few minor
20 modifications. Separate model-data mismatch values were optimized in \mathbf{R} for each continuous
21 measurement location, as well as for flask and aircraft data (with these latter two representing
22 averages across sites). Additionally, covariance parameters are allowed to vary by month. In
23 particular, spatial flux covariance has been found to have a strong seasonal cycle (Huntzinger et
24 al., 2010) that should be appropriately accounted for in order to yield realistic estimates from
25 the inversion. Monthly model-data mismatch values also help to account for seasonal
26 variations in the quality of the transport model and inversion setup. All covariance parameters
27 are estimated simultaneously, per month, using Restricted Maximum Likelihood (RML; e.g.

1 Kitanidis, 1995, Michalak et al., 2004) with the atmospheric measurements, as described
2 further in Gourdjji et al. (2010).

3 The solution method for estimating fluxes (\hat{S}), drift coefficients ($\hat{\beta}$) and their *a posteriori*
4 covariances ($V_{\hat{S}}$ and $V_{\hat{\beta}}$) is described in Gourdjji et al. (2010).

5 **2.3 Atmospheric data, boundary conditions and transport**

6 *2.3.1 Atmospheric CO₂ mixing ratio measurements*

7 This study uses continuous, high-precision, well-calibrated CO₂ mixing ratio
8 measurements from 9 observational locations unevenly spaced across the North American
9 continent in 2004 (Figure 1). These include two tall towers with a height of 457m (Moody,
10 Texas) and 396m (Park Falls, Wisconsin), two coastal towers less than 25m in height (Sable
11 Island, Nova Scotia and Barrow, Alaska), and five other inland, continental towers ranging in
12 height from 30 to 107m (Norman, Oklahoma; Harvard Forest, Massachusetts; Argyle, Maine;
13 Fraserdale, Ontario; Candle Lake, Saskatchewan). In addition, all available flask and aircraft
14 measurements for this year are included, with the exception of flask samples at coincident
15 tower locations and some coastal sites where the atmospheric transport model was deemed
16 unreliable. Appendix A provides additional details on CO₂ data processing and filtering.

17 Although the North American measurement network has now expanded to more than
18 40 sites collecting continuous CO₂ mixing ratio measurements, many new sites are in complex
19 terrain, urban areas, or are very short, and the optimal use of these data in inversions remains a
20 topic of active research (Mueller, 2011; Manning, 2011). This study therefore provides a
21 baseline for improving inversions taking advantage of a more data-rich environment.

22 *2.3.2 Continental boundary conditions*

23 Regional inversions necessitate the use of boundary conditions that represent the CO₂
24 concentrations of air flowing into the domain of interest (i.e. the North American land mass
25 here). The impact of these boundary CO₂ mixing ratios on the observations used in the
26 inversion must be pre-subtracted before inferring CO₂ fluxes. Two plausible sets of CO₂
27 boundary conditions are used in this study: one optimized as part of the CarbonTracker
28 (termed “CT” in this work) global CO₂ data assimilation system (Peters et al., 2007), and the
29 other derived more empirically (termed “EMP” in this work) from marine boundary layer and

1 aircraft observations taken from the GLOBALVIEW-CO₂ (2010) database. Appendix A provides
2 additional details on these datasets. Only results using the EMP boundary conditions are
3 presented at the monthly timescale, but results with both sets of boundary conditions are
4 discussed at the annual timescale, where they were seen to have a larger impact on the
5 conclusions.

6 *2.3.3 Atmospheric transport model*

7 Surface influence functions (“footprints”, or adjoint sensitivities) express the sensitivity
8 of individual CO₂ measurements at specific points in space and time to surface fluxes in the
9 upwind source regions. The Stochastic Time-Inverted Lagrangian Transport (STILT) model (Lin
10 et al., 2003), driven by meteorological fields from the Weather Research and Forecasting (WRF)
11 model (Skamarock and Klemp, 2008), customized for STILT (Nehrkorn et al., 2010), was used to
12 derive these footprints.

13 The WRF-STILT framework is well-suited for this application, because: 1) WRF
14 meteorology is available at higher resolution than that used in most global models, and
15 therefore has the potential to be more realistic (Mass et al., 2002); 2) the Lagrangian approach
16 minimizes numerical diffusion present in Eulerian models (Odman, 1997) and is thus better able
17 to represent plumes in the near-field of the measurement locations (Lin et al., 2003; Wen et al.,
18 2011); 3) the WRF-STILT coupling has been specifically designed to achieve good mass
19 conservation characteristics by using time-averaged winds from WRF within STILT (Nehrkorn et
20 al., 2010); and 4) the Lagrangian approach offers the most efficient way to compute the grid-
21 scale footprints, by running transport backwards in time (Lin et al., 2003). The computational
22 aspects of the footprint calculations are described in more detail in Appendix A.

23 The footprints can also be used to assess which portions of the continent are typically
24 constrained by the measurements included in the inversion. Given the limited network in 2004,
25 not all portions of North America are equally well-constrained, as can be seen in the annual
26 average footprint shown in Figure 2a. Not surprisingly, the best-constrained areas are upwind
27 of the measurement locations, in the Central and Northeastern continental United States (U.S.)
28 and a large portion of central Canada. Figure 2b shows three ecoregions across North America
29 with similar land-cover and/or climatic characteristics (modified from Olson et al., 2001) that

1 are relatively well-constrained by the network (although the Eastern Temperate Forests lack
2 sensitivity in the Southeast U.S.) Inversion results are aggregated *a posteriori* to these three
3 ecoregions for comparison across all presented models.

4 **2.4 Auxiliary variables and variable selection**

5 Geostatistical inversions can estimate fluxes with varying levels of complexity in the flux
6 covariate matrix (\mathbf{X}). In addition to potentially improving flux estimates, introducing auxiliary
7 environmental variables as covariates in \mathbf{X} makes it possible to identify significant flux drivers.

8 As in multi-linear regression, adding all possible covariates can help to improve the fit of
9 the model to the data, although at the risk of introducing spurious relationships that could
10 potentially bias flux estimates in under-constrained regions and time periods. Therefore, for
11 this study, the Bayes Information Criterion (BIC) (Schwarz, 1978) is used to choose covariates
12 that optimally explain the biospheric flux signal in the atmospheric data. The BIC was combined
13 with the Branch-and-Bound algorithm (Yadav et al., in review) in order to reduce computational
14 expense. Appendix A presents the details of the implementation of these techniques.

15 Two main sets of inversion results are presented in this paper. For the first inversion,
16 we include only a fossil fuel inventory dataset in the flux covariate matrix (\mathbf{X}), with no
17 additional information regarding biospheric processes. The fossil fuel inventory is included to
18 help account for the spatial patterns of the fossil fuel emissions, which have a very different
19 structure from the biospheric fluxes. This setup is referred to as the “Simple” inversion, given
20 that the atmospheric observations, fossil fuel inventory and covariance assumptions provide
21 the only constraint on biospheric fluxes in this setup. This inversion is conceptually similar to
22 using a prior of zero in a synthesis Bayesian inversion setup, and provides an independent
23 comparison to process-based, biospheric model output. For the second inversion, we
24 additionally incorporate auxiliary variables from the North American Regional Reanalysis
25 (NARR; Mesinger et al., 2006) to help explain the biospheric signal, which are selected using the
26 combined BIC and Branch-and-Bound algorithm. This case is termed the “NARR” inversion.

27 All included flux covariates are defined at the resolution at which fluxes are estimated,
28 i.e. $1^\circ \times 1^\circ$, 3-hourly, with each variable defined in a single column for all flux locations and time
29 periods. Therefore, the inferred regression coefficients ($\hat{\beta}$) represent average relationships

1 over the entire continent and year, with these averages reflecting the portions of the continent
2 within the measurement footprints.

3 *2.4.1 Fossil fuel inventory*

4 The fossil fuel inventory used in this study is a merged data product providing full
5 coverage for the continent. In the continental United States, we take advantage of diurnally
6 and seasonally varying estimates from version 2.0 of the Vulcan database (Gurney et al., 2009).
7 These estimates for 2002 are scaled up to 2004 total emissions for the region, but without any
8 changes in the underlying spatial and temporal patterns. In Central America, Mexico and
9 Canada, emission estimates are taken from a monthly-varying dataset specifically for 2004,
10 which merges information from British Petroleum fuel statistics, remotely-sensed night lights,
11 and the existing Carbon Dioxide Information Analysis Center (CDIAC) fossil fuel emission
12 inventory (Oda and Maksyutov, 2010).

13 In the NARR inversion, the impact of fossil fuels is removed from the atmospheric
14 observations *a priori*, by multiplying the inventory dataset by the footprints and subtracting the
15 resulting signal from the atmospheric measurements. By pre-subtracting the fossil fuel
16 influence from the measurements, we reduce potential covariance in the inferred regression
17 coefficients between the fossil fuel inventory and biospheric datasets due to covariance in the
18 underlying processes, e.g. re-growing forests and high emissions in the Eastern continental
19 United States, or reduced populations and industrial activity in arid and snow-covered areas.
20 Such covariance would confound flux interpretation by making it more difficult to separate the
21 biospheric and fossil fuel signals *a posteriori*. In both inversions, errors in the fossil fuel
22 inventories will become aliased onto the inferred biospheric fluxes, although these errors are
23 thought to be small relative to the uncertainties in terrestrial biosphere models (Marland et al.,
24 2009).

25 *2.4.2 NARR variables*

26 The NARR data products are a state-of-the-science meteorological reanalysis for North
27 America, and have significantly improved the representation of the hydrological cycle relative
28 to previous datasets (Bukovsky and Karoly, 2007). Eleven datasets with diurnal variability were
29 considered for inclusion in the inversion, as well as two derived precipitation variables (average

1 precipitation over the previous 16 and 30 day intervals, Table 2). This superset of NARR
2 variables primarily relates to water fluxes and availability, although shortwave radiation,
3 evapotranspiration and canopy conductance have a direct physiological relationship with
4 photosynthetic CO₂ fluxes. Vegetative indices from remote-sensing datasets, such as Leaf Area
5 Index or Fraction of Photosynthetically Active Radiation from the MODIS instruments (e.g. Yang
6 et al., 2006), could also provide useful information regarding the seasonal cycle and spatial
7 distribution of CO₂ flux (e.g. Gourdji et al. 2008). However, given that such datasets have a
8 diurnally-varying relationship to CO₂ flux, this would have necessitated the use of diurnally-
9 varying drift coefficients ($\hat{\beta}$), adding substantial complexity to the trend. Sensitivity tests
10 showed that this setup did not help to improve flux estimates, and thus, these datasets were
11 not included. Also, the evapotranspiration and canopy conductance variables from NARR are
12 calculated with the Noah Land Surface Model (Ek et al., 2003), and therefore implicitly include a
13 measure of vegetative biomass.

14 **2.5 Comparison of inferred fluxes to estimates from other models**

15 Biospheric *a posteriori* flux estimates from the GIM inversions are compared with those
16 from previous inversion studies (CarbonTracker 2009, i.e. Peters et al., 2007; Schuh et al., 2010;
17 Butler et al., 2010) for the same domain, and also with a suite of bottom-up flux estimates from
18 16 terrestrial biosphere models that participated in the NACP RCIS (Huntzinger et al., in review).
19 Table 1 compares the features of the GIM inversions conducted here and the synthesis
20 Bayesian inversions included in the inter-comparison. In addition to the details presented in
21 Table 1, each inversion has its own particularities in terms of data processing and selection,
22 identification of covariance parameters, and numerical approaches for implementing the
23 inversion scheme. Despite these differences, the available atmospheric measurements for this
24 year are the same across studies, and the well-constrained areas of the continent should
25 therefore also be similar. The biospheric models from the NACP RCIS included in the inter-
26 comparison are also described in more detail in Huntzinger et al. (in review).

27 Model estimates are compared at monthly and annual timescales, and at grid and
28 aggregated ecoregion and continental spatial scales. The analysis of grid-scale patterns helps to
29 visually assess model output, despite high uncertainties at this fine scale, while the comparison

1 at aggregated spatial scales helps to evaluate the quality of the biospheric models within the
2 inferred 95% uncertainty bounds from the GIM inversions. Net annual flux estimates from all
3 models are less reliable, given that they represent a small residual on a strongly-varying
4 seasonal cycle, although they are particularly important for understanding the carbon budget of
5 North America, and the locations of net sources and sinks within the continent. Overall, this
6 model inter-comparison gives insight into the CO₂ fluxes at various spatiotemporal scales and
7 the strengths and weaknesses of various model formulations. However, an important caveat is
8 that models may still agree with one another for the wrong reasons, e.g. due to systematic
9 errors in the transport models across inversion studies.

10

11 **3. Results and Discussion**

12 ***3.1 Optimized covariance parameters***

13 The monthly flux covariance parameters in **Q** provide insights into the underlying
14 variability of the flux field, and how this variability changes throughout the year, while the
15 inferred monthly model-data mismatch parameters in **R** quantify the ability of the inversion to
16 take advantage of information contained in the CO₂ mixing ratios.

17 The spatial flux covariance parameters in **Q** have a strong seasonal cycle (Figure 3),
18 consistent with that observed in biospheric model estimates (Huntzinger et al., 2011), with the
19 highest variance in July and August and the lowest in the dormant season from November
20 through April. The spatial correlation lengths are shortest during the height of the growing
21 season (~850 and ~600 km respectively for the Simple and NARR inversions in July), with
22 average values across the year of ~1700 and ~1400 km respectively. The temporal correlation
23 range varied from ~5 days in October, a time of sharp seasonal transitions across the continent,
24 to ~50 days in January, with an average value of 22 days throughout the year for both
25 inversions. In the NARR inversion, the variances and correlation lengths of the portion of the
26 flux not explained by the trend $\mathbf{X}\boldsymbol{\beta}$ are reduced relative to the Simple inversion, indicating that
27 the NARR variables explain a portion of the variability in the flux distribution.

28 The yearly weighted average of the monthly model-data mismatch variances for each
29 measurement site (or rather, the square root of this weighted average, $\sigma_{\mathbf{R}}$, with the weights

1 defined by the number of data points per month) is shown for the Simple inversion in Figure 3.
2 The tower with the highest average model-data mismatch is Harvard Forest, which is located in
3 a highly-productive forest (Urbanski et al., 2007) about 100 km west of Boston, and even closer
4 to Worcester and Springfield, Massachusetts, while the $1^\circ \times 1^\circ$ grid-cell containing this site
5 includes several other small towns and developed areas. The difficulty in matching the data at
6 this tower is likely due to spatial aggregation and representation errors associated with fossil
7 fuel emissions and heterogeneous land cover in the surrounding region. The two towers with
8 the lowest model-data mismatch are BRW and CDL, the two northernmost sites in the domain,
9 where the 1° longitudinal grid-cell size is smaller (see Figure 1). This could point to potential
10 improvements in inversion performance that would be obtained by resolving fluxes at finer
11 spatial scales, perhaps the resolution of the driving winds in the transport model (in this case
12 40-km or finer for all of North America).

13 Model-data mismatch can also have significant seasonal variations. For example, the
14 optimized model-data mismatch standard deviation at ARM is 4.7 ppm in April, 0.8 ppm in July,
15 and 0.0004 ppm in September. The high model-data mismatch in April for ARM implies that the
16 full strength of local uptake evident in the measurement data in this month (see Figure A1 in
17 the supplementary material), most likely due to the winter wheat crop planted upwind of the
18 tower (McPherson et al., 2004), is not fully represented by the inversion.

19

20 **3.2 Auxiliary variables and drift coefficients**

21 *3.2.1 Fossil fuel emissions inventory*

22 If the fossil fuel emissions inventory and atmospheric transport model used in this study
23 were perfect, the associated drift coefficient should be approximately one, whereas other
24 values could imply problems with the inversion setup, systematic transport model errors, a lack
25 of atmospheric constraint, covariance between the fossil fuel and biospheric flux signals, and/or
26 errors in the spatiotemporal patterns and magnitudes of emissions in the inventory dataset.
27 The drift coefficients for the Simple inversions were not significantly different from one
28 ($\hat{\beta} = 0.91$ and 0.95 for the EMP and CT boundary conditions, respectively, and $\sigma_{\hat{\beta}} = 0.06$ for
29 both cases), providing support both for the quality of the inventory and the inversion setup. In

1 addition, this result makes it relatively easy to separate the biospheric and fossil fuel
2 contributions to the total flux *a posteriori*.

3 3.2.2 Selected NARR variables

4 The variables selected by the BIC approach (Section 2.4 and Appendix A), and their
5 inferred relationships to CO₂ flux (Table 2) are consistent with process-based understanding of
6 the biospheric carbon cycle. For example, evapotranspiration explains the largest portion of
7 the uptake signal (as indicated by a large negative $\hat{\beta}$), which is consistent with the physiological
8 relationship between plant photosynthetic and transpiration fluxes (Bonan, 2008), and similar
9 relationships between evapotranspiration and CO₂ flux have been found in other regression
10 studies using eddy-covariance measurements (e.g. Mueller et al., 2010; Yadav et al., 2010).
11 Combining evapotranspiration estimates with basin-wide estimates of water-use efficiency has
12 also proven to be a robust method for estimating gross primary production (GPP) at watershed
13 scales (Beer et al., 2007). Canopy conductance, which has a similar mechanistic correlation
14 with photosynthesis, was not selected as a significant variable, potentially due to the difficulty
15 in up-scaling this value to landscape scales (Anderson et al., 2003).

16 The positive $\hat{\beta}$ value associated with specific humidity is consistent with known drivers
17 of heterotrophic respiration (Lloyd & Taylor, 1994; Ise and Moorcroft, 2006), given that this
18 variable, or the mass of water vapor per unit mass of air, scales with both air temperature and
19 surface moisture. The NARR specific humidity and air temperature variables have a correlation
20 coefficient of 0.83 for 2004, and, consequently the $\hat{\beta}$ uncertainties (derived from $\mathbf{V}_{\hat{\beta}}$) on these
21 two variables have a strong *a posteriori* anti-correlation (see Table B1 in the supplementary
22 material). This implies that the air temperature variable is primarily helping to correct the
23 signal associated with specific humidity. The positive $\hat{\beta}$, or source associated with precipitation
24 rate at a 3-hourly timescale is consistent with flux tower studies showing pulses of respiration
25 following rain events (Baldocchi, 2008).

26 While the selected NARR variables and inferred $\hat{\beta}$'s are consistent with process-based
27 understanding of biospheric CO₂ flux, not all processes can be easily included in a statistical
28 regression model like the one used here. For example, disturbance (e.g. storms, flooding,
29 insect infestation) may not be fully reflected in the auxiliary variables available for analysis. In

1 addition, this study only chose to examine diurnally-varying variables from the NARR, and
2 excluded other possible datasets that could help to explain fluxes at daily or weekly timescales
3 (e.g. a fire emission inventory). Third, while evapotranspiration and canopy conductance
4 implicitly incorporate a measure of live biomass, there are no variables within the NARR
5 superset that can directly represent dead substrate availability for heterotrophic respiration,
6 e.g. crop residues after agricultural harvesting or downed woody debris following a storm.
7 Finally, the NARR variables themselves have known biases and limitations (e.g. Bukovsky and
8 Karoly, 2007; West et al., 2007; Markovic et al., 2009). By design, however, any portion of the
9 flux variability that is visible in the atmospheric observations, but that cannot be represented
10 using the available auxiliary environmental datasets, can still be included in the best flux
11 estimates in GIM through the spatiotemporally-correlated stochastic component. (See
12 equation (5) in Gourdj et al., 2010, and Figure B1 in the supplementary material for an example
13 of the contribution to net grid-scale fluxes in April by each component of the best estimate).

14

15 ***3.3 Seasonal cycle of biospheric fluxes***

16 This section compares monthly biospheric fluxes from the GIM Simple and NARR
17 inversions, aggregated *a posteriori* from the fluxes estimated at the 3-hourly timescale, to
18 results from other inversion studies and from biospheric models participating in the NACP RCIS
19 (Huntzinger et al., in review). The median of the biospheric models is used to represent the
20 current consensus of the terrestrial ecosystem modeling community, although it may still be
21 subject to systematic errors across models. Although the mean has also been shown to have
22 high skill relative to individual models in previous studies (Schwalm et al., 2010), the median is
23 used here to reduce the impact of outliers. Both the mean and median showed better
24 agreement with GIM estimates than any individual biospheric model included in the inter-
25 comparison.

26 ***3.3.1 Grid-scale estimates***

27 Grid-scale spatial patterns are similar between the Simple and NARR inversion monthly
28 fluxes (Figure 4), implying that these patterns are primarily informed by the atmospheric
29 observations and spatiotemporal flux correlations, and can therefore be used to evaluate

1 biospheric model estimates. The NARR auxiliary variables add some realistic heterogeneity to
2 the grid-scale flux estimates relative to the Simple inversion, as seen by a slightly stronger
3 correspondence with the biospheric model median, particularly in under-constrained regions
4 like the Pacific coast.

5 The grid-scale GIM estimates have a stronger seasonality relative to the biospheric
6 model median, with larger sources in the winter and stronger sinks in the growing season, but
7 the locations with net uptake and release are generally consistent, especially during months
8 with net uptake. The stronger seasonality of the GIM fluxes may be due to errors in the
9 biospheric model median caused by ignoring models that show the strongest sources or sinks in
10 each month. In addition, GIM inversions that account for both the temporal and spatial
11 covariance of fluxes perform better in terms of capturing grid-scale spatial patterns, but in
12 some cases lead to stronger flux variability relative to inversions that account only for spatial
13 covariance.

14 The GIM estimates exhibit spatial patterns that are more consistent with the biospheric
15 models during the growing, relative to the dormant season. The spatial correlation coefficient
16 between the NARR inversion estimates and the biospheric model median is 0.57 and 0.48
17 respectively in April and July, compared to only 0.27 and -0.14 in January and October,
18 respectively. Similarly, results for the dormant season show a larger number of biospheric
19 models being significantly different from the GIM results in more areas of the continent (Figure
20 4, last column), where the significance is defined as a biospheric model being outside the 95%
21 confidence intervals of the GIM NARR estimates.

22 The greater similarity during the growing season is likely due to, first, both the
23 inversions and biospheric models having greater skill during periods with net uptake. The
24 increased skill during the growing season has previously been documented for biospheric
25 models in model inter-comparison studies using eddy-covariance data (e.g. Schwalm et al.,
26 2010). For inversions, this greater skill is due to the stronger atmospheric signal during this
27 season, thereby making it easier for inversions to constrain fluxes.

28 Second, errors in the magnitude or spatial patterns of the fossil fuel inventories, or an
29 inability to properly interpret fossil fuel plumes within the inversion, impact the GIM biospheric

1 fluxes. These errors would be most evident in the dormant season when fossil fuel emissions
2 represent a larger proportion of the total CO₂ flux. For example, some of the strong sources in
3 the GIM results in the south-central portion of the continent in January may be due to
4 representation errors associated with emission plumes at the Moody, Texas tower.

5 Third, most of the biospheric models in the NACP RCIS do not specifically account for
6 managed agricultural processes (i.e. fertilizer, irrigation, crop harvest and lateral transport,
7 etc.). While this would reduce model skill throughout the year in agricultural areas of the
8 continent (Lokupitiya et al., 2009; Corbin et al., 2010; Huntzinger et al., in review) and in areas
9 with a large consumption of agricultural products (e.g. by human or livestock populations), it
10 would be particularly evident in the presented October fluxes. The strong sources seen in the
11 inversions in this month reflect a strong build-up of CO₂ relative to background air at three
12 towers in heavily agricultural areas (Candle Lake, Saskatchewan, Park Falls, Wisconsin and
13 Norman, Oklahoma; see Figure A1 in the supplementary material), and are most likely
14 associated with the decay of residual biomass after crop harvesting (Johnson et al., 2006). The
15 stronger GIM sinks northwest of the Norman, Oklahoma tower in April and in the agricultural
16 Midwest during July, are also supported by process-based studies showing stronger
17 productivity in well-irrigated and fertilized agricultural croplands relative to unmanaged
18 grasslands, or the native vegetation of these areas as parameterized in many of the biospheric
19 models (Lokupitiya et al., 2009; Corbin et al., 2010; Smith et al., 2010).

20 *3.3.2 Ecoregion-scale estimates*

21 Test inversions using synthetic data showed that monthly inversion results at
22 aggregated spatial scales should be reliable in well-constrained areas of the continent (barring
23 substantial transport errors). Therefore, spatially-aggregated GIM results are compared to
24 other inversions and the biospheric models (Figure 5) for the three ecoregions presented in
25 Figure 2b, as well as for the full continent.

26 At the ecoregion scale, similarly to the grid-scale, inclusion of NARR auxiliary variables is
27 seen to have no significant impact on GIM flux estimates, consistent with results from Gourdj
28 et al. (2008). Yet, the across-model spread for both inversion studies and biospheric models at
29 these aggregated scales is quite large, and generally wider than the GIM confidence intervals

1 throughout the year, particularly in the Eastern Temperate Forest and the Temperate, Grass,
2 Savannah, Shrub ecoregions. More generally, the spread across inversion studies is smaller
3 than that seen in the biospheric models, thereby supporting the use of the atmospheric data
4 constraint to evaluate biospheric models.

5 Compared to the other inversion studies, the seasonal cycle of the GIM estimates is
6 within the spread of the other estimates. The spread across inversions is narrower in the
7 better-constrained ecoregions (i.e. Temperate Grass/ Savannah/ Shrub, and Boreal Forest),
8 pointing to the value of an expanded measurement network for reducing the impact of
9 inversion setup choices and assumptions on flux estimates. The spread between inversions is
10 also narrowest for the two largest examined regions (Boreal Forest and the full continent),
11 indicating a better constraint on flux estimates at progressively larger spatial scales, at least
12 with the limited 2004 measurement network.

13 In terms of individual inversions, GIM flux estimates are relatively similar to those from
14 CarbonTracker, particularly in the Eastern Temperate and Boreal Forests, despite significantly
15 different estimation resolutions and transport models (Table 1). The strong growing season
16 uptake in the Butler et al. (2010) study relative to the other inversions, particularly in the Boreal
17 and Eastern Temperate Forests, may be due to aggregation errors associated with using
18 measurements from highly productive areas, and extrapolating this signal too strongly across
19 that study's coarser estimation regions (see Table 1). The monthly concentration-averaging
20 intervals and flux estimation timescale used in the Butler et al. (2010) study also support this
21 conclusion. Aggregation errors could also be affecting the CarbonTracker results in the
22 Temperate Grass/ Savannah/ Shrub ecoregion, where this inversion shows stronger peak
23 uptake in July and August relative to the other studies. The Schuh et al. (2010) results show a
24 weaker seasonal cycle and an earlier peak uptake relative to the other inversions in the Eastern
25 Temperate Forests, and Temperate Grass/ Savannah/ Shrub. Among other potential factors,
26 this result could be due to a strong adherence to the seasonal cycle of the prior (SiB3), which
27 also has relatively early peak uptake in the continental U.S. relative to other biospheric models.
28 This would imply tighter prior flux uncertainties in Schuh et al. (2010) relative to the Butler et al.

1 (2010) study, where the use of CASA vs. SiB3 as a prior changes flux estimates only slightly at
2 the ecoregion scale.

3 The spread among the biospheric models is generally larger than that seen across
4 inversion studies, especially in the Temperate Grass/ Savannah/ Shrub ecoregion, which has a
5 relatively high proportion of agricultural land-cover. In this ecoregion, the GIM inversions show
6 a stronger, later peak uptake relative to the majority of the biospheric models, as well as
7 stronger sources in the dormant season, particularly in October. The lack of agreement in this
8 region may again reflect the lack of skill in modeling agricultural processes in the biospheric
9 models (Lokupitiya et al., 2009; Corbin et al., 2010). In the Eastern Temperate Forests, the GIM
10 results fall within the wide biospheric model spread. EC-MOD and MOD17+, the two biospheric
11 models with the strongest growing season uptake in the Eastern Temperate Forests, appear
12 unrealistic when compared to GIM estimates and uncertainties. In the Boreal Forests and at
13 the continental scale, the spread in the biospheric models is narrower and also more consistent
14 with the GIM results. In the Boreal Forests, all models agree reasonably well on the timing of
15 the seasonal cycle, and the biospheric model median falls within the GIM 95% confidence
16 intervals for all months. At the continental scale, the spread in both the biospheric model
17 estimates and the inversion studies is the narrowest, pointing to errors that cancel at large
18 spatial scales in both bottom-up and top-down models for the seasonal cycle.

19

20 **3.4 Net annual sources and sinks**

21 Net annual fluxes represent the small residual of a strong seasonal cycle. Therefore,
22 relatively small monthly uncertainties represent a larger proportion of the annual totals. Also,
23 any biases in the inversions or biospheric models may accumulate at longer timescales. In
24 addition, many biospheric models are specifically not designed to capture net annual sources
25 and sinks at all. For these reasons, the annual flux estimates presented here are considered to
26 be less robust than the monthly estimates.

27 **3.4.1 Grid-scale estimates**

28 Although the annual grid-scale GIM flux estimates (Figure 6) show relatively few areas
29 with statistically significant sources or sinks, the spatial patterns are quite consistent between

1 the two sets of boundary conditions and also with inventory-based estimates of CO₂ flux. The
2 GIM inversions show net annual uptake in the Eastern U.S., the midwestern agricultural areas in
3 the U.S. and Canada, and parts of the continental western U.S., which is consistent with
4 bottom-up inventory estimates from the State of the Carbon Cycle Report (SOCCR; CCSP, 2007)
5 and a recent inventory study by Hayes et al. (in press). Results for these regions are also
6 consistent with Crevoisier et al. (2010), who used an independent carbon budgeting method for
7 North America based on vertical profiles of CO₂ mixing ratios collected from aircraft
8 observations.

9 The GIM estimates show net annual sources in the southwest U.S., along the Canadian
10 Pacific Coast, and in the Yucatan peninsula of Mexico. The existence of net sources in the
11 Southwest is consistent with Hayes et al. (in press), who hypothesized that livestock and human
12 consumption of agricultural products grown elsewhere could be contributing to sources in
13 these heavily-populated but arid areas, as did Crevoisier et al. (2010). The lack of annual
14 sources in these areas in the majority of the biospheric models (results not shown) is consistent
15 with the fact that many do not explicitly account for the lateral transport of agricultural
16 products. The net sources from the Mexican tropical forests in GIM are also consistent with
17 inventory-based estimates of emissions from land-use change in this region (Cairns et al., 2000;
18 de Jong et al., 2010), while the GIM sources in the Pacific Northwest most likely represent an
19 artifact of the NARR auxiliary variables in this highly under-constrained region.

20 While inversions with the two boundary condition datasets return similar spatial
21 patterns, magnitudes differ for net annual flux estimates, with stronger sinks and weaker
22 sources evident in almost all regions with the CT relative to the EMP dataset. Most of these
23 differences at the annual timescale are due to a difference in net uptake from March through
24 August, consistent with the seasonally-varying offset between the two sets of boundary
25 conditions (see Figure A2 in the supplementary material).

26 *3.4.2 Ecoregion-scale estimates*

27 At the ecoregion scale (Figure 7), all inversions and biospheric models show a net
28 biospheric uptake in the Eastern Temperate Forests. In this region, the CarbonTracker and
29 Schuh et al. (2010) results fall within the 95% confidence intervals for 3 of the 4 geostatistical

1 inversions, while the majority of the biospheric models fall within the confidence intervals of
2 the GIM Simple inversion with EMP boundary conditions. The strong uptake of approximately
3 1PgC/yr seen here in the Butler et al. (2010) results is inconsistent with the other inversions and
4 all but two of the biospheric models, and may reflect the impact of aggregation errors, as
5 discussed previously. In the Boreal Forests, all inversion studies show net uptake, while the
6 biospheric models span both net sources and sinks. CarbonTracker and the Butler et al. (2010)
7 estimates fall within the confidence intervals of the GIM inversions with EMP and CT boundary
8 conditions, respectively, while the Schuh et al. (2010) inversion does not cover this region. In
9 the Temperate Grass/ Savannah/ Shrub ecoregion, the GIM inversions show a more neutral flux
10 relative to the other inversion models and the biospheric models. It is possible that the
11 biospheric models are under-estimating sources in this region due to their lack of skill in
12 modeling residual biomass and the fate of harvested products, as discussed previously, and the
13 other inversions would then also be biased by their use of these same biospheric models as
14 prior flux estimates. As described previously, the GIM sources in these regions in spring and fall
15 are supported by CO₂ mixing ratio time series at the tower locations, as shown in Figure A1 in
16 the supplementary material.

17 Differences across models in net annual fluxes are most evident at the continental scale
18 (Figure 7). The spread in the continental budget seen here is larger than that for the
19 continental seasonal cycle (Figure 5), although this partially reflects a difference in units
20 between Figure 7 (PgC/yr), which is not normalized by area, and Figure 5 ($\mu\text{mol}/\text{m}^2\text{s}$).

21 At this coarsest scale of comparison, the GIM results are strongly affected by the choice
22 of boundary conditions (as in Göckede et al., 2010a, which estimated fluxes for the state of
23 Oregon), where the consistent offset between these two datasets leads to an additive effect on
24 flux estimates in both space and time. With the EMP boundary conditions, GIM returns a
25 biospheric flux that is not significantly different from zero, and reduces the net North American
26 sink by approximately 0.7 to 0.9 PgC/yr relative to the GIM inversion with CT boundary
27 conditions. The CarbonTracker (Peters et al., 2007) estimates are statistically consistent with
28 the GIM inversions with CT boundary conditions at the annual continental scale, supporting the
29 conclusion that boundary conditions are the primary control on fluxes at this coarsest scale,

1 whereas flux resolution, priors, transport model and data choices, have a stronger impact at
2 sub-domain scales. An inventory-based estimate of the North American carbon balance from
3 Hayes et al. (in press) found a net biospheric uptake of 0.33 PgC/yr, which is statistically
4 consistent with the GIM Simple inversion using the EMP boundary conditions, suggesting that
5 these boundary conditions may be more realistic relative to those from CT. The main
6 conclusion, however, is that the uncertainty associated with boundary conditions must be
7 reduced if regional inversions are to be able to accurately pinpoint net biospheric uptake for
8 the entire spatial domain of interest.

9

10 **4. Conclusions**

11 The primary goal of this study was to perform an inter-comparison of North American
12 CO₂ flux estimates for a single year (2004) across inverse modeling studies and biospheric
13 models, using results from a geostatistical inversion approach as a benchmark. Fluxes were
14 quantified in the GIM inversions at a 1° x 1° spatial and 3-hourly temporal resolution, and
15 covariance parameters and process-based auxiliary information were also optimized using the
16 atmospheric data. By estimating fluxes at substantially finer scales relative to previous
17 inversions, this study reduces spatial and temporal aggregation errors associated with using
18 continental measurements sited in areas with high flux variability, and allows for the recovery
19 of sub-continental spatial patterns from the atmospheric CO₂ measurements. In addition,
20 avoiding the use of prior flux estimates from biospheric models avoids any biases caused by
21 shortcomings in process-based representations, and allows for a more independent comparison
22 to flux estimates from terrestrial ecosystem models.

23 The GIM Simple inversion, that included only a fossil fuel inventory as ancillary data,
24 yielded results that support the quality of the inventory as well as the GIM setup and
25 assumptions. Significant regional-scale spatial and temporal variability was recovered,
26 indicating that the information content of atmospheric observations is greater than implied in
27 past studies. The introduction of NARR auxiliary variables into the second, NARR inversion
28 confirmed that flux patterns in the majority of the continent are constrained by atmospheric
29 observations rather than ancillary data, although these did help to extrapolate the signal to

1 particularly poorly-constrained regions. NARR inversion results are also consistent with
2 process-based understanding of the drivers of CO₂ fluxes from photosynthesis and respiration,
3 with evapotranspiration explaining a substantial portion of the net uptake signal.

4 For the grid-scale seasonal cycle, the GIM inversions were found to have more
5 consistent spatial patterns with biospheric models during the growing relative to the dormant
6 season. This could be due to errors in the fossil fuel inventories that are aliased onto the
7 inferred fluxes, which would be more evident in the dormant season when emissions dominate
8 the total CO₂ flux, or errors in the biospheric models themselves which may have less skill
9 outside of the growing season (e.g. Schwalm et al., 2010). Finally, the fluxes during the growing
10 season are stronger and more variable, and therefore perhaps easier to identify from the
11 atmospheric signal.

12 At the ecoregion-scale, comparisons of inferred seasonal cycles across inversion studies
13 pointed to the strong impact of setup on flux estimates, particularly adherence to the bottom-
14 up prior flux estimates and aggregation errors associated with estimating fluxes at coarse-scales
15 relative to the fine-scale variability embedded in the priors. A strong atmospheric data
16 constraint reduced this impact somewhat, with inversions that estimate fluxes at different
17 spatial scales showing more consistent results in well-constrained regions, i.e. the Boreal
18 Forests and Temperate Grass/ Savannah/ Shrub. This suggests that an expanded measurement
19 network will further help to reduce the sensitivity of inversion results to setup assumptions,
20 although systematic transport model errors will still remain a concern.

21 The comparison of GIM results to the biospheric models at the ecoregion-scale pointed
22 to the need for the biospheric models to better account for crop parameterizations, land-
23 management practices, and the fate of harvested products in the agricultural areas of the
24 continent. For example, the geostatistical inversions showed strong sources in the center of
25 the continent in March and October, which were not seen in the majority of the biospheric
26 models. The fact that these sources were also absent in some of the examined inversion
27 studies may also point to the impact of these biospheric model limitations on *a posteriori* flux
28 estimates for inversions based on these models.

1 At the annual timescale, the GIM inversions showed net uptake in the Eastern
2 Temperate and Boreal Forests, but more of a neutral flux in the Temperate Grass/ Savannah/
3 Shrub. This latter result is inconsistent with other inversion studies and bottom-up models,
4 which may not have properly accounted for the fate of harvested agricultural products and
5 residual biomass. Net annual sources inferred in the Southwest are also consistent with
6 inventory-based estimates of livestock and human consumption of agricultural products in
7 these sparsely-vegetated areas.

8 While the boundary conditions used as input into regional inversions were found to
9 have only minor impact on recovered grid-scale spatial patterns, they were found to lead to
10 large differences in the GIM flux estimates at the coarsest spatial and temporal scale of
11 comparison, i.e. the annual continental scale. The use of an empirically-derived boundary
12 condition dataset eliminated the North American carbon sink for this year relative to an
13 inversion relying on model output from CarbonTracker for boundary CO₂ concentrations. This
14 result points to the importance of accurately pinpointing the CO₂ concentrations of incoming air
15 for appropriate carbon budgeting at the scale of countries in North America.

16 Overall, the North American geostatistical inversion for 2004 presented here provides a
17 robust inversion framework suitable for ingesting the large data volumes associated with the
18 recent expansion of the *in situ* CO₂ monitoring network over North America (Mueller, 2010). In
19 particular, the presented GIM approach estimates fluxes at unprecedented spatiotemporal
20 scales that help to optimally take advantage of the information contained in highly variable
21 continental measurement data. The GIM approach also provides an independent comparison
22 to bottom-up model estimates, thereby helping to provide insight into the currently large
23 spread of biospheric model estimates of regional CO₂ flux, while providing a path forward for
24 improving their formulation of processes at regional scales in future work.

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25

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1 Tables

2 Table 1: Comparison of setup and input data across published inversion studies for North
3 America in 2004.

	Domain	Spatial and temporal resolution	A priori flux covariance	Prior - biospheric	Prior – fossil fuels	Winds & transport model
Butler et al. (2010)	Global	10 sub-regions in North America, monthly	None	SiB3 (hourly) / CASA (monthly mean)	Erickson et al. (2008)	GEOS-4/PCTM
CarbonTracker 2009 (http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/)	Global	25 eco-regions in North America, weekly	Spatial covariance within ecosystem types	CASA-GFEDv2 (3-hourly)	Spatial patterns from EDGAR-4 (http://edgar.jrc.ec.europa.eu/index.php), with additional seasonal cycle	ECMWF/TM5
Schuh et al. (2010)	North America	1°x1°, weekly	Spatial covariance using fixed correlation length scales	SiB3 (hourly)	Vulcan in continental U.S. (Gurney et al., 2009); Andres et al. (1996) elsewhere	RAMS/LPDM
GIM – Simple	North America	1°x1°, 3-hourly	Monthly-varying spatial covariance using correlation length scales and variances estimated with atmospheric data	None	Vulcan in continental U.S. (Gurney et al., 2009); CDIAC/ Night Lights dataset elsewhere (Oda & Maksyutov, 2010)	WRF/STILT
GIM - NARR				Linear trend with 3-hourly NARR variables, calibrated with atmospheric data		

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2

3 Table 2: Candidate NARR environmental covariates, with associated $\hat{\beta}$ values for those
4 variables selected using BIC for inclusion in the NARR inversion with the EMP boundary
5 conditions. Auxiliary variables were normalized to zero mean and unit variance, such that $\hat{\beta}$
6 values are directly comparable. Variables with dashes ('---') were considered but not selected
7 by the BIC/ Branch & Bound algorithm. Also shown are the coefficients of variation (CV) for the
8 selected variables (i.e. $|\sigma_{\hat{\beta}}/\hat{\beta}|$).

	$\hat{\beta}$	CV
Canopy conductance	---	---
Downward shortwave radiation	---	---
Evapotranspiration	-1.16	0.05
Precipitation rate	0.28	0.13
Relative humidity	---	---
Specific humidity	0.48	0.12
Soil moisture	---	---
Air temperature (@ 2m)	-0.22	0.25
Plant canopy water content	---	---
Snow depth	---	---
Snow cover (%)	---	---
16-day average precipitation	---	---
30-day average precipitation	---	---

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10

1 **Figure captions**

2

3 *Figure 1:* Domains of nested WRF winds, flux estimation grid, and the locations of towers, flask
4 & aircraft measurements used in the inversions. See Table A1 in the supplementary material
5 for a key to the tower names.

6 *Figure 2:* a) Sensitivities of all observations used in the inversion (as shown in Table A1 in the
7 supplementary material) to flux estimates, averaged across all 3-hourly flux time periods for the
8 year for each grid-cell location. Black stars represent the nine continuous measurement
9 locations in 2004. b) Three ecoregions (modified from Olson et al., 2001) used for spatial
10 aggregation of flux estimates. These three ecoregions, along with the grey grid-cells, form the
11 domain for the aggregated North American totals in Figures 5 and 7.

12 *Figure 3, a) & b):* Optimized covariance parameters using the RML algorithm with the
13 atmospheric measurements, for the GIM inversions with the EMP boundary conditions. a)
14 Monthly flux standard deviations (σ_Q) for the Simple and NARR inversions. b) Square root of
15 the yearly average model-data mismatch variances (σ_R) (weighted by the number of data-points
16 in each month) for 9 towers, flask and aircraft data from the Simple inversion. Location
17 information for each measurement code is included in Table A1 in the supplementary material.

18 *Figure 4:* Monthly-averaged grid-scale biospheric fluxes for January, April, July and October
19 from the Simple and NARR inversions using the EMP boundary conditions, and the median of
20 biospheric models participating in the NACP RCIS. Also shown are the grid-scale spatial
21 correlation coefficients (ρ) and Root Mean Squared Difference (RMSD; $\mu\text{mol m}^{-2} \text{s}^{-1}$) between
22 the inversion and the biospheric model median fluxes. Please note the different scales for each
23 month. The plots in the right-most column show the percent of individual biospheric models
24 that are outside the 95% confidence intervals of the NARR inversion for each month and
25 location.

26 *Figure 5:* Seasonal cycle of monthly-averaged fluxes aggregated to the three well-constrained
27 ecoregions, as well as to the full continent (Figure 2b). GIM fluxes using the EMP boundary
28 conditions are compared to other inversions and individual biospheric models that have
29 coverage in at least 85% of the given regions. Inversions with the same line color use similar
30 biospheric model output for their prior flux estimates.

31 *Figure 6:* Annually-averaged grid-scale biospheric fluxes from the GIM NARR inversions using
32 the EMP and CT boundary conditions. Also shown are significant sources and sinks (at 67% and
33 95% confidence levels) for each inversion.

34 *Figure 7:* Annual biospheric flux estimates spatially aggregated to the three ecoregions and
35 North America (Figure 2b). Results from the Simple and NARR inversions using the EMP and CT

1 boundary conditions are compared to results from other inversions and the biospheric models
2 participating in the NACP RCIS. GIM results are shown within their 95% confidence intervals.

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