[Technical note] 3-hourly temporal downscaling of monthly global terrestrial biosphere model net ecosystem exchange

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Running title: 3-hourly temporal downscaling of monthly NEE

Abstract

The land surface provides a boundary condition to atmospheric forward and flux inversion models. These models require prior estimates of CO_2 fluxes at relatively high temporal resolutions (e.g., 3-hourly) because of the high frequency of atmospheric mixing and wind heterogeneity. However, land surface model CO_2 fluxes are often provided at monthly time steps, typically because the land surface modeling community focuses more on time steps associated with plant phenology (e.g., seasonal) than on sub-daily phenomena. Here, we describe a new dataset created from 15 global land surface models and 4 ensemble products in the Multi-scale Synthesis and Terrestrial Model Intercomparison Project (MsTMIP), temporally downscaled from monthly to 3-hourly output. We provide 3-hourly output for each individual model over 7 years (2004-2010), as well as an ensemble mean, a weighted ensemble mean, and the multi-model standard deviation. Output is provided in three different spatial resolutions for user preferences: 0.5° x 0.5°, 2.0° x 2.5°, and 4.0° x 5.0° (latitude/longitude). These data are publicly available from: ftp://daac.ornl.gov/data/cms/CMS_NEE_CO2_Fluxes_TBMO/data.

Keywords: CO_2 flux; downscale; land surface; NEE; sub-daily; hourly

This technical note describes the methodological approach employed with temporally downscaling monthly terrestrial biosphere model (TBM) net ecosystem exchange (*NEE*) (i.e., net CO_2 flux between the land and atmosphere) output to 3-hourly time steps (Fisher et al., 2014). These data were created initially for NASA's Carbon Monitoring System (CMS), and are useful to the broader land surface and atmospheric scientific community (Fisher et al., 2011; Fisher et al., 2012). The general downscaling approach follows Olsen and Randerson (2004) with modifications. The logic takes the components of *NEE*, i.e., gross primary production (*GPP*) and ecosystem respiration (*Re*), and links them with incident shortwave solar radiation (*I*) and near surface (2 m) air temperature (T_a), respectively. *I* and T_a are provided at 6-hourly time steps from CRU-NCEP (Wei et al., 2014a; Wei et al., 2014b), which we interpolated to 3-hourly time steps following cosines of solar zenith angle for *I* and linear interpolation for T_a. Hence, *GPP* and *Re* are temporally downscaled to 3-hourly, and re-combined to form *NEE* at 3-hourly time steps.

The 6-hourly to two 3-hourly time steps from the solar zenith angle cosine interpolation follows this equation:

$$I_{t1} = \frac{I_t \times \cos z_{t1}}{\left(\frac{\cos z_{t1} + \cos z_{t-t1}}{2}\right)}, I_{t-t1} = \frac{I_t \times \cos z_{t-t1}}{\left(\frac{\cos z_{t1} + \cos z_{t-t1}}{2}\right)} \quad (1)$$

where *z* is solar zenith angle and I_t is in units of W m^{-2}. As an example, if the 0-6 hour I_t was 100 W m^{-2}, and the 0-3 hour z_{t1} was 0 (i.e., $\cos(z_{t1}) = 1$) and the 4-6 hour z_{t-t1} was 60 (i.e., $\cos(z_{t-t1}) = 0.5$), then the 0-3 hour I_{t1} would be 133.3 W m^{-2}, and the 4-6 hour I_{t-t1} would be 66.7 W m^{-2}.

To scale *GPP* and *Re* to 3-hourly time steps, we followed Olsen and Randerson (2004) with modifications starting first with the calculation of scale factors based on *I* and T_a:

$$Q10_{3hr} = 1.5^{\frac{T_{a,3hr} - 30}{10}} \quad (2a)$$

$$T_{scale} = Q10_{3hr} \Big/ \sum_{30day} Q10_{3hr} \quad (2b)$$

$$I_{scale} = I_{3hr} \Big/ \sum_{30day} I_{3hr} \quad (3)$$

where *Q*10 is the temperature dependency of *Re*, and T_a is in degrees Celsius (converted from Kelvin, as provided by CRU-NCEP). Note that Olsen and Randerson (2004) originally used time integral periods of calendar months, but we observed that this caused unrealistic distinct shifts between months. Instead, we modified the integral period to a 30-day moving window (Figure 1). For the first 15 days of January of the record and the last 15 days of December of the record, we used the last 15 days of December and the first 15 days of January, respectively, within the first (2004) and last (2010) years to complete the 30-day window.

The 3-hourly resolution scale factors are then multiplied by *GPP* and *Re*, respectively, for each 3-hourly time step each month:

$$Re_{3hr} = T_{scale} \times Re_{month} \quad (4)$$

$$GPP_{3hr} = I_{scale} \times GPP_{month} \quad (5)$$

We modified Re_{month} and GPP_{month} from Olsen and Randerson (2004) to be given at a 3-hourly time step, linearly interpolated to 3-hourly time steps based on the present, previous, and subsequent month, maintaining the original units (g C m^{-2} mo^{-1}). Re_{3hr} and GPP_{3hr} are in units of g C m^{-2} $3hr^{-1}$. This modification avoided using the same monthly value for the multiplier for all 3-hourly time steps per month as per Olsen and Randerson (2004), and instead provided a smooth transition from one month to the next. The result of this modification was to eliminate a "ramping" effect whereby values would, for example, increase steadily within a month, then suddenly shift to a new starting point at the beginning of the next month (Figure 1). Note that the original nomenclature of Olsen and Randerson (2004) used $[(2\times NPP_{month}) - NEP_{month}]$ in place of Re_{month}, and $(2\times NPP_{month})$ in place of GPP_{month}, where *NPP* is net primary production (*GPP* minus autotrophic respiration) and *NEP* is net ecosystem production (approximately equivalent to the inverse sign of *NEE*, with caveats (Hayes and Turner, 2012)). The assumption here, therefore, is that $GPP = 2\times NPP$ and $Re = (2\times NPP) - NEP$. The Re assumption misses CO_2 emissions other than respiration, e.g., fire, which we correct for at a later step.

The initial *NEE* calculation simply subtracts *GPP* from *Re*:

$$NEE_{3hr} = Re_{3hr} - GPP_{3hr} \quad (4)$$

where NEE_{3hr} is calculated in units of g C m^{-2} $3hr^{-1}$. However, we applied an additional units conversion for the publicly available data to kg C km^{-2} s^{-1}, as these units are more readily ingestible by atmospheric inversion models (Deng et al., 2014).

Because the downscaling approach uses *Re* (e.g., autotrophic plus heterotrophic respiration) as the primary CO_2 efflux term, other ecosystem CO_2 loss components, such as fire and other disturbances (Hayes and Turner, 2012), are excluded in the downscale. Hence, the sum of the downscaled 3-hourly *NEE* fluxes in a given month did not necessarily equal the original monthly *NEE* flux. So, we included a per-pixel correction whereby we: I) calculated the difference between the sum of the downscaled 3-hourly *NEE* in a given month and the original monthly *NEE*; II) divided that difference by the total 3-hourly time steps in the month, and III) added that difference to each 3-hourly *NEE* flux. In so doing, the sum of the downscaled 3-hourly *NEE* fluxes subsequently summed exactly to the original monthly *NEE*. Nonetheless, this assumption smooths what could otherwise be punctuated fire or disturbance effluxes, so caution should be given when assessing these effluxes at 3-hourly time steps (e.g., relative to observations).

All input data were given in a spatial resolution of 0.5° x 0.5° (latitude/longitude); hence, we provide the 3-hourly *NEE* output in 0.5° x 0.5° (Figure 2). We also provide two additional sets of spatially upscaled *NEE* output in 2.0° x 2.5° and 4.0° x 5.0°. These resolutions are used by the atmospheric modeling community, i.e., the GEOS-Chem atmospheric CO_2 transport model in the NASA CMS (Liu et al., 2014). To generate the coarser resolution data we: I) multiplied each pixel value by the land area of that pixel; II) summed the flux from all pixels that represent one pixel in coarser resolution (e.g., 8 x 10 pixels from 0.5° x 0.5° comprise 1 pixel in 4.0° x 5.0°); III) calculated the total area covered by the pixels summed in step II; and, IV) divided the value in step II by the value in step III. The regridding preserved the total sum flux of the finer grid cells as well as the total global flux. We provide a file containing the land area contained in each latitudinal band for each of the 3 resolutions (folder name: 'latitude_area'). We provide two versions of the 2.0° x 2.5° and 4.0° x 5.0° resolution products—one version with consistent global resolution, and another that conforms to the GEOS-Chem setup whereby the northern and southern most latitudinal bands for the 2.0° x 2.5° resolution are 1.0° x 2.5°, and for the 4.0° x 5.0° they are 2.0° x 5.0°. The orientation of the global grid in the NetCDF files is transposed (i.e., 90°S x 180°W at top-left). The time vector represents the mid-point of each 3-hourly period.

Processing time in R, un-parallelized, on a standard PC for a single year for the forcing data was as follows:

- Interpolation of 6-hourly I and T_a to 3-hourly time step: 1 hr per variable
- 30-day moving window for I: 48 hr
- 30-day moving window for T_a: 68 hr
- *Total time to process forcing data for 7 years: 7*(1*2+48+68) = 826 hr*

Processing time for the application of the modified Olsen and Randerson (2004) downscaling approach for a single model for a single year was:

- Monthly interpolation to 3-hourly time steps for *GPP*: 1 hr
- Monthly interpolation to 3-hourly time steps for *Re*: 1 hr
- *GPP* and *Re* downscaling: 2 hr
- Monthly *NEE* closure correction: 1 hr
- NetCDF generation with additional spatial resolutions: 2 hr
- *Total time to process all 19 products for 7 years: 7*19*(1+1+2+1+2) = 931 hr*

The total storage size of the final NetCDF data products for all 19 products (15 models + 4 ensemble products) for all 7 years is: 374 GB at 0.5° x 0.5°, 38 GB at 2.0° x 2.5°, and 10 GB at 4.0° x 5.0°.

We provide the data in NetCDF with a separate file for each day per product at ftp://daac.ornl.gov/data/cms/CMS_NEE_CO2_Fluxes_TBMO/data (Fisher et al., 2016). Each file contains the global gridded data with the eight 3-hourly intervals in the day. Open water pixels are set to 0, as this was desired by the atmospheric modeling community. However, we realize that *NEE* values can conceivably be 0 (though unlikely as our precision is to 16 decimal places); nonetheless, there are some pixels over land that are calculated as 0, but this is due to missing forcing data (e.g., I in the high latitudes during winter). Our code is set up that we can easily provide a different file output structure and missing value mask by request (contact the corresponding author: jbfisher@jpl.nasa.gov).

Model output (*GPP*, *Re*, and *NEE*) was from the Multi-scale Synthesis and Terrestrial Model Intercomparison Project (MsTMIP) (Huntzinger et al., 2013; Huntzinger et al., 2016), version 1. 15 models were included: 1) BIOME_BGC, 2) CLM, 3) CLM4VIC, 4) CLASS_CTEM, 5) DLEM, 6) GTEC, 7) ISAM, 8) LPJ-wsl, 9) ORCHIDEE, 10) SIB3, 11) SIBCASA, 12) TEM6, 13) TRIPLEX-GHG, 14) VEGAS2.1, and 15) VISIT (Table 1). All models were driven by CRU-NCEP meteorological forcing data, hence our use of the same data source for the downscaling approach applied here. We note that there are other meteorological forcing datasets also available at 3-hourly time steps for those interested in applying our downscaling approach with different data (Sheffield et al., 2006; Weedon et al., 2011; Weedon et al., 2014). Although some models are capable of output at sub-monthly time steps, the standard MsTMIP output is at the monthly time step. Additionally, 4 ensemble products were included: 1) un-weighted (naïve) ensemble mean, 2) un-weighted (naïve) ensemble standard deviation, 3) weighted (optimal) ensemble mean, and 4) weighted (optimal) ensemble standard deviation. Weights for model ensemble integration were derived based on model skill in reproducing *GPP* and biomass (Schwalm et al., 2015). Model output was obtained from: ftp://nacp.ornl.gov/synthesis/2009/reutlingen/CMS/20141006/

To test and confirm that our downscaling approach was applied correctly, we tested our method on a set of ground-truth data of measured *NEE* (and forcing variables) from the FLUXNET database (Baldocchi et al., 2001). We show, for example, a single year for a single site (3-hourly in background with daily-moving window overlaid) (Figure 3) and the scatterplot of calculated versus observed *NEE* values at the 3-hourly time step for that site and year (Figure 4). A full uncertainty analysis of the approach is beyond the scope of this technical note intended to describe the methodological detail of the downscaling.

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Model	Reference
BIOME_BGC	Thornton et al. (2002)
CLM	Mao et al. (2012)
CLM4VIC	Lei et al. (2014)
CLASS_CTEM	Huang et al. (2011)
DLEM	Tian et al. (2012)
GTEC	Ricciuto et al. (2011)
ISAM	Jain and Yang (2005)
LPJ-wsl	Sitch et al. (2003)
ORCHIDEE	Krinner et al. (2005)
SIB3	Baker et al. (2008)
SIBCASA	Schaefer et al. (2008)
TEM6	Hayes et al. (2011)
TRIPLEX-GHG	Peng et al. (2002)
VEGAS2.1	Zeng et al. (2005)
VISIT	Ito (2010)

Table 1. Global terrestrial biosphere models from the Multi-scale Synthesis and Terrestrial Model Intercomparison Project (MsTMIP) downscaled in this activity.

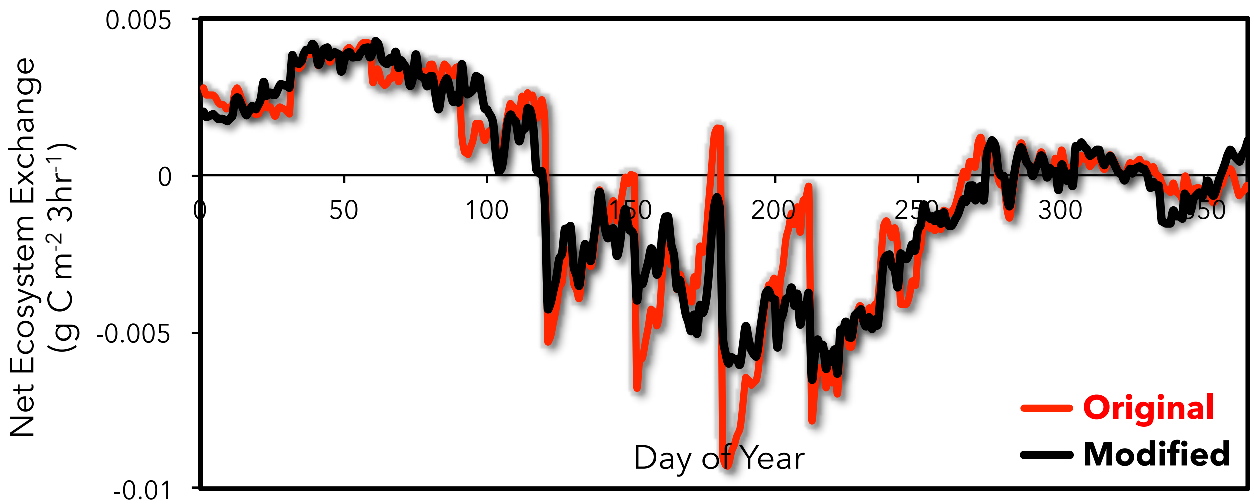

Figure 1.The original downscaling approach of Olsen and Randerson (2004) used monthly fixed values, which led to a "stair-stepping" behavior between months (red). This was eliminated by using a 30-day moving window and interpolating monthly input values to 3-hourly time steps (black). Example shown for LPJ model global mean year 2005.

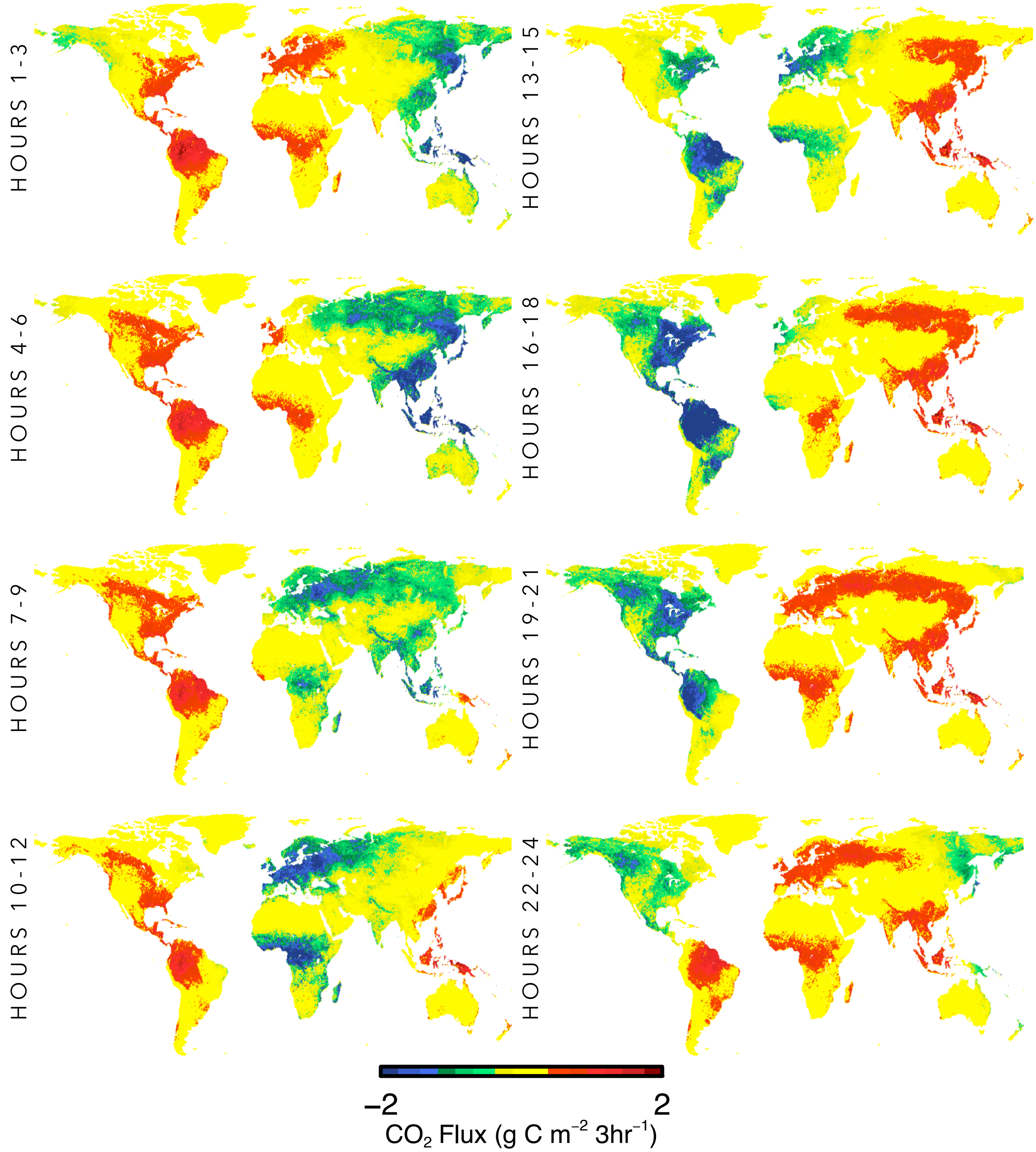

Figure 2. Vegetation productivity (e.g., blues/greens) follows the course of the sun for a single day of net ecosystem exchange (NEE or net CO_2 flux; g C m^{-2} $3hr^{-1}$) for each 3-hourly period. Shown here, for example, is July 1, 2007 for the weighted ensemble mean product.

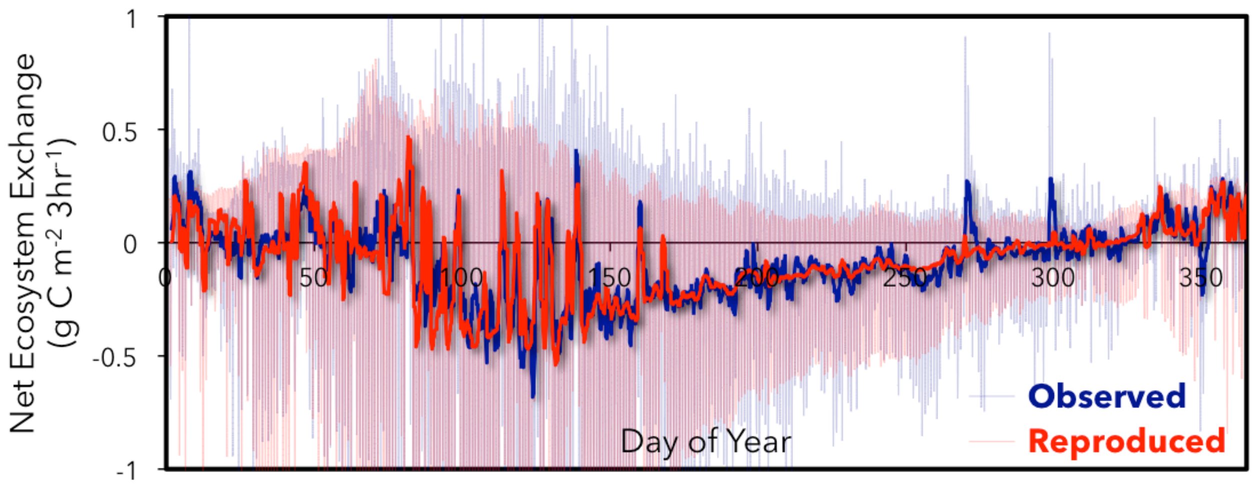

Figure 3. The observed net ecosystem exchange (NEE) (blue) and reproduced NEE (red) shown at the 3-hourly time step with daily moving window overlaid for a single year from the Tonzi Ranch AmeriFlux/FLUXNET site (Baldocchi and Ma, 2013).

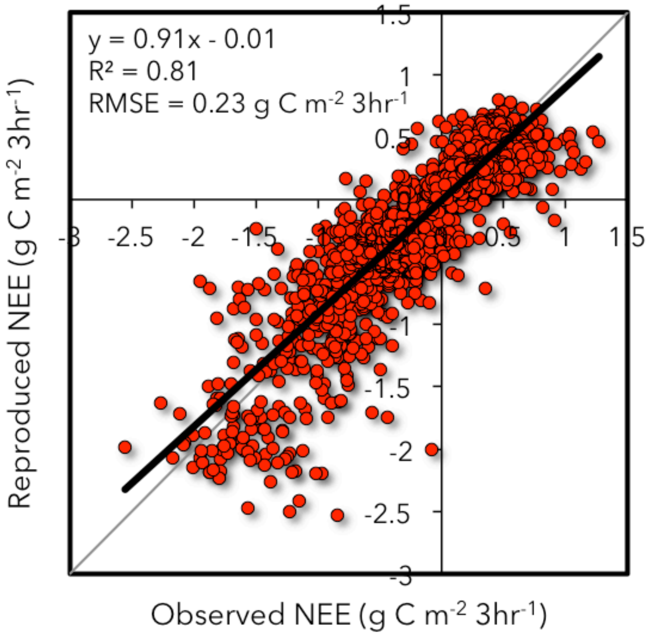

Figure 4. Observed versus reproduced net ecosystem exchange (NEE) at the 3-hourly time step for a single year at the Tonzi Ranch AmeriFlux/FLUXNET site (Baldocchi and Ma, 2013).