

Figure S1. Simulated and observed land-atmosphere fluxes of A) gross primary production (GPP) B) ecosystem respiration (ER) and C) latent heat (LE) for the *limited nitrogen* simulation. The ‘observations’ are taken from the Ameriflux L2 processed eddy covariance flux tower data, partitioned into GPP and ER using the method of Reichstein et al. (2005). The *uncalibrated* simulation represents the CLM simulation without  $V_{cmax}$  scaling and the *calibrated* simulation represents the CLM run using the  $V_{cmax}$  scaling approach.

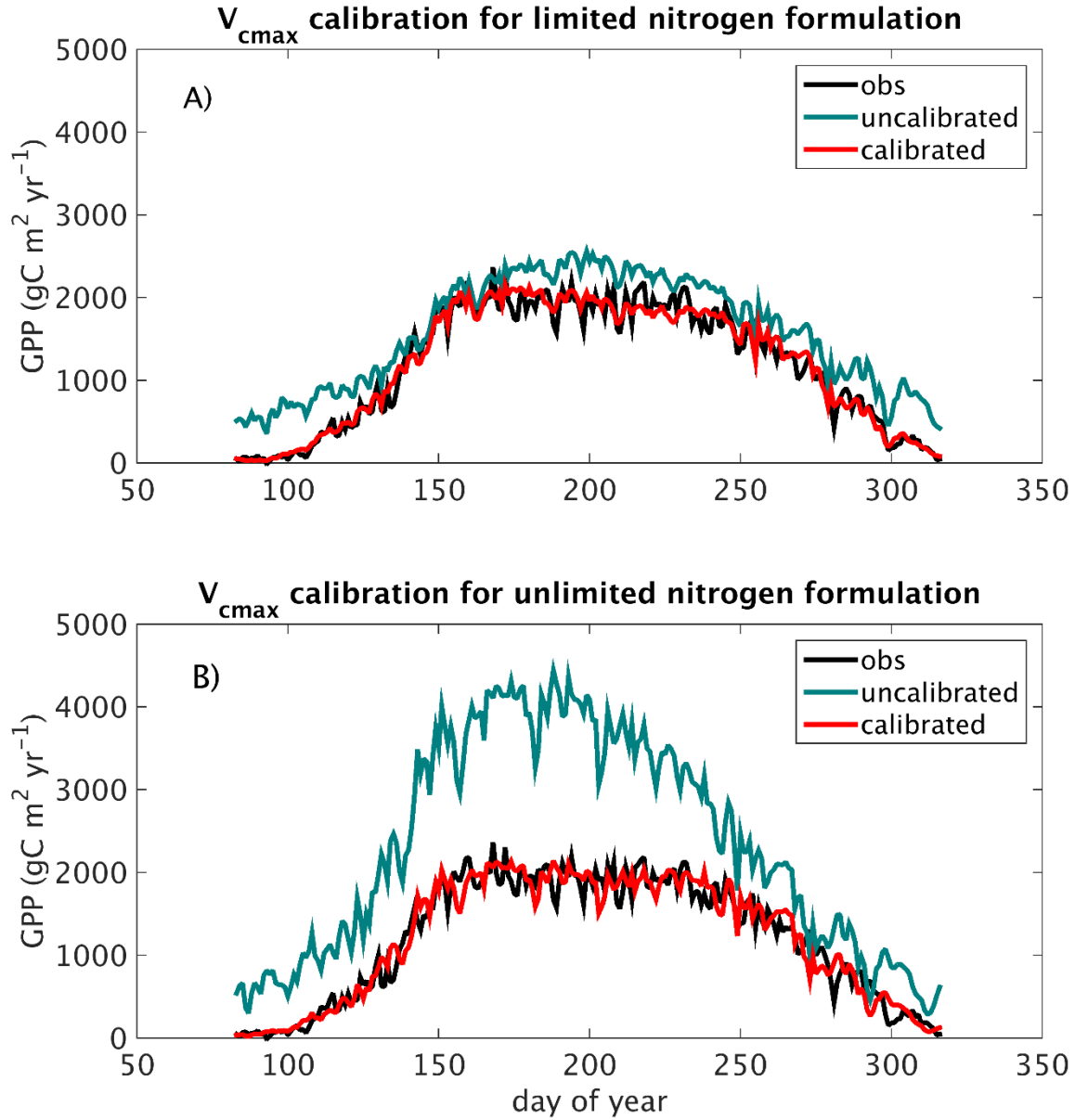


Figure S2. Calibrated and uncalibrated simulations for the *limited nitrogen* formulation (panel A) and *unlimited nitrogen* formulation (panel B). The *limited nitrogen* calibrated run used the  $V_{cmax25}$  calibration parameter: (equation (S1))  $f_{df} = (1.09 \times 10^{-12})x^6 - (1.351 \times 10^{-9})x^5 + (6.722 \times 10^{-7})x^4 - (1.709 \times 10^{-4})x^3 + (2.324 \times 10^{-2})x^2 - (1.584)x + 42.31$ , where  $x$  represents the day of the year. The *unlimited nitrogen* calibrated run used the  $V_{cmax25}$  calibration parameter: (equation (S2))  $f_{df} = (5.01 \times 10^{-13})x^6 - (6.258 \times 10^{-10})x^5 + (3.105 \times 10^{-7})x^4 - (7.803 \times 10^{-5})x^3 + (1.041 \times 10^{-2})x^2 - (0.690)x + 17.93$ .

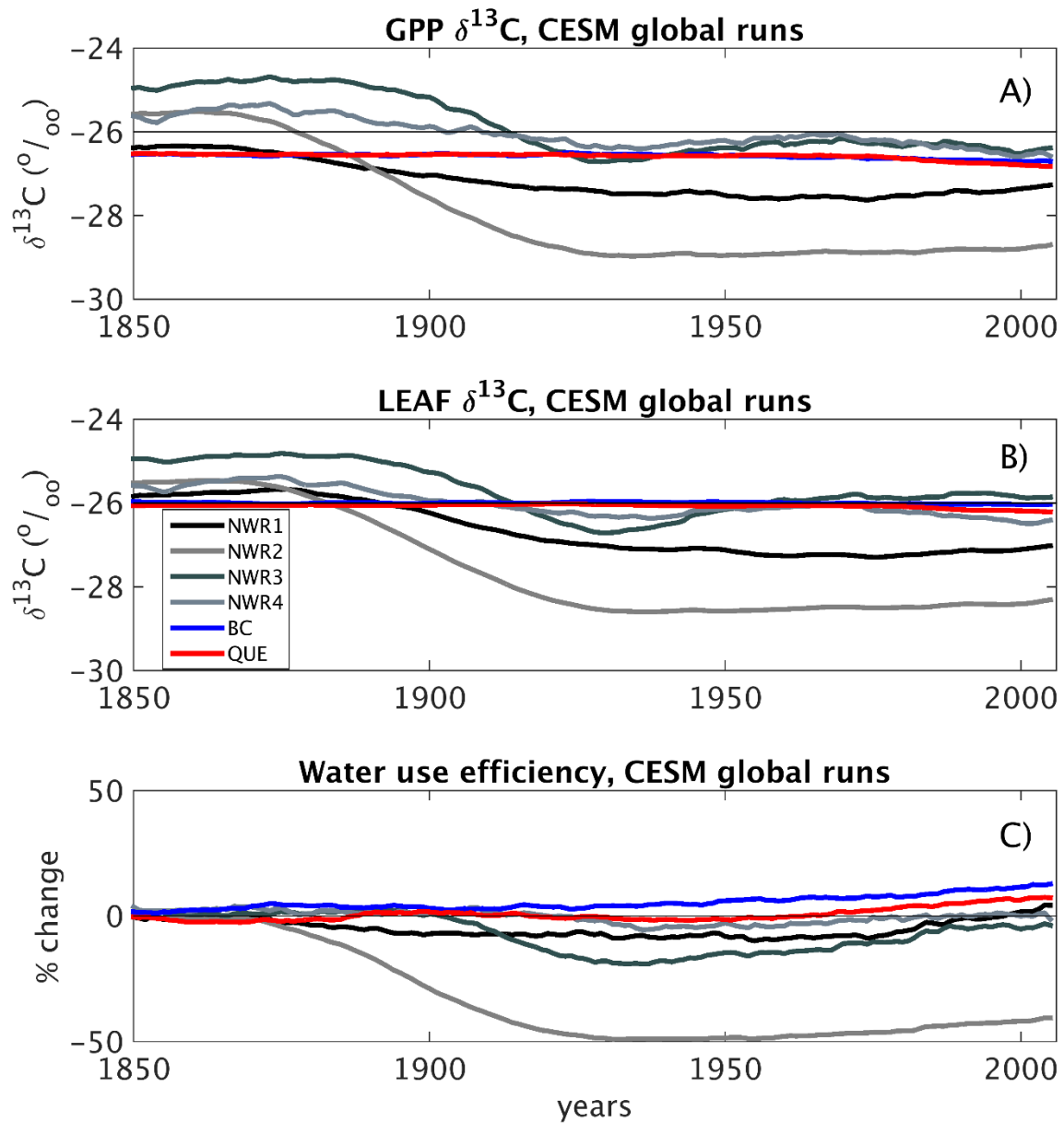


Figure S3. Global CESM1.2 simulation output based upon fully coupled isotope enabled experiment with CAM5 and CLM45BGC (courtesy Keith Lindsay, NCAR) for A)  $\delta^{13}\text{C}$  of GPP B)  $\delta^{13}\text{C}$  of leaves and C) water-use efficiency. NWR1 represents model output from a grid cell that is collocated with coordinates of the site Niwot Ridge (40.0329° N, -105.5464° W), NWR2, NWR3 and NWR4 represent grid cells adjacent to NWR1 and closest to the Niwot Ridge spatial coordinates. QUE and BC represent grid cells of coniferous forest located in Quebec (49.5° N, -70.0° W) and British Columbia (52.3° N, -122.5° W) respectively.

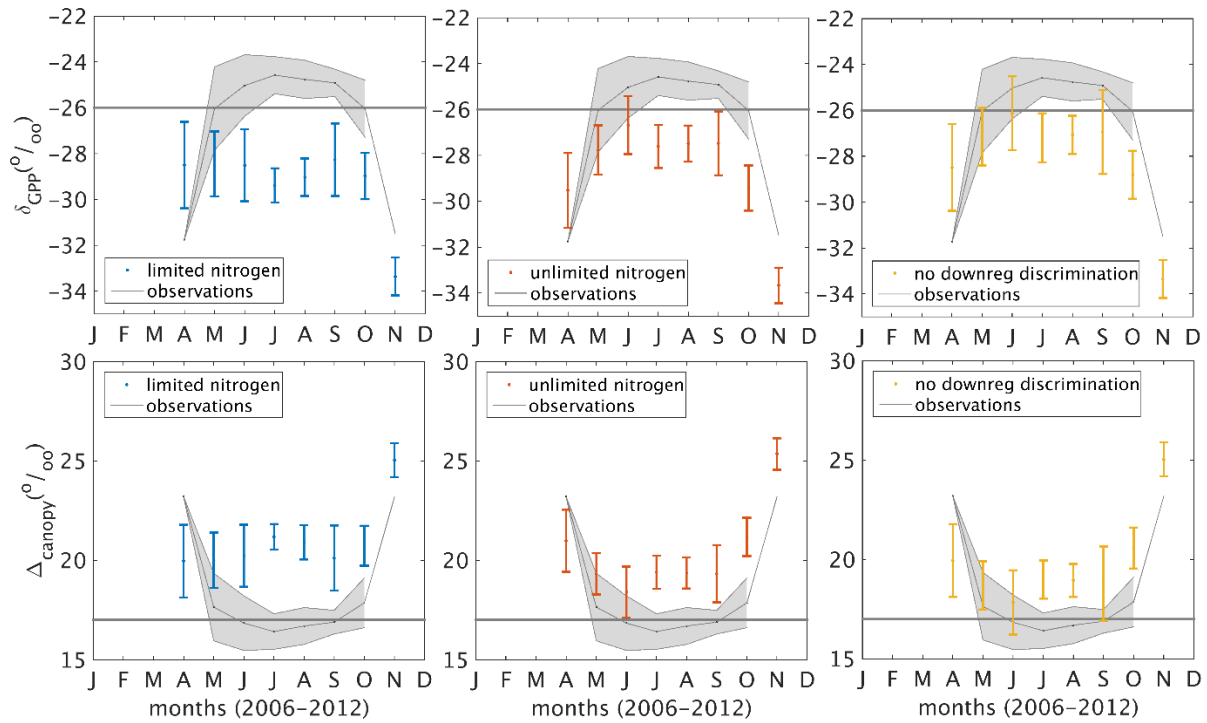


Figure S4. The seasonal photosynthetic discrimination pattern as shown through  $\delta_{GPP}$  (panels A, B and C) and  $\Delta_{canopy}$  (panels D, E and F). Colored uncertainty bars represent 95% confidence bounds of simulated monthly average values from 2006-2012. Gray-shaded observation bounds represent 95% confidence intervals of ‘observed’ monthly average values based upon isotopic mixing model using Lasslop et al., (2010) partitioning of net ecosystem exchange flux (Bowling et al. 2014). Horizontal lines represent  $\delta^{13}C$  of -26 ‰ (panels A, B and C) and 17 ‰ (panels D, E and F) and are included for reference.

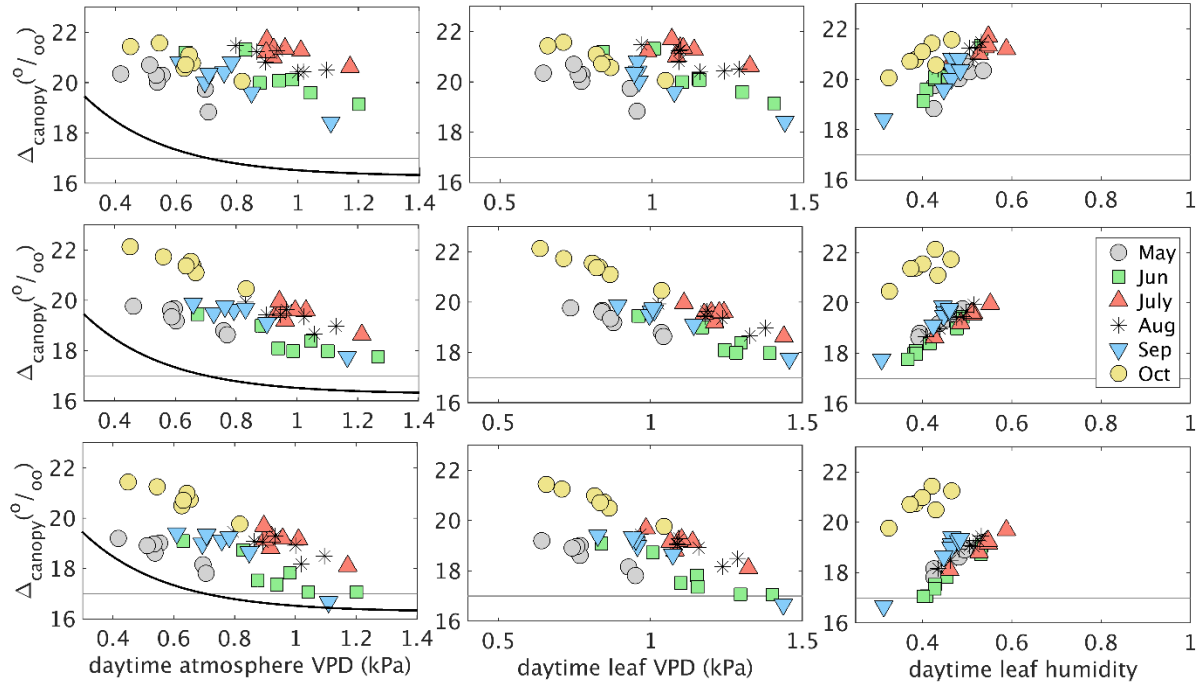


Figure S5. Relationship between monthly average photosynthetic discrimination and monthly average daytime atmosphere VPD (panels A, B and C), leaf VPD (panels D, E and F) and leaf humidity (panels G, H and I) from 2006-2012. The rows represent the *limited nitrogen* (panels A, D and G), *unlimited nitrogen* (panels B, E and H), and *no downregulation discrimination* (panels C, F and I) simulations. The black line in the 1<sup>st</sup> column is based on exponential fitted line from observed relationship at Niwot Ridge (Bowling et al. 2014). The horizontal lines represent  $\delta^{13}\text{C}$  of 17 ‰ and are included for reference.

## Supplement continued

### Derivation of relationship between iWUE and $c_i/c_a$ (discrimination)

Starting with Equation (9) and ending with Equation (17) from main text:

$$c_i^* = c_a - A_n (1 - f_{dreg}) P_{atm} \frac{(1.4g_s) + (1.6g_b)}{g_b g_s}$$

Assume  $f_{dreg} = 0$  for simplicity:

$$c_i^* = c_a - A_n P_{atm} \frac{(1.4g_s) + (1.6g_b)}{g_b g_s}$$

$$\frac{c_i^*}{P_{atm}} = \frac{c_a}{P_{atm}} - A_n \frac{(1.4g_s) + (1.6g_b)}{g_b g_s}$$

$$c_{i \text{ mole fraction}}^* = c_{a \text{ mole fraction}} - A_n \frac{(1.4g_s) + (1.6g_b)}{g_b g_s}$$

$$\frac{c_{i \text{ mole fraction}}^*}{c_{a \text{ mole fraction}}} = 1 - \frac{A_n}{c_{a \text{ mole fraction}}} \frac{(1.4g_s) + (1.6g_b)}{g_b g_s}$$

Removing 'mole fraction' subscript for simplicity:

$$\frac{c_i^*}{c_a} = 1 - \frac{A_n}{c_a} \frac{(1.4g_s) + (1.6g_b)}{g_b g_s}$$

$$\frac{c_i^*}{c_a} = 1 - \frac{A_n}{c_a} \left( \frac{1.4}{g_b} + \frac{1.6}{g_s} \right)$$

Because  $g_b \gg g_s$ , therefore,  $\frac{1.4}{g_b} \ll \frac{1.6}{g_s}$

$$\frac{c_i^*}{c_a} \cong 1 - \frac{A_n}{c_a} \left( \frac{1.6}{g_s} \right)$$

$$\frac{c_i^*}{c_a} \cong 1 - \frac{1.6}{c_a} iWUE$$

## **Methodological Details.**

### **Site-specific atmospheric CO<sub>2</sub> concentration time series:**

Observations were used to create the synthetic product from 1968-2013 by binning flask observations into 20 evenly spaced points each year. These flask observations were taken weekly from Niwot Ridge (Dlugokencky et al., 2015). Prior to 1968, a polynomial fit of the annualized CLM product was created and then adjusted by 1.5 ppm to account for the average difference between the CLM product and the Niwot Ridge observations during those years. Next, the average multi-year seasonal cycle based on the de-trended flask data after 1968 was added to every year of this annualized polynomial before 1968. Finally, the synthetic atmospheric CO<sub>2</sub> time series (pre 1968) was populated with 20 evenly spaced points in time each year.

### **Site-specific $\delta^{13}\text{C}$ atmospheric CO<sub>2</sub> time series:**

After 1990 the flask data were binned into 20 evenly spaced points each year. Prior to 1990 the inter-annual variation was based upon a polynomial fit to ice core data from Law Dome (Francey et al., 1999; see also Rubino et al., 2013). The polynomial was adjusted by 0.20 ‰ to account for the inter-hemispheric difference identified during the common years (1990-1996) between the ice core and flask data. Next the average seasonal cycle (1990-2013) of  $\delta_{atm}$  was added to the adjusted polynomial prior to 1990. The synthetic time series was populated from 1850-1989 with 20 evenly spaced points each year based upon the adjusted polynomial with seasonal cycle included. As released, CLM 4.5 was not compatible with time varying  $\delta_{atm}$ , therefore we modified the source code by following the model procedure for reading in time-varying  $^{14}\text{C}$ . The modified code was designed to temporally interpolate the  $\delta_{atm}$  time series for each time step of the model. This interpolated value was then passed into the photosynthetic discrimination calculation to represent the time-varying  $\delta_{atm}$ .