The Yale Interactive terrestrial Biosphere Model version 1.0: description,
 evaluation and implementation into NASA GISS ModelE2
 X. Yue and N. Unger
 School of Forestry and Environment Studies, Yale University, New Haven, Connecticut
 06511, USA
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#### Abstract

11 The land biosphere, atmospheric chemistry and climate are intricately interconnected yet 12 the modeling of carbon-climate and chemistry-climate interactions have evolved as entirely separate research communities. We describe the Yale Interactive terrestrial 13 14 **B**iosphere (YIBs) model version 1.0, a land carbon cycle model that has been developed 15 for coupling to the NASA Goddard Institute for Space Studies (GISS) ModelE2 global 16 chemistry-climate model. The YIBs model adapts routines from the mature TRIFFID and 17 CASA models to simulate interactive carbon assimilation, allocation, and autotrophic and 18 heterotrophic respiration. Dynamic daily leaf area index is simulated based on carbon 19 allocation and temperature- and drought-dependent prognostic phenology. YIBs 20 incorporates a semi-mechanistic ozone vegetation damage scheme. Here, we validate the present day YIBs land carbon fluxes for three increasingly complex configurations: (i) 21 22 off-line local site-level (ii) off-line global forced with WFDEI (WATCH Forcing Data 23 methodology applied to ERA-Interim data) meteorology (iii) on-line coupled to the 24 NASA ModelE2 (NASA ModelE2-YIBs). Off-line YIBs has hourly and on-line YIBs has 25 half-hourly temporal resolution. The large observational database used for validation 26 includes carbon fluxes from 145 flux tower sites and multiple satellite products. At the 27 site level, YIBs simulates reasonable seasonality (correlation coefficient R > 0.8) of gross 28 primary productivity (GPP) at 121 out of 145 sites with biases in magnitude ranging from -19% to 7% depending on plant functional type. On the global scale, the off-line model 29 30 simulates an annual GPP of  $125 \pm 3$  petagrams of carbon (Pg C) and net ecosystem 31 exchange (NEE) of  $-2.5 \pm 0.7$  Pg C for 1982-2011, with seasonality and spatial 32 distribution consistent with the satellite observations. We assess present day global ozone 33 vegetation damage using the off-line YIBs configuration. Ozone damage reduces global 34 GPP by 2-5% annually with regional extremes of 4-10% in East Asia. The on-line model 35 simulates annual GPP of  $123 \pm 1$  Pg C and NEE of  $-2.7 \pm 0.7$  Pg C. NASA ModelE2-36 YIBs is a useful new tool to investigate coupled interactions between the land carbon 37 cycle, atmospheric chemistry, and climate change.

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39 *Keywords*: terrestrial biosphere model, carbon cycle, photosynthesis, ozone, phenology,

40 gross primary productivity, net ecosystem exchange

#### 41 **1. Introduction**

42 The terrestrial biosphere interacts with the atmosphere through the exchanges of energy, 43 carbon, reactive gases, water, and momentum fluxes. Forest ecosystems absorb an 44 estimated 120 petagrams of carbon (Pg C) per year from the atmosphere (Beer et al., 45 2010) and mitigate about one quarter of the anthropogenic carbon dioxide (CO<sub>2</sub>) 46 emissions (Friedlingstein et al., 2014). This carbon assimilation is sensitive to human-47 caused perturbations including climate change and land use change (Zhao and Running, 48 2010; Houghton et al., 2012), and is affected by atmospheric pollutants such as ozone and 49 aerosols (Sitch et al., 2007; Mercado et al., 2009). Over the past 2-3 decades, a number of 50 terrestrial biosphere models have been developed as tools to quantify the present-day 51 global carbon budget in conjunction with available but sparse observations (e.g., Jung et 52 al., 2009), to understand the relationships between terrestrial biospheric fluxes and 53 environmental conditions (e.g., Zeng et al., 2005), to attribute drivers of trends in the 54 carbon cycle during the anthropogenic era (e.g., Sitch et al., 2015), and to project future 55 changes in the land biosphere and the consequences for regional and global climate 56 change (e.g., Friedlingstein et al., 2006).

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58 Emerging research identifies climatically-relevant interactions between the land 59 biosphere and atmospheric chemistry (e.g., Huntingford et al., 2011). For instance, 60 stomatal uptake is an important sink of tropospheric ozone (Val Martin et al., 2014), but 61 damages photosynthesis, reduces plant growth and biomass accumulation, limits crop 62 yields, and affects stomatal control over plant transpiration of water vapor between the 63 leaf surface and atmosphere (Ainsworth et al., 2012; Hollaway et al., 2012). The indirect 64 CO<sub>2</sub> radiative forcing due to the vegetation damage effects of anthropogenic ozone increases since the industrial revolution may be as large as +0.4 W m<sup>-2</sup> (Sitch et al., 65 2007), which is 25% of the magnitude of the direct  $CO_2$  radiative forcing over the same 66 67 period, and of similar magnitude to the direct ozone radiative forcing. Atmospheric 68 oxidation of biogenic volatile organic compound (BVOC) emissions affects surface air 69 quality and exerts additional regional and global chemical climate forcings (Scott et al., 70 2014; Unger, 2014a, b). Fine mode atmospheric pollution particles affect the land 71 biosphere by changing the physical climate state and through diffuse radiation 72 fertilization (Mercado et al., 2009; Mahowald, 2011). Land plant phenology has 73 experienced substantial changes in the last few decades (Keenan et al., 2014), possibly 74 influencing both ozone deposition and BVOC emissions through the extension of growing seasons. These coupled interactions are often not adequately represented in 75 76 current generation land biosphere models or global chemistry-climate models. Global 77 land carbon cycle models often prescribe off-line ozone and aerosol fields (e.g., Sitch et 78 al., 2007; Mercado et al., 2009), and global chemistry-climate models often prescribe fixed off-line vegetation fields (e.g., Lamarque et al., 2013; Shindell et al., 2013a). 79 80 However, multiple mutual feedbacks occur between vegetation physiology and reactive 81 atmospheric chemical composition that are completely neglected using these previous 82 off-line approaches. Model frameworks are needed that fully 2-way couple the land 83 carbon cycle and atmospheric chemistry, and simulate the consequences for climate 84 change.

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86 Our objective is to present the description and present-day evaluation of the Yale 87 Interactive terrestrial Biosphere (YIBs) model version 1.0 that has been developed for the 88 investigation of carbon-chemistry-climate interactions. The YIBs model can be used in 89 three configurations: (i) off-line local site-level (ii) off-line global forced with WFDEI 90 (WATCH Forcing Data methodology applied to ERA-Interim data) meteorology (iii) on-91 line coupled to the latest frozen version of the NASA GISS ModelE2 (Schmidt et al., 92 2014). The global climate model represents atmospheric gas-phase and aerosol chemistry, 93 cloud, radiation, and land surface processes, and has been widely used for studies of 94 atmospheric components, climate change, and their interactions (Schmidt et al., 2006; 95 Koch et al., 2011; Unger, 2011; Shindell et al., 2013b; Miller et al., 2014). To our 96 knowledge, this study represents the first description and validation of an interactive 97 climate-sensitive closed land carbon cycle in NASA ModelE2. The impacts of the 98 updated vegetation scheme on the chemistry and climate simulations in NASA ModelE2 99 will be addressed in other on-going research. Section 2 describes the observational 100 datasets used to evaluate YIBs land carbon cycle performance. Section 3 describes 101 physical parameterizations of the vegetation model. Section 4 explains the model set up

and simulations in three configurations. Section 5 presents the results of the modelevaluation and section 6 summarizes the model performance.

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#### 105 **1.1 YIBs design strategy**

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107 Many land carbon cycle models already exist (e.g. Sitch et al., 2015 and references 108 therein; Schaefer et al., 2012 and references therein). We elected to build YIBs in a step-109 by-step process such that our research group has intimate familiarity with the underlying 110 scientific processes, rather than adopting an existing model as a "black box". This 111 unconventional interdisciplinary approach is important for discerning the complex mutual 112 feedbacks between atmospheric chemistry and the land carbon sink under global change. The development of YIBs land carbon cycle model has proceeded in three main steps. 113 114 The first step was the implementation of vegetation biophysics, photosynthesis-dependent 115 BVOC emissions and ozone vegetation damage that have been extensively documented, 116 validated and applied in 7 previous publications (Unger, 2013; Unger et al., 2013; Unger, 117 2014a, b; Unger and Yue, 2014; Yue and Unger, 2014; Zheng et al., 2015). The second 118 step was the selection of the YIBs default phenology scheme based on rigorous inter-119 comparison of 13 published phenological models (Yue et al., 2015a). This study 120 represents the third step to simulate the closed climate-sensitive land carbon cycle: 121 implementation of interactive carbon assimilation, allocation, autotrophic and 122 heterotrophic respiration, and dynamic tree growth (changes in both height and LAI). For 123 this third step, we purposefully select the mature, well-supported, well-established, 124 readily available and accessible community algorithms: TRIFFID (Cox, 2001; Clark et 125 al., 2011) and the Carnegie-Ames-Stanford Approach (CASA) (Potter et al., 1993; 126 Schaefer et al., 2008). TRIFFID has demonstrated previous usage in carbon-chemistry-127 climate interactions research.

- 128
- 129 **2.** Observational datasets for validation
- 130

131 **2.1 Site-level measurements** 

132 To validate the YIBs model, we use eddy covariance measurements from 145 flux tower 133 sites (Fig. 1), which are collected by the North American Carbon Program (Schaefer et 134 al., 2012) (K. Schaefer, personal communication) and downloaded from the FLUXNET (http://fluxnet.ornl.gov) network. Among these sites, 138 are located in the Northern 135 136 Hemisphere, with 74 in Europe, 38 in U.S., and 24 in Canada (Table S1). Sites on other 137 continents are limited. Most of the sites have one dominant plant functional type (PFT), 138 including 54 sites of evergreen needleleaf forests (ENF), 20 deciduous broadleaf forests 139 (DBF), 9 evergreen broadleaf forests (EBF), 28 grasslands, 18 shrublands, and 16 140 croplands. We attribute sites with mixed forest to the ENF as these sites are usually at high latitudes. Each site dataset provides hourly or half-hourly measurements of carbon 141 142 fluxes, including gross primary productivity (GPP) and net ecosystem exchange (NEE), and CO<sub>2</sub> concentrations and meteorological variables, such as surface air temperature, 143 144 relative humidity, wind speed, and shortwave radiation.

- 145
- 146 **2.2 Global measurements**
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148 We use global tree height, leaf area index (LAI), GPP, net primary productivity (NPP), 149 and phenology datasets to validate the vegetation model. Canopy height is retrieved using 150 2005 remote sensing data from the Geoscience Laser Altimeter System (GLAS) aboard 151 ICESat satellite (Simard et al., 2011). LAI measurements for 1982-2011 are derived using the Normalized Difference Vegetation Index (NDVI) from Global Inventory 152 153 Modeling and Mapping Studies (GIMMS) (Zhu et al., 2013). Global GPP observations of 154 1982-2011 are estimated based on the upscaling of FLUXNET eddy covariance data with 155 a biosphere model (Jung et al., 2009). This product was made to reproduce a model 156 (LPJmL) using the fraction of absorbed PAR simulated in LPJmL. As a comparison, we 157 also use GPP observations of 1982-2008 derived based on FLUXNET, satellite, and meteorological observations (Jung et al., 2011), which is about 10% lower than that of 158 159 Jung et al. (2009). The NPP for 2000-2011 is derived using remote sensing data from Moderate Resolution Imaging Spectroradiometer (MODIS) (Zhao et al., 2005). We use 160 161 the global retrieval of greenness onset derived from the Advanced Very High Resolution 162 Radiometer (AVHRR) and the MODIS data from 1982 to 2011 (Zhang et al., 2014). All

163 datasets are interpolated to the  $1^{\circ} \times 1^{\circ}$  off-line model resolution for comparisons.

164

## 165 **3. YIBs model description**

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## 167 **3.1 Vegetation biophysics**

168 YIBs calculates carbon uptake for 9 PFTs: tundra, C3/C4 grass, shrubland, DBF, ENF, 169 EBF, and C3/C4 cropland (Table 1). In the gridded large-scale model applications, each 170 model PFT fraction in the vegetated part of each grid cell represents a single canopy. The 171 vegetation biophysics simulates C3 and C4 photosynthesis with the well-established 172 Michealis-Menten enzyme-kinetics scheme (Farquhar et al., 1980; von Caemmerer and 173 Farguhar, 1981) and the stomatal conductance model of Ball and Berry (Ball et al., 1987). The total leaf photosynthesis ( $A_{tot}$ , µmol m<sup>-2</sup> [leaf] s<sup>-1</sup>) is limited by one of three 174 processes: (i) the capacity of the ribulose 1,5-bisphosphate (RuBP) carboxylase-175 176 oxygenase enzyme (Rubisco) to catalyze carbon fixation  $(J_c)$ ; (ii) the capacity of the Calvin cycle and the thylakoid reactions to regenerate RuBP supported by electron 177 178 transport  $(J_e)$ ; (iii) the capacity of starch and sucrose synthesis to regenerate inorganic 179 phosphate for photo- phosphorylation in C3 plants and phosphoenolpyruvate (PEP) in 180 C4 plants  $(J_s)$ .

181

$$A_{tot} = \min(J_c, J_e, J_s) \tag{1}$$

183

184 The  $J_c$ ,  $J_e$ , and  $J_s$  are parameterized as functions of environmental variables (e.g. 185 temperature, radiation, and CO<sub>2</sub> concentrations) and the maximum carboxylation capacity 186 ( $V_{cmax}$ , µmol m<sup>-2</sup> s<sup>-1</sup>) (Collatz et al., 1991; Collatz et al., 1992):

187

188 
$$J_{c} = \begin{cases} V_{cmax} \left( \frac{c_{i} - \Gamma_{*}}{c_{i} + K_{c} \left( 1 + O_{i} / K_{o} \right)} \right) & \text{for C3 plant} \\ V_{cmax} & \text{for C4 plant} \end{cases}$$
(2)

190 
$$J_{e} = \begin{cases} a_{leaf} \cdot PAR \cdot \alpha \cdot \left(\frac{c_{i} - \Gamma_{*}}{c_{i} + 2\Gamma_{*}}\right) & \text{for C3 plant} \\ a_{leaf} \cdot PAR \cdot \alpha & \text{for C4 plant} \end{cases}$$
(3)

192 
$$J_{s} = \begin{cases} 0.5V_{cmax} & \text{for C3 plant} \\ K_{s} \cdot V_{cmax} \cdot \frac{C_{i}}{P_{s}} & \text{for C4 plant} \end{cases}$$
(4)

193

194 where  $c_i$  and  $O_i$  are the leaf internal partial pressure (Pa) of CO<sub>2</sub> and oxygen,  $\Gamma_*$  (Pa) is 195 the CO<sub>2</sub> compensation point,  $K_c$  and  $K_o$  (Pa) are Michaelis-Menten parameters for the carboxylation and oxygenation of rubisco. The parameters  $K_c$ ,  $K_o$ , and  $\Gamma_*$  vary with 196 temperature according to a Q<sub>10</sub> function. PAR (µmol m<sup>-2</sup> s<sup>-1</sup>) is the incident 197 198 photosynthetically active radiation,  $a_{leaf}$  is leaf-specific light absorbance, and  $\alpha$  is intrinsic 199 quantum efficiency.  $P_s$  is the ambient pressure and  $K_s$  is a constant set to 4000 following Oleson et al. (2010).  $V_{cmax}$  is a function of the optimal  $V_{cmax}$  at 25 °C ( $V_{cmax25}$ ) based on a 200 201 Q<sub>10</sub> function.

202

#### 203 Net carbon assimilation $(A_{net})$ of leaf is given by:

- 204
- 205

$$A_{net} = A_{tot} - R_d \tag{5}$$

206

where  $R_d$  is the rate of dark respiration set to 0.011  $V_{cmax}$  for C3 plants (Farquhar et al., 1980) and 0.025  $V_{cmax}$  for C4 plants (Clark et al., 2011). The stomatal conductance of water vapor ( $g_s$  in mol [H<sub>2</sub>O] m<sup>-2</sup> s<sup>-1</sup>) is dependent on net photosynthesis:

210

211 
$$g_s = m \frac{A_{net} \cdot RH}{c_s} + b$$
(6)

212

where *m* and *b* are the slope and intercept derived from empirical fitting to the Ball and Berry stomatal conductance equations, *RH* is relative humidity, and  $c_s$  is the CO<sub>2</sub> concentration at the leaf surface. In the model, the slope *m* is influenced by water stress, so that drought decreases photosynthesis by affecting stomatal conductance. Appropriate
photosynthesis parameters for different PFTs are taken from Friend and Kiang (2005) and
the Community Land Model (Oleson et al., 2010) with updates from Bonan et al. (2011)
(Table 1). In future work, we will investigate the carbon-chemistry-climate impacts of
updated stomatal conductance models in YIBs (Berry et al., 2010; Pieruschka et al.,
2010; Medlyn et al., 2011).

222

223 The coupled equation system of photosynthesis, stomatal conductance and CO<sub>2</sub> diffusive 224 flux transport equations form a cubic in  $A_{net}$  that is solved analytically (Baldocchi, 1994). 225 A simplified but realistic representation of soil water stress  $\beta$  is included in the vegetation 226 biophysics following the approach of Porporato et al. (2001). The algorithm reflects the 227 relationship between soil water amount and the extent of stomatal closure ranging from 228 no water stress to the soil moisture stress onset point (s<sup>\*</sup>) through to the wilting point ( $s_{wilt}$ ). Stomatal conductance is reduced linearly between the PFT-specific values of  $s^*$ 229 230 and swilt based on the climate model's soil water volumetric saturation in 6 soil layers 231 (Unger et al., 2013).

232

The canopy radiative transfer scheme divides the canopy into an adaptive number of layers (typically 2-16) for light stratification. Each canopy layer distinguishes sunlit and shaded portions of leaves, so that the direct and diffuse photosynthetically active radiation (PAR) is used for carbon assimilation respectively (Spitters et al., 1986). The leaf photosynthesis is then integrated over all canopy layers to generate the GPP:

238

- $GPP = \int_{0}^{LAI} A_{tot} \, dL \tag{7}$
- 240

## 241 **3.2 Leaf phenology**

Phenology determines the annual cycle of LAI. Plant phenology is generally controlled by temperature, water availability, and photoperiod (Richardson et al., 2013). For deciduous trees, the timing of budburst is sensitive to temperature (Vitasse et al., 2009) and the autumn senescence is related to both temperature and photoperiod (Delpierre et al., 2009). For small trees and grasses, such as tundra, savanna, and shrubland, phenology is controlled by temperature and/or soil moisture, depending on the species type and locations of the vegetation (Delbart and Picard, 2007; Liu et al., 2013). In the YIBs model, leaf phenology is updated on a daily basis. For the YIBs model, we build on the phenology scheme of Kim et al. (2015) and extend it based on long-term measurements of leaf phenology at 5 U.S. sites (Yue et al., 2015a, hereinafter Y2015) and GPP at the 145 flux tower sties. A summary of the phenological parameters adopted is listed in Table 2.

254

# 255 **3.2.1 Deciduous broadleaf forest (DBF)**

We predict spring phenology of DBF using the cumulative thermal summation (White et al., 1997). The accumulative growing degree day (GDD) is calculated for the *n*th day from winter solstice if the 10-day average air temperature  $T_{10}$  is higher than a base temperature  $T_b$ :

260

$$GDD = \sum_{i=1}^{n} \max(T_{10} - T_{b}, 0)$$
(8)

262

Here  $T_b$  is set to 5°C as that in Murray et al. (1989). Similar to the approach outlined in Kim et al. (2015), the onset of greenness is triggered if the GDD exceeds a threshold value  $G_b$  and a temperature-dependent phenological factor  $f_T$  is calculated as follows:

267 
$$f_T = \begin{cases} \min\left(1, \frac{GDD - G_b}{L_g}\right), & \text{if } GDD \ge G_b \\ 0, & \text{otherwise} \end{cases}$$
(9)

268

Following Murray et al. (1989), the threshold  $G_b = a + b \exp(r \cdot NCD)$  is dependent on the number of chill days (NCD), which is calculated as the total days with < 5°C from winter solstice.

272

The autumn phenology is more uncertain than budburst because it is affected by both temperature and photoperiod (White et al., 1997; Delpierre et al., 2009). For the temperature dependent phenology, we adopted the cumulative cold summation method
(Dufrene et al., 2005; Richardson et al., 2006), which calculates the accumulative falling
degree day (FDD) for the *m*th day from summer solstice as follows,

278

279

$$FDD = \sum_{i=1}^{m} \min(T_{10} - T_s, 0)$$
(10)

280

where  $T_s$  is 20°C as that in Dufrene et al. (2005). Similar to the budburst process, we determine autumn phenological factor based on a fixed threshold  $F_s$ :

283

284 
$$f_{T} = \begin{cases} \max\left(0, 1 + \frac{FDD - F_{s}}{L_{f}}\right), & \text{if } FDD \leq F_{s} \\ 1, & \text{otherwise} \end{cases}$$
(11)

285

286 In addition, we assume photoperiod regulates leaf senescence as follows,

287

288 
$$f_{P} = \begin{cases} \max\left(0, \frac{P - P_{i}}{P_{x} - P_{i}}\right), & \text{if } P \leq P_{x} \\ 1, & \text{otherwise} \end{cases}$$
(12)

289

where  $f_P$  is the photoperiod-limited phenology. *P* is daylength in minutes.  $P_i$  and  $P_x$  are the lower and upper limits of daylength for the period of leaf fall. Finally, the autumn phenology of DBF is determined as the product of  $f_T$  (Equation 11) and  $f_P$  (Equation 12). Both the spring and autumn phenology schemes have been evaluated with extensive ground records over the U.S. in Y2015.

295

## 296 **3.2.2 Shrubland**

Shrub phenology is sensitive to temperature and/or water availability. We calculate correlation coefficients between observed GPP and soil meteorology at 18 shrub sites (Fig. 2). For 10 sites with annual mean soil temperature < 9 °C, the GPP-temperature correlations are close to 1 while the GPP-moisture correlations are all negative (Fig. 2a),

suggesting that temperature is the dominant phenological driver for these plants. In 301 302 contrast, for 8 sites with average soil temperature > 14 °C, GPP-moisture correlations are 303 positive and usually higher than the GPP-temperature correlations, indicating that 304 phenology is primarily regulated by water availability at climatologically warm areas. 305 The wide temperature gap (9-14 °C) is due to the limit in the availability of shrub sites. 306 Here, we select a tentative threshold of 12 °C to distinguish cold and drought species. We 307 also try to identify phenological drivers based on soil moisture thresholds but find that 308 both temperature- and drought-dependent phenology may occur at moderately dry 309 conditions (Fig. 2b).

310

In the model, we apply the temperature-dependent phenology  $f_T$  for shrubland, if the site has annual mean soil temperature <12 °C. We use the same  $f_T$  as that for DBF (Equations 9 and 11), due to the lack of long-term phenology measurements at the shrub sites. However, if the soil temperature is >12 °C, the plant growth is controlled by droughtlimit phenology  $f_D$  instead:

316

317 
$$f_{D} = \begin{cases} \max\left(0, \frac{\beta_{10} - \beta_{\min}}{\beta_{\max} - \beta_{\min}}\right), & \text{if } \beta_{10} \leq \beta_{\max} \\ 1, & \text{otherwise} \end{cases}$$
(13)

318

where  $\beta_{10}$  is 10-day average water stress calculated based on soil moisture, soil ice 319 320 fraction, and root fraction of each soil layer (Porporato et al., 2001). The value of  $\beta_{10}$ 321 changes from 0 to 1, with lower value indicating drier soil. Two thresholds,  $\beta_{\text{max}}$  and  $\beta_{\text{min}}$ , 322 represent the upper and lower thresholds that trigger the drought limit for woody species. 323 The values of these thresholds are set to  $\beta_{\text{max}} = 1$  and  $\beta_{\text{min}} = 0.4$  so that the predicted 324 phenology has the maximum correlations with the observed GPP seasonality (Fig. S1a). 325 The shrub phenology applies for shrubland in tropical and subtropical areas, as well as 326 tundra at the subarctic regions, though the phenology of the latter is usually dependent on 327 temperature alone because the climatological soil temperature is <12 °C.

328

#### 329 3.2.3 Grassland

In the model, we consider temperature-dependent phenology for grassland based on soiltemperature (ST) accumulation (White et al., 1997):

332

333 
$$SGDD = \sum_{i=1}^{n} \max(ST_{10} - ST_{b}, 0)$$
(14)

334

where  $ST_{10}$  is 10-day average soil temperature and  $ST_b = 0$  °C. Similar to DBF, the onset of grass greenness is triggered if *SGDD* is higher than a threshold value  $SG_b$  (Kim et al., 2015):

338

339 
$$f_{T} = \begin{cases} \min\left(1, \frac{SGDD - SG_{b}}{SL_{g}}\right), & \text{if } SGDD \ge SG_{b} \\ 0, & \text{otherwise} \end{cases}$$
(15)

340

where  $SL_g$  determines the grow length of grass. Both  $SG_b$  and  $SL_g$  are calibrated based on 341 342 observed GPP seasonality at FLUXNET sites (Table 2). Grass phenology at warm sites is 343 also sensitive to water stress (Fig. 2c). We apply the same drought-limit phenology  $f_D$  as shrubland (Equation 13) for grassland but with calibrated threshold  $\beta_{max} = 0.9$  and  $\beta_{min}$ 344 345 =0.3 (Fig. S1b). Different from shrubland whose phenology is dominated by drought when ST > 12 °C (Fig. 2a), grassland phenology is jointly affected by temperature and 346 347 soil moisture (Fig. 2c). As a result, the final phenology for grassland at warm regions is the minimum of  $f_T$  and  $f_D$ . 348

349

#### **350 3.2.4 Other PFTs**

YIBs considers two evergreen PFTs, ENF at high latitudes and EBF in tropical areas. Observations do suggest that evergreen trees experience seasonal changes in LAI, following temperature variations and/or water availability (Doughty and Goulden, 2008; Schuster et al., 2014). However, due to the large uncertainty of evergreen phenology, we set a constant phenology factor of 1.0 for these species, following the approach adopted in other process-based vegetation models (Bonan et al., 2003; Sitch et al., 2003). We implement a parameterization for the impact of cold temperature (frost hardening) on the maximum carboxylation capacity ( $V_{cmax}$ ) so as to reduce cold injury for ENF during winter (Hanninen and Kramer, 2007). EBF may experience reduced photosynthesis during the dry season through the effects of water stress on stomatal conductance(Jones et al., 2014).

362

Crop phenology depends on planting and harvesting dates. In YIBs, we apply a global dataset of crop planting and harvesting dates (Sacks et al., 2010; Unger et al., 2013). Crop budburst occurs at the plant date and the crop continues to grow for a period of 30 days until reaching full maturity (f = 1). The crop leaves begin to fall 15 days prior to the harvest date, after which phenology is set to 0. A similar treatment has been adopted in CLM model (Bonan et al., 2003). Thus, crop productivity but not crop phenology is sensitive to the imposed meteorological forcings.

370

## **371 3.3 Carbon allocation**

We adopt the autotrophic respiration and carbon allocation scheme applied in the dynamic global vegetation model (DGVM) TRIFFID (Cox, 2001; Clark et al., 2011). On a daily basis, the plant LAI is updated as follows:

375

376

- $LAI = f \cdot LAI_b \tag{16}$
- 377

378 where *f* is the phenological factor, and  $LAI_b$  is the biomass-balanced (or available 379 maximum) LAI related to tree height.  $LAI_b$  is dependent on the vegetation carbon content 380  $C_{veg}$ , which is the sum of carbon from leaf ( $C_l$ ), root ( $C_r$ ), and stem ( $C_w$ ):

381

$$382 C_{veg} = C_l + C_r + C_w (17)$$

383

384 where each carbon component is a function of 
$$LAI_b$$
:

385

 $386 C_l = \sigma_l \cdot LAI (18a)$ 

$$387 C_r = \sigma_l \cdot LAI_b (18b)$$

$$C_w = a_{wl} \cdot LAI_b^{b_{wl}}$$
(18c)

here  $\sigma_l$  is the specific leaf carbon density.  $a_{wl}$  and  $b_{wl}$  are PFT-specified allometric parameters (Table 1). The vegetation carbon content  $C_{veg}$  is updated every 10 days based on the carbon balance of assimilation, respiration, and litter fall.

393

394 
$$\frac{dC_{veg}}{dt} = (1 - \lambda) \cdot NPP - \Lambda_l$$
(19)

395

396 The net primary productivity (NPP) is the net carbon uptake:

397

$$398 \qquad NPP = GPP - R_a \tag{20}$$

399

400 here GPP is the total photosynthesis rate integrated over LAI. Autotrophic respiration 401 ( $R_a$ ) is split into maintenance ( $R_{am}$ ) and growth respiration ( $R_{ag}$ ) (Clark et al., 2011):

402

$$403 R_a = R_{am} + R_{ag} (21)$$

404

405 The maintenance respiration is calculated based on nitrogen content in leaf  $(N_l)$ , root  $(N_r)$ , 406 and stem  $(N_w)$  as follows,

407

408 
$$R_{am} = 0.012 R_d \left(\beta + \frac{N_r + N_w}{N_l}\right)$$
 (22)

409

410 where  $R_d$  is the dark respiration of leaf, which is dependent on leaf temperature and is 411 integrated over whole canopy LAI. The factor of 0.012 is the unit conversion from mol 412 CO2 m<sup>-2</sup> s<sup>-1</sup> to kg C m<sup>-2</sup> s<sup>-1</sup> and  $\beta$  is water stress representing soil water availability. The 413 nitrogen contents are given by:

$$415 N_l = n_0 \cdot C_l (23a)$$

416 
$$N_r = n_{rl} \cdot n_0 \cdot C_r \tag{23b}$$

417 
$$N_{w} = n_{wl} \cdot n_{0} \cdot \eta \cdot H \cdot LAI$$
(23c)

here  $n_0$  is leaf nitrogen concentration,  $n_{rl}$  and  $n_{wl}$  are ratios of nitrogen concentrations of root and stem to leaves,  $\eta$  is a factor scaling live stem mass to LAI and tree height *H*. We adopt the same values of  $n_0$ ,  $n_{rl}$ ,  $n_{wl}$  and  $\eta$  as that of TRIFFID model (Table 1) except that  $n_{rl}$  is set to 0.5 following observations of deciduous trees by Sugiura and Tateno (2011). The growth respiration is dependent on the residual between *GPP* and  $R_{am}$  based on a ratio  $r_g$  set to 0.2 for all PFTs (Knorr, 2000):

425

$$R_{ag} = r_g \cdot \left(GPP - R_{am}\right) \tag{24}$$

427

428 The  $\lambda$  in Equation (19) is a partitioning coefficient determining the fraction of NPP used 429 for spreading:

430

431 
$$\lambda = \begin{cases} 1, & \text{if } LAI_b > LAI_{\max} \\ \frac{LAI_b - LAI_{\min}}{LAI_{\max} - LAI_{\min}}, & \text{if } LAI_{\min} \le LAI_b \le LAI_{\max} \\ 0, & \text{if } LAI_b < LAI_{\min} \end{cases}$$
(25)

432

433 where  $LAI_{min}$  and  $LAI_{max}$  are minimum and maximum LAI values for a specific PFT 434 (Table 1). In the current model version, we turn off the fractional changes by omitting 435  $\lambda$ NPP in the carbon allocation but feeding it as input for the soil respiration. The litter fall 436 rate  $\Lambda_l$  in Equation (19) consists of contributions from leaf, root, and stem as follows,

- 437
- 438

$$\Lambda_l = \gamma_l \cdot C_l + \gamma_r \cdot C_r + \gamma_w \cdot C_w \tag{26}$$

439

440 here  $\gamma_l$ ,  $\gamma_r$ , and  $\gamma_w$  are turnover rate (yr<sup>-1</sup>) for leaf, root, and stem carbon respectively. 441 The leaf turnover rate is calculated based on the phenology change every day. The root 442 and stem turnover rates are PFT-specific constants (Table 1), derived based on the metaanalysis by Gill and Jackson (2000) for root and Stephenson and van Mantgem (2005) forstem.

445

## 446 **3.4 Soil respiration**

447 The soil respiration scheme is developed based on the Carnegie-Ames-Stanford 448 Approach (CASA) model (Potter et al., 1993; Schaefer et al., 2008), which considers 449 carbon flows among 12 biogeochemical pools. Three live pools, including leaf  $C_l$ , root  $C_r$ , and wood  $C_w$ , contain biomass carbon assimilated from photosynthesis. Litterfall 450 451 from live pools decomposes and transits in nine dead pools, which consist of one coarse 452 woody debris (CWD) pool, three surface pools, and five soil pools. The CWD pool is 453 composed of dead trees and woody roots. Both surface and soil have identical pools, 454 namely structural, metabolic, and microbial pools, which are distinguished by the content 455 and functions. The structural pool contains lignin, the metabolic pool contains labile 456 substrates, and the microbial pool represents microbial populations. The remaining two 457 soil pools, the slow and passive pools, consist of organic material that decays slowly. The 458 full list of carbon flows among different pools has been illustrated by Schaefer et al. 459 (2008) (c.f. their Fig. 1).

460

461 When carbon transfers from pool *j* to pool *i*, the carbon loss of pool *j* is:

462 463

$$L_{j2i} = f_{j2i}k_jC_j \tag{27}$$

464

where  $C_j$  is the carbon in pool *j*,  $k_j$  is the total carbon loss rate of pool *j*, and  $f_{j2i}$  is the fraction of carbon lost from pool *j* transferred to pool *i*. The coefficient  $k_j$  is dependent on soil temperature, moisture, and texture. Meanwhile, the carbon gain of pool *i* is:

468

$$G_{j2i} = e_{j2i} \cdot L_{j2i} = e_{j2i} f_{j2i} k_j C_j$$
(28)

470

471 where  $e_{j2i}$  is the ratio of carbon received by pool *i* to the total carbon transferred from 472 pool *j*. The rest of the transferred carbon is lost due to heterotrophic respiration: 473

474 
$$R_{j2i} = (1 - e_{j2i}) \cdot L_{j2i}$$
(29)

476 As a result, the carbon in the *i*th pool is calculated as

477

478 
$$\frac{dC_i}{dt} = \sum_{j=1}^n G_{j2i} - \sum_{k=1}^m L_{i2k}$$
(30)

479

480 The total heterotrophic respiration ( $R_h$ ) is the summation of  $R_{j2i}$  for all pair pools where 481 carbon transitions occur. The total soil carbon is the summation of carbon for all dead 482 pools:

483

484

$$C_{soil} = \sum_{i=1}^{9} C_i \tag{31}$$

485

486 The net ecosystem productivity (NEP) is calculated as

487

$$488 \qquad NEP = -NEE = NPP - R_h = GPP - R_a - R_h \tag{32}$$

489

where NEE is the net ecosystem exchange, representing net carbon flow from land to
atmosphere. YIBs does not yet account for NEE perturbations due to dynamic
disturbance.

493

# 494 **3.5 Ozone vegetation damage effects**

We apply the semi-mechanistic parameterization proposed by Sitch et al. (2007) to account for ozone damage to photosynthesis through stomatal uptake. The scheme simulates associated changes in both photosynthetic rate and stomatal conductance. When photosynthesis is inhibited by ozone, stomatal conductance decreases accordingly to resist more ozone molecules. We employed an off-line regional version of YIBs to show that present-day ozone damage decreases GPP by 4-8% on average in the eastern U.S. and leads to larger decreases of 11-17% in east coast hotspots (Yue and Unger, 502 2014). In the current model version, the photosynthesis and stomatal conductance 503 responses to ozone damage are coupled. In future work, we will update the ozone 504 vegetation damage function in YIBs to account for decoupled photosynthesis and 505 stomatal conductance responses based on recent extensive meta-data analyses (Wittig et 506 al., 2007; Lombardozzi et al., 2013).

507

## 508 **3.6 Biogenic volatile organic compound (BVOC) emissions**

509 YIBs incorporates two independent leaf-level isoprene emission schemes embedded 510 within the exact same host model framework (Zheng et al., 2015). The photosynthesis-511 based isoprene scheme simulates emission as a function of the electron transport-limited 512 photosynthesis rate ( $J_e$ , Equation 3), canopy temperature, intercellular CO<sub>2</sub> ( $c_i$ ) and  $\Gamma_*$ 513 (Arneth et al., 2007; Unger et al., 2013). The MEGAN scheme applies the commonly 514 used leaf-level functions of light and canopy temperature (Guenther et al., 1993; 515 Guenther et al., 1995; Guenther et al., 2012). Both isoprene schemes account for 516 atmospheric CO<sub>2</sub>-sensitivity (Arneth et al., 2007). Long-term increases (decreases) in 517 atmospheric CO<sub>2</sub> decrease (increase) isoprene emissions (Unger et al., 2013). The CO<sub>2</sub>-518 sensitivity is higher under lower atmospheric  $CO_2$  levels than present day. Leaf-level 519 monoterpene emissions are simulated using a simplified temperature dependent algorithm 520 (Lathiere et al., 2006). The leaf-level isoprene and monoterpene emissions are integrated 521 over the multiple canopy layers in the exact same way as GPP to obtain the total canopy-522 level emissions.

523

## 524 3.7 Implementation of YIBs into NASA ModelE2 (NASA ModelE2-YIBs)

525 NASA ModelE2 has a spatial resolution of 2°×2.5° latitude by longitude with 40 vertical 526 levels extending to 0.1 hPa. In the on-line configuration, the global climate model 527 provides the meteorological drivers to YIBs and the land-surface hydrology submodel 528 provides the soil characteristics (Rosenzweig and Abramopoulos, 1997; Schmidt et al., 529 2014). Recent relevant updates to NASA ModelE2 include a dynamic fire activity 530 parameterization from Pechony and Shindell (2009) and climate-sensitive soil NO<sub>x</sub> emissions based on Yienger and Levy (1995) (Unger and Yue, 2014). Without the YIBs 531 532 implementation, the default NASA ModelE2 computes dry deposition using fixed LAI 533 and vegetation cover fields from Olson et al. (2001), which are different from the climate 534 model's vegetation scheme (Shindell et al., 2013b). With YIBs embedded in NASA 535 ModelE2, the YIBs model provides the vegetation cover and LAI for the dry deposition 536 scheme. The on-line simulated atmospheric ozone and aerosol concentrations influence 537 terrestrial carbon assimilation and stomatal conductance at the 30-minute integration time 538 step. In turn, the on-line vegetation properties, and water, energy and BVOC fluxes affect 539 air quality, meteorology and the atmospheric chemical composition. The model simulates 540 the interactive deposition of inorganic and organic nitrogen to the terrestrial biosphere. 541 However, the YIBs biosphere currently applies fixed nitrogen levels and does not yet 542 account for the dynamic interactions between the carbon and nitrogen cycles, and the 543 consequences for carbon assimilation, which are highly uncertain (e.g., Thornton et al., 544 2007; Koven et al., 2013; Thomas et al., 2013; Zaehle et al., 2014; Houlton et al., 2015).

- 545
- 547

# 546 **4. Model setup and simulations**

548 **4.1 Site-level simulations (YIBs-site)** 

549 We perform site-level simulations with offline YIBs model at 145 eddy covariance flux 550 tower sites for the corresponding PFTs (Fig. 1). Hourly in situ measurements of 551 meteorology (Sect. 2.1) are used as input for the model. We gap filled missing 552 measurements with the Global Modeling and Assimilation Office (GMAO) Modern Era-553 Retrospective Analysis (MERRA) reanalysis (Rienecker et al., 2011), as described in Yue 554 and Unger (2014). All grasslands and most croplands are considered as C3 plants, except 555 for some sites where corn is grown. Meteorological measurements are available for a 556 wide range of time periods across the different sites ranging from the minimum of 1 year 557 at some sites (e.g. BE-Jal) and the maximum of 16 years at Harvard Forest (US-HA1). 558 The soil carbon pool initial conditions at each site are provided by the 140-year spin up 559 procedure using YIBs-offline (Supplement). An additional 30-year spin up is conducted 560 for each site-level simulation using the initial height  $H_0$  for corresponding PFT (Table 1) 561 and the fixed meteorology and  $CO_2$  conditions at the first year of observations. Then, the 562 simulation is continued with year-to-year forcings at the specific site for the rest of measurement period. For all grass and shrub sites, two simulations are performed. One 563

applies additional drought controls on phenology as described in Sects. 3.2.2 and 3.2.3, while the other uses only temperature-dependent phenology. By comparing results of these two simulations, we assess the role of drought phenology for plants in arid and semi-arid regions.

568

# 569 **4.2 Global off-line simulation (YIBs-offline)**

570 The global off-line YIBs applies the CLM land cover dataset (Oleson et al., 2010). Land 571 cover is derived based on retrievals from both MODIS (Hansen et al., 2003) and AVHRR 572 (Defries et al., 2000). Fractions of 16 PFTs are aggregated into 9 model PFTs (Table 1). 573 The soil carbon pool and tree height initial conditions are provided by the 140-year spin 574 up procedure using YIBs-offline (Supplement). The global off-line YIBs model is driven with WFDEI meteorology (Weedon et al., 2014) at 1°×1° horizontal resolution for the 575 576 period of 1980-2011. Observed atmospheric  $CO_2$  concentrations are adopted from the 577 fifth assessment report (AR5) of the Intergovernmental Panel on Climate Change (IPCC) 578 (Meinshausen et al., 2011). We evaluate the simulated long-term 1980-2011 average tree 579 height/LAI and carbon fluxes with available observations and recent multi-model inter-580 comparisons. Attribution of the decadal trends in terrestrial carbon fluxes are explored in 581 a separate follow-on companion study (Yue et al., 2015b).

582

#### 583 4.3 Global on-line simulation in NASA ModelE2-YIBs

584 The global land cover data is identical to that used in YIBs-offline (Sect. 4.2) based on 585 the CLM cover. Because our major research goal is to study short-term (seasonal, annual, 586 decadal) interactions between vegetation physiology and atmospheric chemistry, we elect 587 to prescribe the PFT distribution in different climatic states. We perform an on-line 588 atmosphere-only simulation representative of the present day (~2000s) climatology by 589 prescribing fixed monthly-average sea surface temperature (SST) and sea ice temperature 590 for the 1996-2005 decade from the Hadley Center as the boundary conditions (Rayner et 591 al., 2006). Atmospheric CO<sub>2</sub> concentration is fixed at the level of the year 2000 (370 592 ppm). In NASA ModelE2-YIBs, initial conditions for soil carbon pools and tree heights 593 are provided by the 140-year spin-up process described in the Supplement using YIBs-594 offline but for year 2000 (not 1980) fixed WFDEI meteorology and atmospheric  $CO_2$  595 conditions. The NASA ModelE2-YIBs global carbon-chemistry-climate model is run for 596 an additional 30 model years. The first 20 years are discarded as the on-line spin-up and 597 the last 10-year results are averaged for the analyses including comparisons with 598 observations and the YIBs-offline.

599

# 600 4.4 Ozone vegetation damage simulation (YIBs-ozone)

601 We perform two simulations to quantify ozone vegetation damage with the off-line YIBs 602 model based on the high and low ozone sensitivity parameterizations (Sitch et al., 2007). 603 Similar to the set up in Yue and Unger (2014), we use off-line hourly surface ozone 604 concentrations simulated with the NASA ModelE2 based on the climatology and 605 precursor emissions of the year 2000 (Sect. 4.3). In this way, atmospheric ozone 606 photosynthesis damage affects plant growth, including changes in tree height and LAI. 607 We compare the simulated ozone damage effects with the previous results in Yue and 608 Unger (2014) that used prescribed LAI. For this updated assessment, we do not isolate 609 possible feedbacks from the resultant land carbon cycle changes to the surface ozone 610 concentrations themselves, for instance through concomitant changes to BVOC emissions 611 and water fluxes. The importance of these feedbacks will be quantified in future research 612 using the on-line NASA ModelE2-YIBs framework.

613

#### 614 **5. Results**

615

# 616 5.1 Site-level evaluation

617 The simulated monthly-average GPP is compared with measurements at 145 sites for different PFTs (Fig. 3). GPP simulation biases range from -19% to 7% depending on 618 619 PFT. The highest correlation of 0.86 is achieved for DBF, mainly contributed by the 620 reasonable phenology simulated at these sites (Fig. S2). The correlation is also high for 621 ENF sites even though phenology is set to a constant value of 1.0. A relatively low 622 correlation of 0.65 is modeled for EBF sites (Fig. S2). However, the site-specific 623 evaluation shows that the simulations reasonably capture the observed magnitude and 624 seasonality, including the minimum GPP in summer due to drought at some sites (e.g. 625 FR-Pue and IT-Lec). Predictions at crop sites achieve a medium correlation of 0.77, 626 because the prescribed crop phenology based on the planting and harvesting dates dataset 627 matches reality for most sites with some exceptions (e.g. CH-Oe2). Measured GPP at 628 shrub and grass sites show varied seasonality. For most sites, the maximum carbon fluxes 629 are measured in the hemispheric summer season. However, for sites with arid or 630 Mediterranean climate, the summer GPP is usually the lowest during the year (e.g. ES-631 LMa and US-Var in Fig. S2) while the peak flux is observed during the wet season when 632 the climate is cooler and moister. Implementing the drought-dependent phenology helps 633 improve the GPP seasonality and decrease the root-mean-square error (RMSE) at most 634 warm climate shrub and grass sites (Fig. S3).

635

636 A synthesis of the site-level evaluation is presented in Fig. 4. Among the 145 sites, 121 637 have correlations higher than 0.8 for the GPP simulation (Fig. 4a). Predictions are better 638 for PFTs with larger seasonal variations. For example, high correlations of >0.8 are 639 achieved at 95% ENF and DBF sites, but only 70% for grass and 45% for EBF sites. Low 640 relative biases (-33%-50%) are achieved at 94 sites (Fig. 4b). For most PFTs, a similar 641 fraction (65%) of the sites have low biases falling into that range, except for cropland, where only 7 sites (45%) have the low biases. The RMSE is lower than 3 g [C] day<sup>-1</sup> for 642 643 107 out of 145 sites (Fig. 4c). The highest RMSE is predicted for crop sites, where the 644 model misses the large interannual variations due to crop rotation at some sites (e.g. BE-645 Lon, DE-Geb, and US-Ne2). YIBs model performs simulations at the PFT level while 646 measurements show large uncertainties in the carbon fluxes among biomes/species within 647 the same PFT (Luyssaert et al., 2007). The simulated intraspecific variations (in the form 648 of standard deviation) are smaller than the measured/derived values for most PFTs (Table 649 S2), likely because of the application of fixed photosynthetic parameters for each PFT 650 (Table 1).

651

Compared with GPP, the NEE simulations have smaller correlations with measurements because of the limited seasonality in the observations at most sites (Fig. S4). 74 sites (51%) have correlation coefficients higher than 0.6 (Fig. 4d) and 75 sites (52%) have absolute biases within  $\pm$  0.5 g [C] day<sup>-1</sup> (Fig. 4e). For most ENF sites, the maximum net carbon uptake (the minimum NEE) is observed in spring or early summer, when GPP 657 begins to increase while soil respiration is still at low rate due to the cool and wet 658 conditions (e.g. CA-Ojp and ES-ES1). Compared with other PFTs, the DBF trees usually 659 have larger seasonality with the NEE peak in the early summer. Such seasonality helps 660 promote correlations between model and measurements, resulting in high R (>0.8) for 17 661 out of 20 sites (Fig. 4d). For shrub and grass sites, the observed seasonality of NEE is not 662 regular, though most show maximum carbon uptake in spring or early summer. 663 Implementation of drought-dependent phenology helps improve the simulated NEE 664 seasonality at some sites of these PFTs (e.g. ES-LMa and IT-Pia), however, such 665 improvement is limited for others (Fig. S4). Simulated crop NEE reaches maximum 666 magnitude in summer at most sites, consistent with observations and leading to a high R667 (> 0.8) for 10 out 16 sites (Fig. 4d). The RMSE of simulated NEE is larger for crop relative to other PFTs because the model does not treat crop rotation (Fig. 4f). 668

669

#### 670 **5.2 Evaluation of YIBs-offline**

671 YIBs-offline forced with WFDEI meteorology simulates reasonable spatial distributions 672 for tree height, LAI, and GPP, all of which show maximums in the tropical rainforest 673 biome and medium values in the Northern Hemisphere high latitudes (Fig. 5). Compared 674 with the satellite observations, the simulated height is underestimated by 30% on the 675 annual and global mean basis (Fig. 5b). Regionally, the prediction is larger by only 4% 676 for tropical rainforest and temperate DBF, but by 27% for boreal ENF, for which the 677 model assumes a constant phenology of 1.0 all the year round. However, for the vast 678 areas covered with grass and shrub PFTs, the simulated height is lower by 41% with 679 maximum underestimation in Eastern Siberia, where the model land is covered by short 680 tundra. The modeled LAI is remarkably close to observations on the annual and global 681 mean basis (Figs. 5c-d). However, there are substantial regional biases in model LAI. Model LAI prediction is higher by 0.8 m<sup>2</sup> m<sup>-2</sup> (70%) for boreal ENF and by 0.1 m<sup>2</sup> m<sup>-2</sup> 682 (5%) for tropical rainforest. In contrast, the simulation underestimates LAI of tropical C4 683 grass by 0.4 m<sup>2</sup> m<sup>-2</sup> (30%) and shrubland by 0.2 m<sup>2</sup> m<sup>-2</sup> (30%). The GPP simulation is 684 lower than the FLUXNET-derived value by 5% on the global scale, which is contributed 685 686 by the minor underestimation for all PFTs except for tropical rainforest, where model 687 predicts 9% higher GPP than observations (Fig. 5f).

689 The model simulates reasonable seasonality for LAI and land carbon fluxes (Fig. 6). Tree 690 height shows limited seasonal variations, especially for DBF, ENF, and EBF trees. LAI, 691 GPP, and NPP also exhibit small seasonality over tropical areas, such as the Amazon, 692 Central Africa, and Indonesia. However, for temperate areas, such as North America, 693 Europe and East Asia, these variables show large seasonal variations with minimum in 694 winter and maximum in summer. The LAI is overestimated by 20% in Amazon during 695 the December-January-February season but underestimated by 25% in Indonesia during 696 summer (Fig. 6b). For GPP and NPP, the positive bias in Indonesia is even larger at 45% 697 during summer (Figs. 6c-d).

698

On the global scale, YIBs-offline simulates GPP of  $124.6 \pm 3.3$  Pg C a<sup>-1</sup> and NEE of -2.5 699  $\pm$  0.7 Pg C a<sup>-1</sup> for 1982-2011. These values are consistent with estimates upscaled from 700 701 the FLUXNET observations (Jung et al., 2009; Friedlingstein et al., 2010; Jung et al., 702 2011) and simulations from 10 other carbon cycle models (Piao et al., 2013) (Fig. 7). The 703 net biome productivity (NBP) is in opposite sign to NEE. Tropical areas (23°S-23°N) 704 account for 63% of the global GPP, including 27% from Amazon rainforest, 21% from 705 central Africa, and 5% from Indonesia forest (Table 3). A lower contribution of 57% 706 from tropics is predicted for both NPP and heterotrophic respiration. However, for NEE, 707 only 40% of the land carbon sink is contributed by tropical forests and grasslands, while 708 56% is from temperate forests and grasslands in North America, Europe, and East Asia. 709

710 We compare the simulated budburst dates with observations from satellite retrieval (Fig. 711 8). The model captures the basic spatial pattern of spring phenology with earlier to later 712 budburst dates from lower to higher latitudes. On average, the observed budburst date in Northern Hemisphere (NH) is 133 DOY (May 13<sup>th</sup>) and simulation is 132 DOY (May 713 12<sup>th</sup>). Such close estimate results from the regional delay of 10 days (119 versus 129 714 715 DOY) in Europe and advance of 4 days (140 versus 136 DOY) in East Asia. In Y2015, 716 extensive (~75000 records) ground-based measurements have been used to validate the 717 simulated spring and autumn phenology in U.S. and both the spatial distribution and 718 interannual variation of simulation are reasonable.

#### 720 5.3 Evaluation of NASA ModelE2-YIBs

721 NASA ModelE2-YIBs simulations of global land carbon fluxes show similar spatial 722 distribution and magnitude as the YIBs-offline model (Figs. S6-S8). However, due to 723 differences in the meteorological forcings (Figs. S9-S12), regional discrepancies between 724 the two configurations occur. The predicted LAI with NASA ModelE2-YIBs is lower by 725 20% in Amazon region than YIBs-offline (Fig. S6), following the similar magnitude of 726 differences in regional GPP and NPP (Figs. S7-S8). We performed driver attribution 727 sensitivity simulations, in which the YIBs-offline configuration is driven with the same 728 meteorological forcings simulated by NASA ModelE2 except for one selected field from 729 the WFDEI reanalysis. We found that the anomalously warmer climate over the Amazon 730 in the global climate model (Fig. S9) causes the lower GPP in that region in NASA 731 ModelE2-YIBs. The temperature optimum for C3 photosynthesis is around 30 °C, above 732 which the maximum rate of electron transport (Equation 3) decreases dramatically 733 (Farguhar et al., 1980). As a result, the higher NASA ModelE2-YIBs surface temperature 734 in the tropical rainforest results in the lower photosynthesis rates there. With the 735 exception of the Amazon, the NASA ModelE2-YIBs June-July-August GPP and NPP 736 show low biases in central Africa and high latitudes in North America and Asia, but high biases in Europe, western U.S., and eastern China (Figs. S7-S8). The sensitivity tests 737 738 attribute these discrepancies to differences in canopy humidity (Fig. S11) and soil 739 wetness (Fig. S12). Low soil wetness decreases water stress  $\beta$ , reduces the slope *m* of 740 Ball-Berry equation (Equation 6), and consequently limits photosynthesis by declining 741 stomatal conductance in combination with low humidity. On the global scale, the ModelE2-YIBs simulates annual GPP of 122.9 Pg C, NPP of 62 Pg C, and NEE of -2.7 742 743 Pg C, all of which are close to the YIBs-offline simulation (Table 3) and consistent with 744 results from observations and model inter-comparison (Fig. 7).

745

# 746 **5.4 Assessment of global ozone vegetation damage**

747

Ozone dampens GPP and consequently affects tree growth and LAI. In North America,
 the annual average reductions range from 2% to 6%, depending on the plant sensitivity to

750 ozone damage (Table 3). Locally, average damages reach as high as 5-11% in the eastern 751 U.S. with maximums up to 11-23% (Figs. 9a-b). These values are higher than the 752 estimate of 4-8% (maximum 11-17%) by Yue and Unger (2014), because the latter used 753 prescribed LAI in the simulation and did not consider the LAI reductions due to ozone 754 damage (Figs. 9c-d). The YIBs model predicts similar magnitude of damages in Europe 755 compared to North America, but almost doubled effects in East Asia (Table 3) due to the 756 high ozone concentrations there, especially in boreal summer (Fig. S5). Ozone-induced 757 GPP-reductions are limited in tropical areas (Fig. 5e) because the surface ozone levels 758 there are very low, for example, especially over the Amazon forest (Fig. S5). The damage 759 to LAI generally follows the pattern of GPP reductions but the response signal is weaker 760 than that of GPP (Figs. 9c-d).

- 761
- 762

# 6. Conclusions and discussion

763

764 We describe and evaluate the process-based YIBs interactive terrestrial biosphere model. 765 YIBs is embedded into the NASA ModelE2 global chemistry-climate model and is an 766 important urgently needed development to improve the biological realism of interactions 767 between vegetation, atmospheric chemistry and climate. We implement both 768 temperature- and drought-dependent phenology for DBF, shrub, and grass species. The 769 model simulates interactive ozone vegetation damage. The YIBs model is fully validated 770 with land carbon flux measurements from 145 ground stations and global observations of 771 canopy height, LAI, GPP, NPP, and phenology from multiple satellite retrievals.

772

773 There are several limitations in the current model set up. The vegetation parameters,  $V_{cmax}$ 774  $_{25}$ , m, and b (Table 1), are fixed at the PFT level, which may induce uncertainties in the 775 simulation of carbon fluxes due to intraspecific variations (Kattge et al., 2011). The 776 model does not yet include a dynamic treatment of nitrogen and phosphorous availability 777 because current schemes suffer from large uncertainties (Thornton et al., 2007; Zaehle et 778 al., 2014; Houlton et al., 2015). Phenology is set to a constant value of 1 for ENF and 779 EBF, which is not consistent with observations (O'Keefe, 2000; Jones et al., 2014). The 780 ozone damage scheme of Sitch et al. (2007) considers coupled responses of photosynthesis and stomatal conductance while observations suggest a decoupling(Lombardozzi et al., 2013).

783

784 Despite these limitations, the YIBs model reasonably simulates global land carbon fluxes 785 compared with both site-level flux measurements and global satellite observations. YIBs 786 is primed for on-going development, for example, incorporating community dynamics 787 including mortality, establishment, seed transport and dynamic fire disturbance 788 (Moorcroft et al., 2001). NASA ModelE2-YIBs is available to be integrated with 789 interactive ocean and atmospheric carbon components to offer a full global carbon-790 climate model, for example for use in interpreting and diagnosing new satellite datasets 791 of atmospheric CO<sub>2</sub> concentrations. In the current form, NASA ModelE2-YIBs provides 792 a useful new tool to investigate the impacts of air pollution on the carbon budget, water 793 cycle, and surface energy balance, and, in turn, the impacts of changing vegetation 794 physiology on the atmospheric chemical composition. Carbon-chemistry-climate 795 interactions, a relatively new interdisciplinary research frontier, are expected to influence 796 the evolution of the Earth's climate system on multiple spatiotemporal scales.

797

## 798 Code availability

799

800 The **YIBs** model (version 1.0) site-level source code is available at 801 https://github.com/YIBS01/YIBS site. The source codes for the global off-line and 802 global on-line versions of the YIBs model (version 1.0) are available through 803 collaboration. Please submit request to X. Yue (xu.yue@yale.edu) and N. Unger 804 (nadine.unger@yale.edu). Auxiliary forcing data and related input files must be obtained 805 independently.

806

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PFT <sup>a</sup>	TDA	GRAC3	GRAC4	SHR	DBF	ENF	EBF	CROC3	CROC4
Carboxylation	C3	C3	C4	C3	C3	C3	C3	C3	C4
$V_{cmax 25}$ (µmol m <sup>-2</sup> s <sup>-1</sup> )	33	43	24	38	45	43	40	40	40
т	9	9	5	9	9	9	9	11	5
$b \pmod{m^{-2} s^{-1}}$	2	2	2	2	2	2	2	8	2
$a_{wl}$ (kg C m <sup>-2</sup> )	0.1	0.005	0.005	0.1	0.95	0.85	0.95	0.005	0.005
$b_{wl}$	1.667	1.667	1.667	1.667	1.667	1.667	1.667	1.667	1.667
$\sigma_l (\mathrm{kg}\mathrm{C}\mathrm{m}^{-2}\\mathrm{LAI}^{-1})$	0.05	0.025	0.05	0.05	0.0375	0.1	0.0375	0.025	0.05
$\eta (\text{kg C m}^{-1} \text{LAI}^{-1})$	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
$n_0 (\text{kg N} [\text{kg C}]^{-1})$	0.06	0.073	0.06	0.06	0.046	0.033	0.046	0.073	0.06
<i>n<sub>rl</sub></i>	0.5	1	1	0.5	0.5	0.75	0.5	1	1
$n_{wl}$	0.1	1	1	0.1	0.1	0.1	0.1	1	1
rg	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2
LAImin	1	1	1	1	1	1	1	1	1
LAI <sub>max</sub>	3	3	3	3	9	5	9	3	3
$\gamma_r (360 \text{ days})^{-1}$	0.5	0.75	0.75	0.5	0.75	0.25	0.75	0.75	0.75
$\gamma_w (360 \text{ days})^{-1}$	0.1	0.2	0.2	0.1	0.015	0.01	0.015	0.2	0.2
$H_{0}\left(\mathrm{m} ight)$	1	0.8	1.3	1	19	16.5	19	0.8	1.3

1223 Table 1. Photosynthetic and allometric parameters for the vegetation model.1224

<sup>a</sup> Plant functional types (PFTs) are tundra (TDA), C3 grassland (GRAC3), C4
savanna/grassland (GRAC4), shrubland (SHR), deciduous broadleaf forest (DBF),
evergreen needleleaf forest (ENF), evergreen broadleaf forest (EBF), and C3/C4 cropland
(CROC3/CROC4).

1233	Table 2.	Phenological	parameters	for the	vegetation	model.
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Variables	Description	Units	Value	Reference
$T_b$	Base temperature for budburst forcing	°C	5	Murray et al. (1989)
а	Parameters for budburst threshold $G_b$	Degree day	-110	Calibrated (Y2015)
b	Parameters for budburst threshold $G_b$	Degree day	550	Calibrated (Y2015)
r	Parameters for budburst threshold $G_b$	Dimensionless	-0.01	Murray et al. (1989)
$L_g$	Growing length	Degree day	380	Calibrated (Y2015)
$T_s$	Base temperature for senescence forcing	°C	20	Dufrene et al. (2005)
$F_s$	Threshold for leaf fall	Degree day	-140	Calibrated (Y2015)
$L_{f}$	Falling length	Degree day	410	Calibrated (Y2015)
$P_x$	Daylength threshold for leaf fall	Minutes	695	White et al. (1997)
$P_i$	Daylength threshold for full dormancy	Minutes	585	Calibrated (Y2015)
$T_d$	Threshold for drought phenology	°C	12	Calibrated (Fig. 2)
$eta_{\min}$	Lower threshold of drought limit for shrub	Dimensionless	0.4	Calibrated (Fig. S1)
$\beta_{\max}$	Upper threshold of drought limit for shrub	Dimensionless	1	Calibrated (Fig. S1)
$ST_b$	Base soil temperature for budburst forcing	°C	0	White et al. (1997)
$SG_b$	Threshold for budburst with soil temperature	Degree day	100	Calibrated
$SL_g$	Growing length with soil temperature	Degree day	100	Calibrated
$ST_s$	Base soil temperature for senescence forcing	°C	10	Calibrated
$SF_s$	Threshold for leaf fall with soil temperature	Degree day	-80	Calibrated
$SL_f$	Falling length with soil temperature	Degree day	100	Calibrated
$eta_{\min}$	Lower threshold of drought limit for herbs	Dimensionless	0.3	Calibrated (Fig. S1)
$\beta_{\rm max}$	Upper threshold of drought limit for herbs	Dimensionless	0.9	Calibrated (Fig. S1)

**Table 3.** Summary of carbon fluxes and ozone vegetation damage in different domains

and for tropics  $(23^{\circ}S-23^{\circ}N)$ . 

Regions	Amazon	North America	Central Africa	Europe	East Asia	Indonesia	Tropics	Global
GPP (Pg C a <sup>-1</sup> )	33.4	12.3	25.7	11.5	17.9	6.7	77.9	124.6
NPP (Pg C $a^{-1}$ )	15.5	7.5	12.1	7.3	10.3	2.9	36.8	65
NEE (Pg C a <sup>-1</sup> )	-0.4	-0.5	-0.3	-0.4	-0.5	-0.1	-1.0	-2.5
Ra (Pg C $a^{-1}$ )	17.9	4.8	13.6	4.2	7.6	3.8	41.1	59.6
Rh (Pg C $a^{-1}$ )	15.1	7	11.8	6.9	9.8	2.8	35.8	62.5
Low ozone damage to GPP (%)	-0.9	-2.4	-1.8	-2.5	-4.3	-3	-1.7	-2.1
High ozone damage to GPP (%)	-2.6	-5.8	-4.4	-6.1	-9.6	-7.3	-4.4	-5
Low ozone damage to LAI (%)	-0.3	-0.5	-0.6	-0.5	-0.9	-0.8	-0.5	-0.5
High ozone damage to LAI (%)	-0.8	-1.2	-1.6	-1.4	-2.4	-2.1	-1.4	-1.4

- 1250 Figure captions
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Figure 1. Distribution of 145 sites from the FLUXNET and the North American Carbon Program (NACP) network. The duplicated sites have been removed. The color indicates different plant functional types (PFTs) as evergreen needleleaf forest (ENF, blue), evergreen broadleaf forest (EBF, cyan), deciduous broadleaf forest (DBF, magenta), shrubland (SHR, yellow) grassland (GRA, green), and cropland (CRO, red). "Mixed Forests" are classified as ENF, "Permanent Wetlands", "Savannas", and "Woody Savannas" as SHR. The PFT of each site is described in supplemental Table S1.

1259

Figure 2. Correlations between monthly gross primary productivity (GPP) and soil variables at (a, b) shrub and (c, d) grass sites. For each site, we calculate correlation coefficients of GPP-soil temperature (red points) and GPP-soil moisture (blue squares). These correlation coefficients are then plotted against the annual mean (a, c) soil temperature (°C) or (b, d) soil moisture (fraction) at each site.

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1266 Figure 3. Comparison between observed and simulated monthly GPP from FLUXNET 1267 and NACP networks grouped by PFTs. Each point represents the average value of one 1268 month at one site. The red lines indicate linear regression between observations and 1269 simulations. The regression fit, correlation coefficient, and relative bias are shown on 1270 each panel. The PFTs include evergreen needleleaf forest (ENF), evergreen broadleaf 1271 forest (EBF), deciduous broadleaf forest (DBF), shrubland (SHR), grassland (GRA), and 1272 cropland (CRO). The detailed comparison for each site is shown in Fig. S2. Units of GPP:  $g C m^{-2} day^{-1}$ . 1273

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Figure 4. Bar charts of (a, d) correlation coefficients (R), (b, e) biases, and (c, f) RMSE for monthly (a, b, c) GPP and (d, e, f) net ecosystem exchange (NEE) between simulations and observations at 145 sites. Each bar represents the number of sites where the R, bias, or RMSE of simulations fall between the specific ranges as defined by the xaxis intervals. The minimum and maximum of each statistical metric are indicated as the two ends of x-axis in the plots. The values of x-axis are not even. The absolute biases instead of relative biases are shown for NEE because the long-term average NEE (the
denominator) is usually close to zero at most sites. The PFT definitions are: ENF,
Evergreen Needleleaf Forest; EBF, Evergreen Broadleaf Forest; DBF, Deciduous
Broadleaf Forest; SHR, Shrubland; GRA, Grasslands; CRO, Croplands. Detailed
comparisons at each site are shown in Figs. S2 and S4.

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Figure 5. Simulated (a) tree height, (c) leaf area index (LAI), and (e) GPP and their differences relative to observations (b, d, f). GPP dataset is from Jung et al. (2009). Simulations are performed with WFDEI reanalysis. Statistics are the annual average for period 1982-2011. The boxes in (a) represent six regions used for seasonal comparison in Fig. 6.

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**Figure 6.** Comparison of annual (a) tree height and seasonal (b) LAI, (c) GPP, and (d) net primary productivity (NPP) between simulations and observations for the six regions shown in Fig. 5a. GPP dataset is from Jung et al. (2009). Values at different regions are marked using different symbols, with distinct colors indicating seasonal means for winter (blue, December-February), spring (green, March-May), summer (red, June-August), and autumn (magenta, September-November).

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1300 Figure 7. Comparison of simulated global GPP and net biome productivity (NBP) from 1301 (red) YIBs-offline and (blue) ModelE2-YIBs models with 10 other carbon cycle models 1302 for 1982-2008. Each black symbol represents an independent model as summarized in 1303 Piao et al. (2013). Error bars indicate the standard deviations for interannual variability. 1304 The gray shading represents global residual land sink (RLS) calculated in Friedlingstein 1305 et al. (2010). The green line on the top represents range of GPP for 1982-2008 estimated 1306 by Jung et al. (2011) and the magenta line represents GPP for 1982-2011 from Jung et al. 1307 (2009).

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Figure 8. Comparison of simulated budburst dates in Northern Hemisphere with remote
sensing. Simulated phenology in each grid square is the composite result from DBF,
tundra, shrubland, and grassland based on PFT fraction and LAI in that grid box. Both

simulations and observations are averaged for period 1982-2011. Results for Southern
Hemisphere are not shown due to the limit coverage of deciduous forests and cold grass
species.

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1316 Figure 9. Percentage of ozone vegetation damage to (top) GPP and (bottom) LAI with (a,

1317 c) low and (b, d) high sensitivity. Both damages of GPP and LAI are averaged for 1982-

1318 2011. Offline surface ozone concentrations (Fig. S5) are simulated by GISS ModelE2

1319 with climatology of the year 2000.

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**Figure 1.** Distribution of 145 sites from the FLUXNET and the North American Carbon Program (NACP) network. The duplicated sites have been removed. The color indicates different plant functional types (PFTs) as evergreen needleleaf forest (ENF, blue), evergreen broadleaf forest (EBF, cyan), deciduous broadleaf forest (DBF, magenta), shrublands (SHR, yellow) grasslands (GRA, green), and croplands (CRO, red). "Mixed Forests" are classified as ENF, "Permanent Wetlands", "Savannas", and "Woody Savannas" as SHR. The PFT of each site is described in supplemental Table S1.

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Figure 2. Correlations between monthly gross primary productivity (GPP) and soil
variables at (a, b) shrub and (c, d) grass sites. For each site, we calculate correlation
coefficients of GPP-soil temperature (red points) and GPP-soil moisture (blue squares).
These correlation coefficients are then plotted against the annual mean (a, c) soil
temperature (°C) or (b, d) soil moisture (fraction) at each site.







Figure 3. Comparison between observed and simulated monthly GPP from FLUXNET and NACP networks grouped by PFTs. Each point represents the average value of one month at one site. The red lines indicate linear regression between observations and simulations. The regression fit, correlation coefficient, and relative bias are shown on each panel. The PFTs include evergreen needleleaf forest (ENF), evergreen broadleaf forest (EBF), deciduous broadleaf forest (DBF), shrublands (SHR), grasslands (GRA), and croplands (CRO). The detailed comparison for each site is shown in Fig. S2. Units of GPP:  $gCm^{-2}day^{-1}$ . 



1371 Figure 4. Bar charts of (a, d) correlation coefficients (R), (b, e) biases, and (c, f) RMSE 1372 for monthly (a, b, c) GPP and (d, e, f) net ecosystem exchange (NEE) between 1373 simulations and observations at 145 sites. Each bar represents the number of sites where 1374 the R, bias, or RMSE of simulations fall between the specific ranges as defined by the xaxis intervals. The minimum and maximum of each statistical metric are indicated as the 1375 1376 two ends of x-axis in the plots. The values of x-axis are not even. The absolute biases 1377 instead of relative biases are shown for NEE because the long-term average NEE (the denominator) is usually close to zero at most sites. The PFT definitions are: ENF, 1378 1379 Evergreen Needleleaf Forest; EBF, Evergreen Broadleaf Forest; DBF, Deciduous Broadleaf Forest; SHR, Shrubland; GRA, Grasslands; CRO, Croplands, Detailed 1380 1381 comparisons at each site are shown in Figs. S2 and S4.



**Figure 5.** Simulated (a) tree height, (c) leaf area index (LAI), and (e) GPP and their differences relative to observations (b, d, f). GPP dataset is from Jung et al. (2009). Simulations are performed with WFDEI reanalysis. Statistics are the annual average for period 1982-2011. The boxes in (a) represent six regions used for seasonal comparison in Fig. 6.

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**Figure 6.** Comparison of annual (a) tree height and seasonal (b) LAI, (c) GPP, and (d) net primary productivity (NPP) between simulations and observations for the six regions shown in Fig. 5a. GPP dataset is from Jung et al. (2009). Values at different regions are marked using different symbols, with distinct colors indicating seasonal means for winter (blue, December-February), spring (green, March-May), summer (red, June-August), and autumn (magenta, September-November).

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Figure 7. Comparison of simulated global GPP and net biome productivity (NBP) from (red) YIBs-offline and (blue) ModelE2-YIBs models with 10 other carbon cycle models for 1982-2008. Each black symbol represents an independent model as summarized in Piao et al. (2013). Error bars indicate the standard deviations for interannual variability. The gray shading represents global residual land sink (RLS) calculated in Friedlingstein et al. (2010). The green line on the top represents range of GPP for 1982-2008 estimated by Jung et al. (2011) and the magenta line represents GPP for 1982-2011 from Jung et al. (2009).



Figure 8. Comparison of simulated budburst dates in Northern Hemisphere with remote sensing. Simulated phenology in each grid square is the composite result from DBF, tundra, shrubland, and grassland based on PFT fraction and LAI in that grid box. Both simulations and observations are averaged for period 1982-2011. Results for Southern Hemisphere are not shown due to the limit coverage of deciduous forests and cold grass species.

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**Figure 9.** Percentage of ozone vegetation damage to (top) GPP and (bottom) LAI with (a, 1455 c) low and (b, d) high sensitivity. Both damages of GPP and LAI are averaged for 1982-1456 2011. Offline surface ozone concentrations (Fig. S5) are simulated by GISS ModelE2 1457 with climatology of the year 2000.