



The seasonal cycle of satellite chlorophyll fluorescence observations and its relationship to vegetation phenology and ecosystem atmosphere carbon exchange



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ABSTRACT

Mapping of terrestrial chlorophyll fluorescence from space has shown potential for providing global measurements related to gross primary productivity (GPP). In particular, space-based fluorescence may provide information on the length of the carbon uptake period. Here, for the first time we test the ability of satellite fluorescence retrievals to track seasonal cycle of photosynthesis as estimated from a diverse set of tower gas exchange measurements from around the world. The satellite fluorescence retrievals are obtained using new observations near the 740 nm emission feature from the Global Ozone Monitoring Experiment 2 (GOME-2) instrument offering the highest temporal and spatial resolution of available global measurements. Because GOME-2 has a large ground footprint ($\sim 40 \times 80 \text{ km}^2$) as compared with that of the flux towers and the GOME-2 data require averaging to reduce random errors, we additionally compare with seasonal cycles of upscaled GPP estimated from a machine learning approach averaged over the same temporal and spatial domain as the satellite data surrounding the tower locations. We also examine the seasonality of absorbed photosynthetically-active radiation (APAR) estimated from satellite measurements. Finally, to assess whether global vegetation models may benefit from the satellite fluorescence retrievals through validation or additional constraints, we examine seasonal cycles of GPP as produced from an ensemble of vegetation models. Several of the data-driven models rely on satellite reflectance-based vegetation parameters to derive estimates of APAR that are used to compute GPP. For forested (especially deciduous broadleaf and mixed forests) and cropland sites, the GOME-2 fluorescence data track the spring onset and autumn shutoff of photosynthesis as delineated by the upscaled GPP estimates. In contrast, the reflectance-based indicators and many of the models, particularly those driven by data, tend to overestimate the length of the photosynthetically-active period for these biomes. Satellite fluorescence measurements therefore show potential for improving the seasonal dependence of photosynthesis simulated by global models at similar spatial scales.

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1. Introduction

Vegetation phenology, the study of the timing and length of the terrestrial growing season and its connection to climate, has shown important relationships with climate change, surface meteorology, and the carbon cycle; it influences both spatial and temporal variability

in ecosystem productivity (Gu et al., 2003; White & Nemani, 2003; Churkina, Schimel, Braswell, & Xiao, 2005; Piao et al., 2008; Gu et al., 2009; Richardson et al., 2009, 2010, 2012). For example, the timing of leaf out, particularly for deciduous forests, is an important indicator of responses to climate change. It has major implications for the seasonal variation of numerous interactions between the biosphere and atmosphere including the partitioning of available energy into sensible and latent heat exchange as well as impacts to surface radiation budgets and dynamics (Randerson, Field, Fung, & Tans, 1999; Baldocchi et al., 2004; Churkina et al., 2005). The duration of the carbon uptake period

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(CUP), controlled by leaf out and senescence, can explain 80% of the spatial variance in annual net carbon exchange of ecosystems (NEE), defined as the amount of carbon entering and leaving an ecosystem (Baldocchi et al., 2001). Bauerle et al. (2012) have shown that while temperature is an important driver of seasonal changes in photosynthetic physiology, photoperiod also regulates leaf activity, particularly following summer solstice. They further show that proper accounting for this effect can significantly improve predictions of seasonal variations in atmospheric CO₂ within a global carbon-cycle model.

Several studies in North American forests (Richardson et al., 2009, 2010; Dragoni et al., 2010) show that earlier spring onset consistently results in higher gross ecosystem photosynthesis (GEP), as well as smaller increases in ecosystem respiration, leading to increased net ecosystem productivity (NEP) for both spring and annual flux integrals. Piao et al. (2008) find that autumnal warming produces increases in both photosynthesis and respiration, with greater increases in respiration. Dragoni et al. (2010) further show that in a North American deciduous forested site, the sensitivity of the carbon cycle to climate variability depends on the timing of the climate change with respect to phenological stages as well as to its sign and magnitude.

Terrestrial biosphere models have a large spread in the magnitude of predicted gross primary productivity (GPP) and show substantial differences in the temporal and biome-related (spatial) variability of GPP (Huntzinger et al., 2012). They show generally poor performance as compared with flux tower GPP estimates (Schaefer et al., 2012) and consistently predict that the growing season begins too early and ends late for deciduous forests; this results in an over-prediction of gross ecosystem photosynthesis during spring and autumn (Richardson et al., 2012). There is need for additional data to validate and improve these models.

The CUP and other phenological indicators have been estimated using satellite vegetation indices such as the Normalized Differential Vegetation Index (NDVI) and the Enhanced Vegetation Index (EVI) (e.g., Churkina et al., 2005; Ma et al., 2013; Zhang et al., 2003; Zhou et al., 2001). These indices have also been used within parameterized models to estimate gross primary productivity (GPP), defined as the total amount of carbon dioxide taken up from the atmosphere via photosynthesis (e.g., Running et al., 2004; Wang, Xiao, & Yan, 2010; Xiao et al., 2008). Many of these estimates are based on the light-use efficiency (LUE) model (Monteith, 1972) given by

$$GPP(t) = LUE(t) \times fPAR_{chl}(t) \times PAR_{chl}(t) = LUE(t) \times APAR_{chl}(t), \quad (1)$$

where $fPAR_{chl}$ is the fractional absorbed (by chlorophyll) photosynthetically-active radiation (PAR_{chl}), LUE is defined as the amount of carbon a specific vegetation type can fix biochemically per unit of absorbed solar energy, $APAR_{chl}$ is the absorbed PAR (for convenience the subscript 'chl' is henceforth dropped), and t is time. For example, satellite reflectance-based $fPAR$ estimates are given in the MOD15A2 product from the MODerate-resolution Imaging Spectroradiometer (MODIS), and LUE can be parameterized as a function of meteorological parameters for a given biome. However, the use of reflectance-based indicators such as $fPAR$ can be problematic in areas where vegetation indices do not drop when vegetation stays green while photosynthesis declines, (e.g., in evergreen needleleaf forests), in regions affected by seasonal snow cover under the canopy, and possibly in areas with high heterogeneity within a satellite pixel (e.g., Churkina et al., 2005; Xiao et al., 2004). In these cases, LUE models must rely more heavily on their LUE parameterizations.

Fluorescence measurements, particularly global observations from space, offer an alternative means of remotely sensing the functional status of vegetation. Fluorescence is generated during the photosynthetic process. The excitation for chlorophyll fluorescence in nature is provided by sunlight. The broad-band emission has two chlorophyll-related peaks at red and far-red wavelengths near 685 and 740 nm, respectively (e.g., Campbell, Middleton, Corp, & Kim, 2008; Corp et al., 2003).

At the canopy level, steady-state fluorescence from chlorophyll in vegetation at emission wavelength $\lambda_{em} = 740$ nm, henceforth denoted F_{740} , in general can be expressed as an integral of contributions over all excitation wavelengths from ultraviolet to near-infrared wavelengths, i.e.,

$$F_{740}(t) = e(\lambda_{em} = 740 \text{ nm}, t) \int_{\lambda_{ex}} \Theta_F(\lambda_{ex}, \lambda_{em}, t) fPAR_F(\lambda_{ex}, t) I(\lambda_{ex}, t) d\lambda_{ex}, \quad (2)$$

where λ_{ex} is the excitation wavelength, I is incident radiation at the surface, e is the fractional amount of fluorescence that escapes the canopy, and Θ_F is the fluorescence efficiency. Here it is recognized (by use of the subscript F) that $fPAR$ for chlorophyll fluorescence ($fPAR_F$) may differ slightly from $fPAR$ for photosynthesis ($fPAR_{chl}$). $fPAR_F$ and e are determined by canopy structure and vegetation biochemistry, captured in spectral optical properties.

A more simplified formulation has also been used to express steady state fluorescence (e.g., Berry et al., 2013; Louis et al., 2005), i.e.,

$$F_{740}(t) \approx e(t) \Theta_F(t) \times fPAR_F(t) \times PAR_F(t) = e(t) \Theta_F(t) \times APAR_F(t). \quad (3)$$

Again, we recognize that PAR_F may differ somewhat from PAR_{chl} (typically assumed to be 400–700 nm) as the action spectrum for fluorescence may weight ultraviolet wavelengths more heavily (Chappelle & Williams, 1987; Middleton, Corp, & Campbell, 2008; Rosema, Verhoef, Schoote, & Snel, 1991). Eq. (3) is similar in form to Eq. (1). Conversely, Eq. (1) could also be written in a somewhat more complex form similar to Eq. (2) as an integral over photosynthetically-active wavelengths. Eq. (3) may be used to approximate Eq. (2) provided that the spectral structure of Θ_F , $fPAR_F$, and I remains relatively constant with time.

If Eq. (3) is taken as is and $APAR_F(t) \approx APAR_{chl}(t)$, then the ratio of $GPP(t)$ to $F_{740}(t)$ is proportional to the ratio of $LUE(t)$ to $e(t)\Theta_F(t)$. There is theoretical evidence to support that under strong illumination, the ratio of LUE to Θ_F remains relatively constant, at least for fluorescence from photosystem II (Berry et al., 2013). Experimental studies have also shown that in high light conditions (i.e., in the early afternoon and late morning when many satellite measurements are made), chlorophyll fluorescence is positively correlated with $APAR$, LUE, and GPP (e.g., Amoros-Lopez et al., 2008; Flexas et al., 2002; Gunter et al., 2014; Louis et al., 2005; Meroni et al., 2008; van der Tol, Verhoef, & Rosema, 2009; Zarco-Tejada et al., 2009). Therefore, we may expect similar seasonal variability in GPP and F_{740} for a given vegetation type as long as e remains relatively constant.

The main objective of this study is to test the ability of F_{740} to accurately track the seasonal cycle of GPP across different vegetation types. A new F_{740} data set derived from observations from the GOME-2 satellite instrument provides the temporal and spatial resolution needed for a first direct comparison with global flux tower gas exchange measurements in terms of the seasonality of photosynthesis. Towards our goal, we compare the seasonal cycle of GOME-2 F_{740} , averaged over multiple years, with that of GPP from a diverse set of flux towers from around the world at middle latitudes where there is a distinct cycle in photosynthesis. Because the spatial scale of the tower measurements is much smaller than the large footprint GOME-2 satellite measurements (additionally averaged over time and space to reduce random errors), we also compare with upscaled GPP estimated with the Max Planck Institute for Biogeochemistry (MPI-BGC) machine learning algorithm; these upscaled GPP estimates are averaged at the same spatial resolution and over the same time period as the GOME-2 F_{740} retrievals. This allows us to assess potential representativeness errors in the comparison between GOME-2 F_{740} and GPP from flux towers. We perform additional comparisons to determine whether the seasonal cycle of fluorescence more closely tracks photosynthesis as compared with absorbed photosynthetically-active radiation (APAR),

derived from satellite reflectances. Finally, in order to assess whether fluorescence data may provide additional validation of and/or constraints for global vegetation models, we compare seasonal cycles of GOME-2 F_{740} and GPP generated from an ensemble of state-of-the-art physically-based and data driven models; the mostly global models are typically run at similar spatial resolutions as compared with the GOME-2 F_{740} data set.

2. Data

2.1. GOME-2 fluorescence at 740 nm (F_{740})

2.1.1. Background on remote sensing of terrestrial chlorophyll fluorescence

Fluorescence from chlorophyll in terrestrial vegetation has been measured with ground-, aircraft, and satellite-based instrumentation at wavelengths in and surrounding the O_2 A- and B-bands (e.g., Amoros-Lopez et al., 2008; Guanter et al., 2007, 2013; Meroni et al., 2009; Middleton et al., 2010; Moya et al., 2004; Rascher et al., 2009). The filling-in of solar Fraunhofer lines by terrestrial fluorescence at wavelengths on both shoulders of the O_2 -A absorption band (755 and 770 nm) has been observed using the Japanese Greenhouse gases Observing SATellite (GOSAT) (Frankenberg et al., 2011, Guanter et al., 2012; Joiner et al., 2011, 2012). Joiner et al. (2012) found a small filling-in of the broad solar Fraunhofer ionized calcium (Ca II) line at 866 nm consistent with fluorescence using the SCanning Imaging Absorption spectrometer for Atmospheric CHartography (SCIAMACHY) instrument flying on the European Space Agency's (ESA's) EnviSat.

Joiner et al. (2013) demonstrated that fluorescence can be retrieved near the 740 nm emission peak using atmospheric hyperspectral satellite-based instrumentation. They applied their approach to data from the Global Ozone Monitoring Experiment 2 (GOME-2) flying on operational European meteorological (MetOp) satellites. GOME-2 provides the highest fidelity satellite fluorescence data set currently available; the data, gridded to a spatial resolution of about 0.5° latitude by 0.5° longitude at a monthly time resolution, have estimated errors of 0.1–0.4 $\text{mW}/\text{m}^2/\text{nm}/\text{sr}$.

2.1.2. The GOME-2 instrument

GOME-2 is a grating spectrometer that measures backscattered sunlight in a nadir-viewing geometry at wavelengths between 270 and 800 nm in four separate channels (Munro et al., 2006). It has been launched on the MetOp A and B platforms on 19 October 2006 and 17 September 2012, respectively. Both MetOp A and B are in sun-synchronous orbits with an equator crossing time near 09:30 AM, but approximately 45 min (half an orbit) apart.

Here, we use data from MetOp A covering 2007–2011. We use radiances from channel 4 at a spectral resolution of ~ 0.5 nm with a signal-to-noise ratio of ~ 1000 . The nominal ground pixel lengths at nadir are approximately 40 and 80 km in the along- and across-track directions, respectively. The default swath width is 1920 km. This enables global coverage of the Earth's surface within about 1.5 days. The actual coverage for fluorescence retrievals is reduced because data in heavily clouded overcast conditions are filtered out as described in more detail below.

2.1.3. Retrieval of far-red fluorescence from GOME-2

We derive GOME-2 F_{740} primarily from the filling-in of solar Fraunhofer lines in the vicinity of the 740 nm far-red fluorescence emission peak as in Joiner et al. (2013). The basis for the retrieval relies on the fact that an additive signal such as fluorescence produces a filling-in of a solar line when an Earth backscattered spectrum is normalized with respect to the solar spectrum or a reference spectrum that does not contain fluorescence. The retrieval uses a principal component analysis approach with a simplified radiative transfer model to disentangle the spectral signatures of three basic components: atmospheric absorption, surface reflectance, and fluorescence emission. GOME-2 F_{740} is given in

radiance units ($\text{mW}/\text{m}^2/\text{nm}/\text{sr}$) and varies somewhat with viewing geometry (Guanter et al., 2012; Joiner et al., 2012).

The retrieval algorithm performed well when tested with simulated data and was applied to radiances from GOME-2 (Joiner et al., 2013). Fluorescence from GOME-2 compared well in terms of spatial and temporal variability with that from GOSAT (Guanter et al., 2012) obtained with a more simple retrieval approach. The GOME-2 fluorescence data set provides substantially improved sampling and precision (and therefore spatial resolution) as compared with GOSAT; therefore only GOME-2 data are used in this study.

We have made some minor changes to the approach of Joiner et al. (2013) that bring the GOME-2 results into slightly better agreement with GOSAT and reduce small biases where no fluorescence is expected. We use a spectral fitting window between 715 and 758 nm and a single set of principal components (PCs), derived from cloudy data over ocean, to estimate the spectral structure of atmospheric absorption; absorption is dominated by water vapor over this spectral range. The O_2 A-band is not included in the fitting window. The principal components are derived from radiance spectra here as opposed to the logarithm of the radiance spectra as in Joiner et al. (2013). We also attempted to correct for drift in the absolute instrument calibration by fitting a degradation factor to the GOME-2 solar spectra.

2.1.4. Processing of GOME-2 fluorescence retrievals

For cloud screening of GOME-2 data as in Joiner et al. (2013), we make use of the concept of the effective cloud fraction, f_e , described in detail by Stammes et al. (2008). f_e can be computed by inverting the following equation:

$$I_m = I_{\text{clr}}(1 - f_e) + I_{\text{cld}}f_e, \quad (4)$$

where I_m is the measured radiance, and I_{clr} and I_{cld} are considered to be clear and cloudy subpixels (i.e., the independent pixel approximation). I_{clr} is computed using a surface albedo data set as described in Joiner et al. (2013) and I_{cld} is modeled as a Lambertian surface with an effective reflectivity of 0.8. In this mixed Lambertian model of cloudy scenes, f_e is not a true geometrical cloud fraction, but rather represents an estimated fraction of the surface that is completely shielded by clouds (i.e., the satellite sensor sees only the clear fraction of a pixel approximated by $1 - f_e$).

Here, we retain only pixels with $f_e < 40\%$. The impact of this empirically chosen threshold is described in more detail in Section 3. Due to uncertainties in the GOME-2 absolute calibration and the surface albedo data set used in the calculation of f_e , our cloud screening procedure primarily removes heavily clouded (overcast) pixels; cases of thin and broken clouds are retained in the sample. Clouds do not affect the spectral signature of fluorescence as is the case for vegetation indices derived from satellite reflectances. Therefore, the main effect of clouds on fluorescence measurements is a shielding effect, i.e., a fraction of the surface is shielded by clouds/aerosol from satellite observation. Radiative transfer simulations show that a substantial fraction of the fluorescence signal ($\sim 80\%$) can penetrate through clouds/aerosols of low to moderate optical thickness (up to 5) (Frankenberg, O'Dell, Guanter, & McDuffie, 2012). Joiner et al. (2012) similarly estimate that with a 40% geometrical cloud cover, 80% or more of the surface will be seen for cloud optical thicknesses up to 10.

We generate climatological 8 day mean GOME-2 F_{740} values using GOME-2 data averaged over the time period Jan. 2007 through Dec. 2011. The 8-day intervals were chosen to match those of the MODIS fPAR (MOD15) data set as described below. For comparison with data from a given flux tower site, we average quality-controlled pixels that have centers within 1° latitude and 1° longitude of the tower location; we apply quality control checks as described in Joiner et al. (2013) In addition, we use only GOME-2 pixels with solar zenith angles (SZA) less than 70° to avoid possible biases due to rotational-Raman scattering (Vasilkov, Joiner, & Spurr, 2013).

Table 1
Network sites used in analysis (see text for more details).

Code	State/country & name	Years	IGBP ^a	IGBP ^b	%	Reference
AU-Fog	Fogg Dam, Australia	2006–2007	WET	SAV	72.2	Beringer, Livesley, Randle, and Hutley (2013), Ma et al. (2013)
AU-How	Howard Springs, Australia	2001–2006	WSA	SAV	61.1	Beringer et al. (2011), Ma et al. (2013)
AU-Tum	Tumbarumba, Australia	2001–2006	EBF	EBF	41.0	Bonan et al. (2011)
AU-Wac	Wallaby Creek, Australia	2005–2007	EBF	EBF	43.8	Kilinc, Beringer, Hutley, Tapper, and McGuire (2013)
BW-Ma1	Maun–Mopane Woodland, Botswana	1999–2001	WSA	SAV	91.0	Veenendaal, Kolle, and Lloyd (2004)
CA-Mer	Quebec Eastern Peatland–Mer Bleue	1998–2005	WET	DBF	70.1	Lafleur, Roulet, and Admiral (2001), Kross (2011)
CA-Qcu	Quebec Boreal Cutover Site	2001–2007	ENF	ENF	72.2	Giasson, Coursolle, and Margolis (2006)
DE-Tha	Anchor Station Tharandt, Germany	1996–2007	ENF	MF	67.4	Grünwald and Bernhofer (2007)
IL-Yat	Yatir, Israel	2001–2006	ENF	SH	45.1	Rotenberg and Yakir (2010)
IT-Amp	Amplero, Italy	2002–2006	GRA	MF	67.4	Gilmanov et al. (2010)
IT-Cpz	Castelporziano, Italy	1997–2007	EBF	WAT	45.1	Garbulsky, Penuelas, Papale, and Filella (2008)
IT-Ro1	Roccarespampani, Italy	2000–2007	DBF	MF	53.5	Migliavacca et al. (2010)
NL-Hor	Horstermeer, Netherlands	2004–2007	GRA	CRO	54.9	Hendriks, van Huissteden, Dolman, and van der Molen (2007, 2008)
NL-Loo	Loobos, Netherlands	1996–2007	ENF	CRO	48.6	Elbers, Jacobs, Kruijt, Jans, and Moors (2011)
US-ARM	OK ARM Southern Great Plains–Lamont	2000–2007	CRO	GRA	44.4	Billesbach, Fischer, Torn, and Berry (2004)
US-Aud	AZ Audubon Research Ranch	2002–2006	GRA	SAV	47.2	Gilmanov et al. (2010)
US-Bar	NH Bartlett Experimental Forest	2004–2006	DBF	DBF	70.1	Jenkins et al. (2007)
US-Bkg	SD Brookings	2004–2006	GRA	CRO	79.2	Gilmanov et al. (2005)
US-Blo	CA Blodgett Forest	1997–2007	ENF	ENF	53.5	Goldstein et al. (2000)
US-Bo1	IL Bondville	1996–2007	CRO	CRO	77.1	Turner, Urbansky et al. (2003)
US-Dk3	NC Duke Forest Loblolly Pine	1998–2005	ENF	MF	45.8	Luo et al. (2001), Stoy et al. (2008)
US-FPe	MT Fort Peck	2000–2006	GRA	GRA	66.7	Gilmanov et al. (2003)
US-Goo	MS Goodwin Creek	2002–2006	GRA	DBF	50.0	Yuan et al. (2007)
US-Ha1	MA Harvard Forest EMS Tower (HFR1)	1991–2006	DBF	DBF	97.2	Urbanski et al. (2007), Goulden, Munger, Fan, Daube, and Wofsy (1996)
US-Ho1	ME Howland Forest (main tower)	1996–2004	ENF	MF	61.8	Thornton et al. (2002)
US-Ho2	ME Howland Forest (west tower)	1999–2005	ENF	MF	61.8	Thornton et al. (2002)
US-IB1	IL Fermi Agricultural	2005–2007	CRO	CRO	50.7	Xiao et al. (2008)
US-IB2	IL Fermi Prairie	2004–2007	GRA	CRO	50.7	Xiao et al. (2008)
US-Los	WI Lost Creek	2000–2006	CSH	MF	92.4	Sulman, Desai, Cook, Saliendra, and Mackay (2009), Desai et al. (2008)
US-MMS	IN Morgan Monroe State Forest	1999–2006	DBF	MF	37.5	Schmid, Grimmond, Cropley, Offerle, and Su (2000), Dragoni, Schmid, Grimmond, and Loescher (2007)
US-MOz	MO Missouri Ozark Site	2004–2007	DBF	DBF	59.7	Gu et al. (2003, 2006, 2012)
US-Me2	OR Metolius Intermed. Pine	2002–2007	ENF	ENF	56.2	Loescher et al. (2006)
US-Me3	OR Metolius Second Young Pine	2004–2005	ENF	ENF	56.2	Loescher et al. (2006)
US-Me4	OR Metolius-old aged ponderosa pine	1996–2000	ENF	ENF	56.2	Loescher et al. (2006)
US-Me5	OR Metolius First Young Pine	1999–2002	ENF	ENF	56.2	Loescher et al. (2006)
US-NR1	CO Niwot Ridge	1998–2007	ENF	ENF	41.0	Monson et al. (2002)
US-Ne1	NE Mead – irrigated continuous maize	2001–2006	CRO	CRO	97.9	Suyker, Verma, Burba, and Arkebauer (2005), Verma et al. (2005)
US-Ne2	NE Mead – irrigated maize–soybean rot.	2001–2006	CRO	CRO	97.9	Suyker et al. (2005), Verma et al. (2005)
US-Ne3	NE Mead – rainfed maize–soybean rot.	2001–2006	CRO	CRO	98.6	Suyker et al. (2005), Verma et al. (2005)
US-Oho	OH Oak Openings	2004–2005	DBF	CRO	69.4	Sun et al. (2010)
US-PFa	WI Park Falls/WLEF	1995–2005	MF	MF	96.5	Davis et al. (2003) Desai et al. (2008)
US-SO2	CA Shy Oaks Old	1998–2006	CSH	SH	72.9	Stylinski, Gamon, and Oechel (2002)
US-SP1	FL Slashpine–Austin Cary–65 yr nat regen	2000–2006	ENF	MF	47.2	Powell et al. (2008)
US-SP2	FL Slashpine–Mize–clearcut–3 yr regen	1998–2005	ENF	MF	47.2	Bracho et al. (2012)
US-SP3	FL Slashpine–Donaldson–mid–rot–12 yr	1999–2005	ENF	MF	47.2	Bracho et al. (2012)
US-Shd	OK Shidler Tallgrass Prairie	1997–2000	GRA	GRA	44.4	Gilmanov et al. (2003)
US-Syv	MI Sylvania Wilderness Area	2001–2006	MF	MF	88.9	Desai, Bolstad, Cook, Davis, and Carey (2005)
US-Ton	CA Tonzi Ranch	2001–2007	WSA	SAV	55.6	Sims et al. (2005)
US-UMB	MI Univ. Mich. Biological Station	1999–2006	DBF	MF	84.7	Gough, Hardiman, Vogel, Nave, and Curtis (2010)
US-Var	CA Vaira Ranch–Ione	2000–2007	GRA	SAV	55.6	Sims et al. (2005)
US-WBW	TN Walker Branch Watershed	1995–2000	DBF	MF	49.3	Misson et al. (2007)
US-WCr	WI Willow Creek	1998–2006	DBF	MF	99.3	Cook et al. (2004)
ZA-Kru	Skukuza–Kruger Natl. Park, South Africa	2001–2003	SAV	SAV	75.7	Scholes et al. (2001)

^a IGBP vegetation type at site – CRO: Croplands; CSH: Closed Shrublands; DBF: Deciduous Broadleaf Forest; EBF: Evergreen Broadleaf Forest; ENF: Evergreen Needleleaf Forest; GRA: Grasslands; GMF: Grass + Mixed Forest; MF: Mixed Forest; OSH: Open Shrublands; SAV: Savannas; SH: Shrublands; WET: Wetlands; WSA: Woody Savannas.

^b Predominant IGBP type within satellite averaging area (see text) where WSA and SAV are combined as SAV, CSH and OSH as SH, and MF and GMF as MF.

We estimated uncertainties in each 8-day bin as the root sum square of the standard error of the mean (of all samples in the bin) and a nominal GOME-2 F_{740} constant error of $0.2 \text{ mW/m}^2/\text{nm/sr}$. The standard errors alone appear to underestimate the uncertainties as the large numbers of samples used in the averaging process lead to relatively small standard errors in most bins. The constant error is introduced to account for other error sources such as cloud contamination.

2.2. AmeriFlux and FluxNet tower measurements

We use quality-controlled 1/2 hourly GPP from the FluxNet synthesis project (<http://www.fluxdata.org/>) (Baldocchi et al., 2001) and additional US stations in the AmeriFlux site synthesis project (Barr, Ricciuto et al., 2013; Barr, Richardson et al., 2013). Table 1 provides tower station details including the starting and ending years of the observational record used here and the International Geosphere Biosphere Programme (IGBP) vegetation type at the station. Table 1 also lists the dominant vegetation type, according to an IGBP land cover map, corresponding to the area over which the GOME-2 F_{740} data are averaged (within 1° latitude, 1° longitude of a station location), denoted IGBP_{avg}. Here, we combined open and closed shrublands into a single type (shrublands), and woody savannas and savannas into one type (savannas). Our mixed forest type contains the IGBP type ‘grass + mixed forest’ in addition to ‘mixed forest’. We provide the approximate percentage (%) of the satellite-averaging box covered by the dominant vegetation type IGBP_{avg} in Table 1. Fig. 1 displays locations and vegetation types in a mapped format.

We compute 8-day means of GPP estimated from the tower data in a manner similar to our processing of GOME-2 data. Each 8-day value is

an average over all available years for a particular tower. The 8-day intervals match those of the MOD15 data set. We do not include gap-filled data in our data processing. We use all available GPP data regardless of the cloud conditions and average data over all hours. We checked that the derived seasonal cycle of GPP does not change substantially if we use only data near the satellite overpass time.

For inclusion of a site in our analysis, at least 40 quality-controlled GOME-2 pixels must have been collected for a given 8 day period and at least 75% of the 8-day bins within the year must be filled. Unfortunately, the tower observational time records do not generally coincide with those of GOME-2. Therefore, we must compare seasonal cycles that have been averaged over different sets of years (for each site). This may produce some differences between the tower and other satellite data sets as there can be interannual variability, particularly in the initiation of photosynthesis (e.g., Gu et al., 2008). Comparisons of derived seasonal cycles of photosynthesis from flux towers and GOME-2 satellite data are considered to be climatological. By using averages over several years, we may smooth out some of the interannual variability.

Uncertainties in the GPP derived from flux tower measurements have been computed for the Ameriflux sites (Schaefer et al., 2012); total uncertainties include contributions from random errors, threshold friction velocity uncertainty, and partitioning uncertainty (owing to uncertainty in the estimated ecosystem respiration). The partitioning uncertainty is based on the variance produced by different partitioning algorithms (Desai et al., 2008). Random uncertainty is the largest contributor to the total uncertainties (50–90%).

Using the available Ameriflux data, we find that total uncertainties in the weekly-mean GPP (GPP_{weekly}) varies with GPP_{weekly} . We fit a general exponential function to the Ameriflux data to approximate the weekly-averaged total GPP uncertainties ($\sigma_{GPP_{\text{tot}}}$), i.e.,

$$\sigma_{GPP_{\text{tot}}} = 0.5085 * e^{0.1088 * GPP_{\text{weekly}}} \tag{5}$$

We then apply this formulation to all tower sites to approximate uncertainties in the derived 8-day GPP.

2.3. The MPI-BGC data-driven model of GPP

Estimates of GPP from the Max Planck Institute for Biogeochemistry (MPI-BGC) originate from upscaling a global dataset of eddy covariance based measurements (Jung et al., 2011). A machine learning algorithm (Model Tree Ensembles, MTE) as described by Jung, Reichstein, & Bondeau (2009) was trained to predict monthly observed GPP at the tower sites based on remotely sensed fPAR, climate, and vegetation type data. The trained model was then applied using spatial grids of the explanatory variables to generate global monthly GPP estimates at a 0.5° spatial resolution (see Jung et al., 2011, for details).

We averaged monthly MPI-BGC GPP estimates from Jan. 2007–Dec. 2011, the same time period used for GOME-2 data. We then averaged all gridboxes within 1° latitude and longitude of each flux tower location, the same spatial scale as represented by the GOME-2 data. We may then use the upscaled MPI-BGC GPP estimates to assess the effect of the different spatial scales of the flux tower and GOME-2 satellite data. We use Eq. (5) to estimate uncertainties in the upscaled GPP.

2.4. GPP model ensemble

We also examine seasonal cycles (weekly output) of GPP as produced by an ensemble of 24 models that were used in the study of Schaefer et al. (2012). MPI-BGC is not included in the ensemble. The models were driven with gap-filled meteorological data from each tower site. Other input parameters and biophysical characteristics

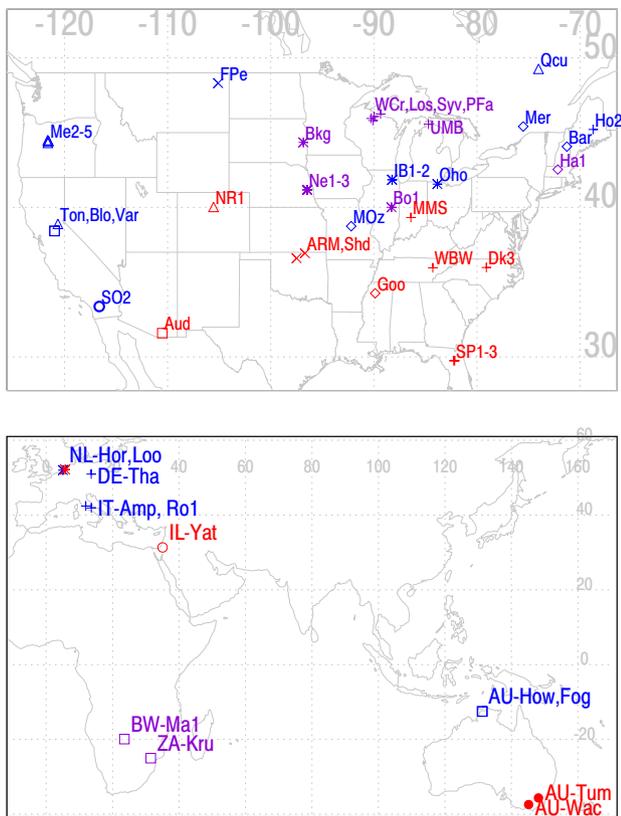


Fig. 1. Locations of flux towers and their designations used in this study; purple, blue, and red indicate that the primary vegetation type (IGBP) covers approximately 75–100%, 50–75%, and 0–50%, respectively, of the surrounding satellite averaging area; symbols show dominant vegetation type for the satellite averaging area; +: Mixed Forest (including ‘grass + MF’); *: Croplands; x: Grasslands; ◊: Deciduous Broadleaf Forest; △: Evergreen Needleleaf Forest; square: Savannas (including woody); ○: Shrublands (open and closed); ●: Evergreen Broadleaf Forest. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

were derived from local observations as discussed in Schaefer et al. (2012).

The model ensemble includes 14 physically-based models that have prognostic phenology and 10 data-driven models that use remote sensing data to determine leaf area index (LAI) and/or GPP. The models were classified in Schaefer et al. (2012) as either enzyme-kinetic (EK) (17 models) or LUE (7) models. Both EK and LUE groupings include a combination of data-driven and physically-based approaches to estimate LAI and/or GPP. Because some of the models are targeted for a particular biome (e.g., forest or agriculture), not all of the models produced a simulation for a given site. Therefore, each site has a different model ensemble associated with it.

2.5. MODIS fPAR/APAR (MOD15)

We used 8-day means of the canopy fPAR derived from the Terra MODIS collection 5 (MOD15A2) (Myneni et al., 2002) obtained from the Oak Ridge National Laboratory's Distributed Active Archive Center (ORNL DAAC, 2010). We used quality controlled data averaged over approximately 7 km × 7 km regions centered on a flux tower. The original data are produced as an 8-day maximum value composite at 1 km spatial resolution. Because the MODIS data set is produced as a composite using maxima rather than means (as was done for the F_{740} and tower GPP data) and are then specified as a single value at the midpoint of the compositing period, it should be noted that the values may be weighted towards earlier dates in spring during the onset of greening (by up to ~4 days or half the compositing period) and similarly towards later dates in autumn as greenness is declining.

APAR values are computed using the MOD15A2 fPAR × cos(θ), where θ is the average solar zenith angle for each time period near the MetOp-A and Terra local overpass times; cos(θ) is a proxy for the seasonal cycle of potential PAR. We compute a climatological seasonal cycle of APAR by averaging data for each 8-day interval over the time period Feb. 2000–Oct. 2011. The averaged data are then plotted at the midpoint of the time interval. We estimate uncertainties similar to what was done for GOME-2 F_{740} as described above; for each 8-day bin, we estimate the uncertainty as the root sum square of the standard error of the mean (for each 8-day interval) and a nominal constant error of 0.03 intended to account for additional error sources such as cloud contamination and compositing effects.

3. Results and discussion

3.1. Seasonal variations in tower-based and upscaled GPP, MODIS-based APAR, and GOME-2 F_{740}

In this section, we assess the ability of GOME-2 F_{740} to track the seasonality of photosynthesis as delineated by tower-based and upscaled GPP estimates. Figs. 2–3 show average seasonal cycles of GPP (normalized to unity at the maxima) from towers along with the upscaled GPP from MPI-BGC, GOME-2 F_{740} , and MODIS-based estimates of APAR, for sites representing a variety of biomes. Similar plots for the other sites listed in Table 1 are provided in the Supplemental information (SI). All GOME-2 pixels with centers within 1° latitude and longitude of the flux tower site are averaged here, and similarly all MPI-BGC gridboxes within 1° latitude and longitude of the site are averaged. The GOME-2 F_{740} and MPI-BGC GPP data are averaged over the same years (2007–2011). Therefore, we expect better agreement of GOME-2 F_{740} with MPI-BGC GPP as compared with tower-based GPP due to the closer collocation in both time and space of GOME-2 F_{740} with MPI-BGC GPP.

The tower data indicate a relatively short growing season for the agricultural Nebraska site US-Ne1 (Fig. 2a), composed of continuous maize crops. This short duration of photosynthesis is similarly shown by both GOME-2 F_{740} and the upscaled MPI-BGC GPP estimates. The upscaled GPP and GOME-2 F_{740} display a slightly wider mean growing season as compared with the tower-based GPP. This may be expected

as GOME-2 F_{740} and the upscaled GPP estimates are analyzed at similar and larger spatial scales as compared with the tower measurements. The larger footprints of GOME-2 F_{740} and MPI-BGC GPP likely contain contributions from different crops such as soybeans that have somewhat lengthier growing seasons and vegetation types other than croplands; this may explain the more gradual increases (decreases) in spring (autumn). It should be noted that monthly mean MPI-BGC GPP estimates are in excellent agreement with 8-day mean GOME-2 F_{740} ; this indicates that monthly-mean values are adequate for the present analysis.

A significantly earlier springtime rise and later autumn decline is seen in MODIS-based APAR as compared with GOME-2 F_{740} and the GPP estimates for the US-Ne1 agricultural site and similarly for the agricultural US-IB1 site (see SI). The later decline in autumn may be expected as APAR does not contain information about LUE and therefore may remain high in the presence of green vegetation that is not engaging in photosynthesis. However, the almost symmetrical early rise in spring is more difficult to explain as green vegetation in spring should be photosynthetically-active.

One explanation is that the reflectances used to generate MODIS (MOD15) fPAR are sensitive to pigments in vegetation and soil other than chlorophyll. It has been shown that the MOD15 estimate of fPAR applies to the whole vegetation canopy, both photosynthetic and nonphotosynthetic components, and does not provide consistent relationships to photosynthetic processes at the ecosystem scale (Turner, Ritts et al., 2003; Turner, Urbansky et al., 2003; Turner et al., 2006; Zhang et al., 2009). Alternative methods have emerged to improve estimates of fPAR related to only the photosynthetic component (see Zhang, Middleton, Cheng, & Landis, 2013, and references therein). One such approach involves the retrieval of a new fPAR parameter related only to the chlorophyll-containing foliage (called fPAR_{chl}) (Zhang et al., 2005, 2006, 2009; Zhang, Middleton, Gao, & Cheng, 2012). This parameter shows a seasonal cycle more consistent with tower-based GPP for several tower sites used in our study including the agricultural sites US-Ne2 and US-Ne3, and a deciduous broadleaf forest site (US-Bar) (Cheng, Zhang, Lyapustin, Wang, & Middleton, 2014).

The MODIS-based APAR also shows a slightly earlier spring onset of activity for the northern deciduous broadleaf forest (DBF) and mixed-forest (MF) sites (US-UMB and US-Ha1) in Fig. 2b and c, respectively, and is lagged in the autumn decline with respect to the tower GPP at these sites. We note that MODIS fPAR typically stays above 0.2 throughout the year for these sites. For some sites such as US-Ha1, fPAR remains very high (~0.5) throughout the winter, possibly owing to contributions from evergreen needleleaf vegetation or other pigments in the woody parts of the vegetation. While multiplication of fPAR by the PAR-proxy brings MODIS-based APAR to near zero in winter, GOME-2 F_{740} minimum winter values are at or closer to zero. MODIS-based APAR shows a much closer relationship with tower-based GPP at the more southern US-Dk3 site (Fig. 2d) where GPP does not drop to zero in winter.

GOME-2 F_{740} tracks the sharp springtime rise and autumn drop in GPP, as shown in the upscaled MPI-BGC GPP product, at sites composed primarily of DBF and MF in the northeast, midwest, and southern US shown in (US-Ha1, US-UMB, and US-Dk3 sites in Fig. 2b–d, respectively). Similar results are obtained at other US DBF and MF sites in the northeast and midwest US (see SI) such as US-Syv, US-PFa, US-WCr, and US-MMS (stations in Wisconsin and Indiana) and New England sites (US-Bar and US-Ho1,2). The GOME-2 F_{740} and MPI-BGC GPP seasonal variations also closely follow those from the tower-based GPP estimates at these relatively homogeneous sites.

For most forested sites, GOME-2 F_{740} appears to begin to decline slightly earlier than both GPP estimates. This decline, starting near summer solstice, is consistent with seasonal changes in leaf photosynthetic capacity (V_{cmax}) across a variety of tree species reported by Bauerle et al. (2012). It should be noted that the uncertainties in the tower GPP, particularly due to partitioning, are relatively large at this

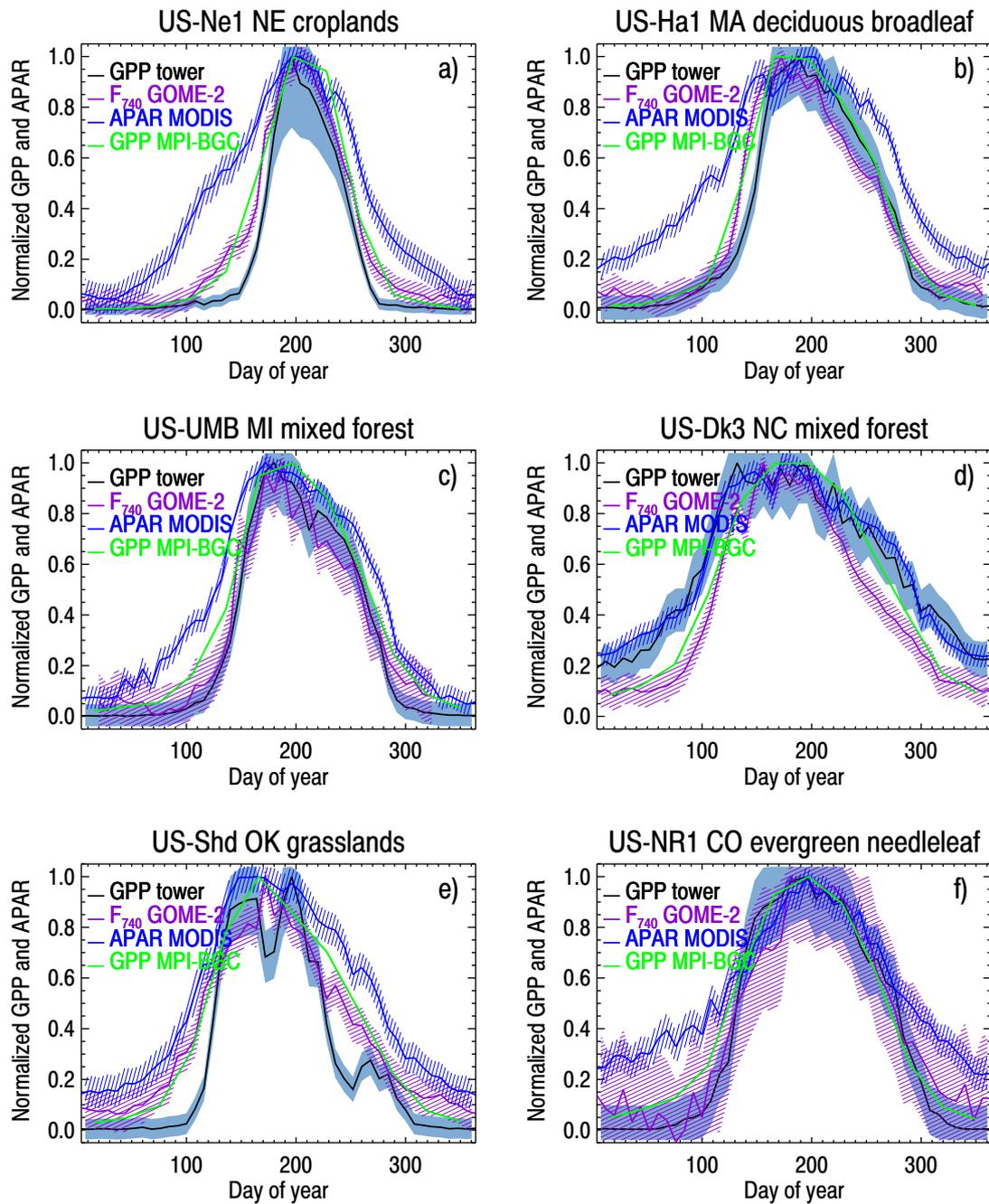


Fig. 2. Seasonal cycle (means) of tower-based and upscaled GPP from MPI-BGC, GOME-2 F_{740} , and MODIS-based APAR for a variety of vegetation types. Curves are normalized with respect to unity at the maximum annual value. Contours indicate estimated uncertainties as discussed in the text. Site names, US state, and majority vegetation type within the satellite averaging area are indicated.

time of year. Another explanation is that the seasonal variations in fluorescence efficiency differ slightly from those of light use efficiency.

The Oklahoma US-Shd site shown in Fig. 2e is relatively heterogeneous in terms of vegetation type in the surrounding satellite averaging area and is composed primarily of grasslands. The upscaled GPP from MPI-BGC shows a somewhat more broad and smooth seasonal cycle as compared with the tower-estimated GPP. GOME-2 F_{740} agrees to within estimated uncertainties with the MPI-BGC GPP at this site, while the MODIS APAR shows a more lengthy duration of activity.

GOME-2 F_{740} and MPI-BGC upscaled GPP compare reasonably well with each other as well as with tower GPP at the evergreen needleleaf forest (ENF) US-NR1 site (Fig. 2f). MODIS-based APAR does not show a drop to near zero in winter. This is likely a result of the evergreen vegetation or other non-photosynthetic components that are absorbing

PAR in winter but not engaging in photosynthesis. The GOME-2 F_{740} errors are proportionally higher for this site as compared with the others owing to the overall lower observed values. Therefore, the empirically-derived constant component of the error ($0.2 \text{ mW/m}^2/\text{nm/sr}$) produces an effectively lower signal-to-noise ratio for sites with lower fluorescence signals. Other examples are shown in the Supplemental material for shrublands and savannas that also display low fluorescence values.

The seasonality of GPP and GOME-2 F_{740} at the savanna tower sites in Africa and Australia (see Fig. 3a and c) shows similar patterns. In both cases MODIS-based APAR does not display as much variability as GOME-2 F_{740} or the GPP estimates. In contrast, the evergreen broadleaf forest site in Australia (Fig. 3b) shows different seasonality of both upscaled MPI-BGC GPP and GOME-2 F_{740} as compared with MODIS-

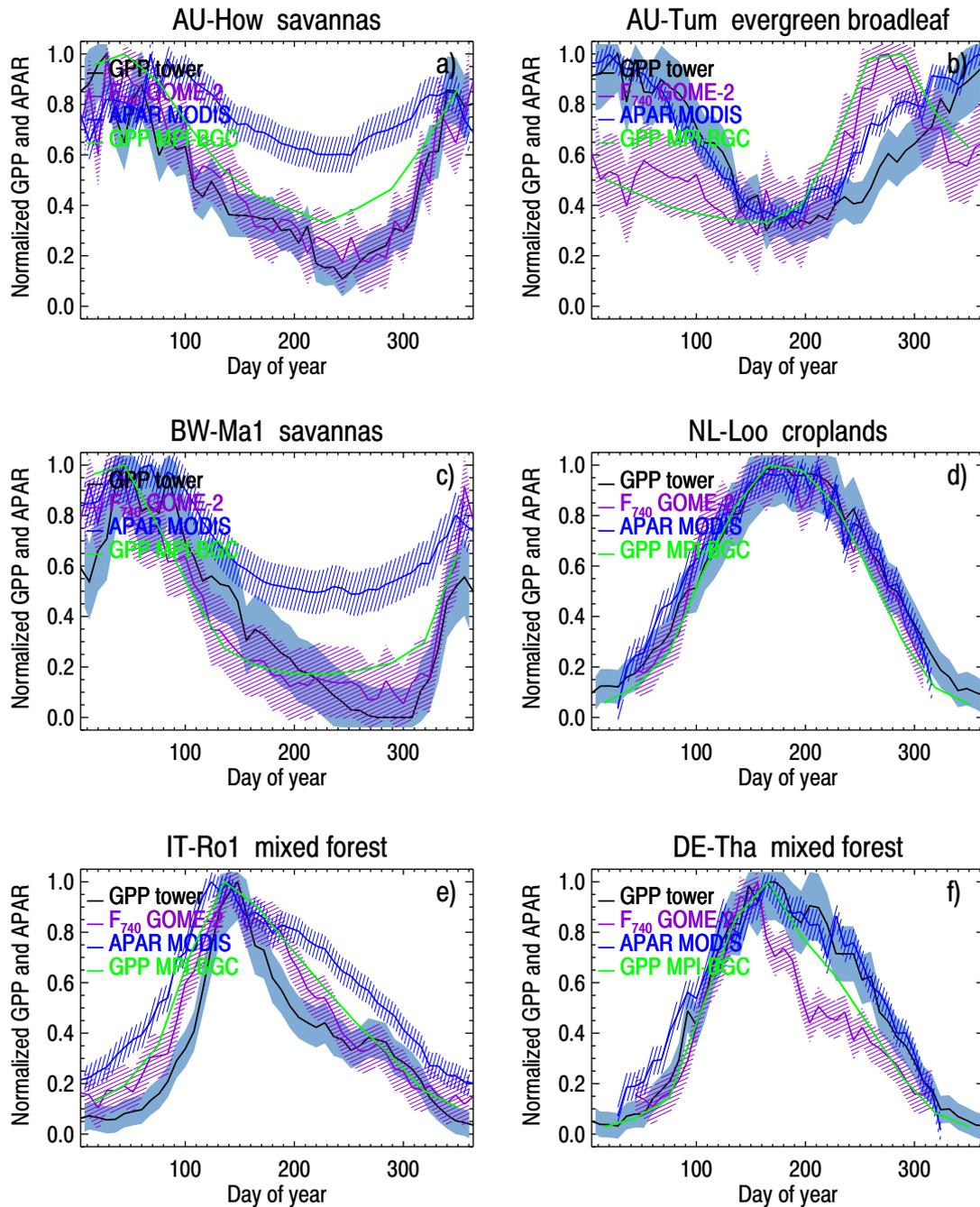


Fig. 3. Similar to Fig. 2 but showing sites from Australia, Africa, and Europe for a variety of vegetation types.

based APAR and tower GPP. This is likely due to spatial heterogeneity around the site that is surrounded by pastures that display a peak in GPP around day 280 similar to that shown in MPI-BGC GPP and GOME-2 F_{740} (J. Beringer, private communication, 2014).

GOME-2 F_{740} tracks the seasonality of GPP reasonably well for the European sites dominated by croplands and mixed-forest within the satellite averaging area (Fig. 3d–f). It should be noted that these sites are also relatively heterogeneous as indicated by differences shown in sites contained within approximately the same satellite averaging area (see SI). In these cases, GOME-2 F_{740} is in good agreement with the upscaled MPI-BGC GPP estimates. However, as shown for the mixed-forest dominated US sites and discussed above, a somewhat earlier decline at the start of senescence is shown for GOME-2 F_{740} as compared with the GPP estimates for the DE-Tha site (Fig. 3f).

In order to show that the displayed seasonal variability of GPP is not driven primarily by the seasonality of PAR, we alternatively repeated this comparison by normalizing GPP estimates and GOME-2 F_{740} with respect to incoming potential PAR (results not shown). This analysis showed that the seasonality of GPP (and GOME-2 F_{740}) is dictated largely by that of LUE and fPAR. Results in Cheng et al. (2014) support this conclusion.

The general conclusions discussed above were not substantially impacted by varying the value of the f_e threshold for the GOME-2 F_{740} data. We also checked whether the conclusions hold if tower data are filtered for clouds using the reported incident short-wave radiation. While cloud filtering quantitatively affects monthly-mean GPP and to some extent GOME-2 F_{740} values (changes absolute values), it does not substantially alter the qualitative spatio-temporal variations of normalized GPP.

3.2. Comparisons with multi-model mean weekly GPP

In this section, we examine whether GOME-2 F_{740} offers a means to constrain or validate global vegetation models in terms of the simulated seasonality of photosynthesis. Fig. 4 shows the multi-model weekly mean GPP from data driven (DD) and prognostic (Prog) models along with the tower-based GPP and GOME-2 F_{740} for the same sites as in Fig. 2. The multi-model means, particularly for the DD models, show a somewhat lengthier duration of photosynthesis for northern and midwestern DBF and MF sites such as US-Ha1 and US-UMB, the agricultural US-Ne1 site, and the grasslands US-Shd site as compared with tower-based GPP. Like the MODIS APAR estimates, the models, especially DD models, show better agreement of the estimated GPP seasonal cycle with the tower data for the southern MF-dominated US-Dk3 site.

The models also generally fall within the range of observational uncertainties for the ENF-dominated US-NR1 site.

Some of the DD models contained in the multi-model means calculate GPP using the LUE model as in Eq. (1). Errors in these types of models can result from errors in $fPAR$ and/or LUE. In areas containing dormant green vegetation, such as MF and ENF in winter, APAR may remain high owing to the greenness of the vegetation (including non-chlorophyll containing pigments) when solar radiation is being absorbed but not used for photosynthesis. In this situation, models that utilize reflectance-based parameters like $fPAR$ must then depend upon their LUE parameterization to control GPP.

In regions with cold winters, low winter temperatures are generally sufficient to reduce LUE and subsequently GPP; when LUE can be estimated reliably as near or equal to zero (e.g., temperatures near or

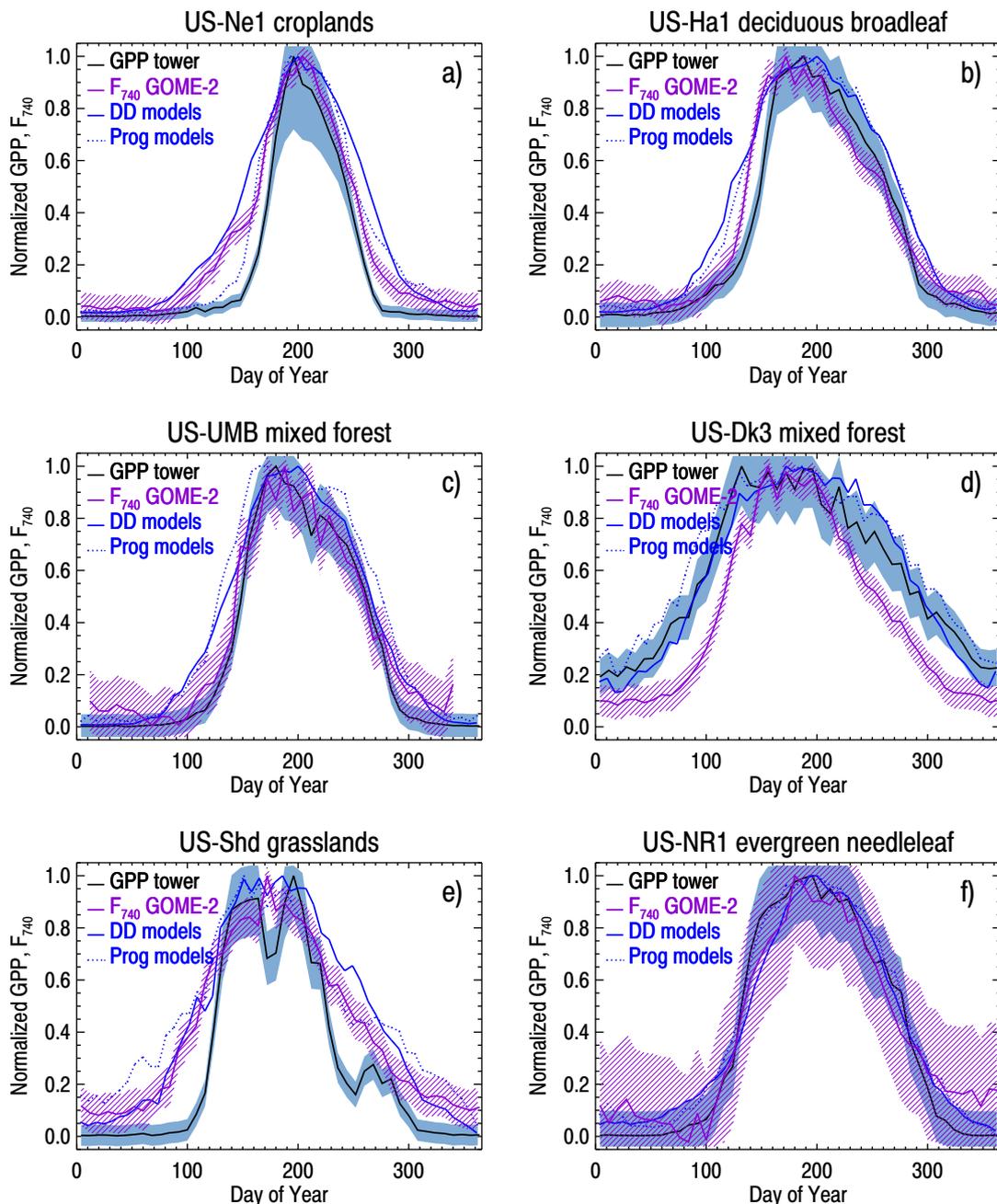


Fig. 4. Similar to Fig. 2 showing seasonal variability in tower-based GPP, GOME-2 F_{740} , and multi-model ensemble means that use data-driven (DD) and prognostic (Prog) approaches to estimate LAI/GPP.

below freezing), it can be assumed that GPP is likewise near or equal to zero. Under these conditions, the GPP estimate is not influenced by any errors in fPAR/APAR.

However, in areas where temperatures are near or above freezing outside of the main part of growing season and fPAR remains high, it is more challenging to estimate the spring initiation and autumn decline of photosynthesis through the LUE parameterization. As a result, an incorrect GPP may be generated outside the main growing season when fPAR is at a moderate value. This has been reported previously for the MODIS GPP product (MOD17) (Heinsch et al., 2006; Turner, Ritts et al., 2003; Turner et al., 2006); MOD17 is one of the models contained in our data-driven ensemble and one that specifically uses the MOD15 fPAR product. Improved seasonal cycles of GPP have been obtained in an LUE model by using fPAR_{chl} as compared with MODIS fPAR (fPAR_{canopy}) (Cheng et al., 2014).

Our results suggest that GOME-2 F_{740} may provide an additional constraint for estimating the seasonal rise and fall of GPP, particularly for the deciduous and mixed forest sites. Given the results shown in the previous subsection, it is suggested that F_{740} can offer estimates of the seasonality of photosynthesis in areas not well covered by flux tower measurements that can be used for model validation. In addition, GOME-2 F_{740} provides a global data set at a spatial resolution similar to that of global models.

3.3. Timing indicators associated with different stages of photosynthetic activity

There is no standard way to compute phenological indicators, such as onset of greenness or photosynthetic activity in spring, using satellite data (Fisher, Mustard, & Vadeboncoeur, 2006; Gu et al., 2003). It has been shown for deciduous vegetation and many crops that the spring pattern of leaf emergence, followed by rapid growth, and then a stable period of maximum leaf area can be represented using a logistical model (e.g., Zhang et al., 2003, and references therein). A reverse pattern can be modeled for the transition from senescence to dormancy.

We identify various timing indicators following the approach of Zhang et al. (2003) as illustrated in Fig. 5 for the US-Bar site. We have augmented the approach by computing uncertainties for the indicators as described below. The first step is to fit either the greenup or senescence portions of the seasonal cycle of the various parameters (GPP, MODIS APAR, or GOME-2 F_{740}) to a function of the form

$$y(t) = \frac{c}{1 + e^{a+bt}} + d. \quad (6)$$

Then, using the fitted parameters in Eq. (6), the rate of change in the curvature can be computed analytically. Transition dates are defined for the times when the rate of change in the curvature reaches local minima or maxima.

In the greenup (or declining) portion of the seasonal cycle, the photosynthetic (or senescence) onset is defined as the first peak/valley in the curvature-change rate. The next large peak is known as the inflection or stability point where GPP or satellite parameters are changing at a large rate. The last peak occurs at the onset of maximum photosynthetic activity in the greenup portion or at the onset of dormancy in the declining phase.

Here, we focus exclusively on forested and cropland sites in North America for which this fitting approach works well. We inspected the results for each site and discarded a few sites (e.g., US-Bkg, US-MOz, US-SP1–3) where the fitting procedure was not well behaved (e.g., owing to a too narrowly peaked maximum, multiple peaks, or incomplete dormancy).

To compute the uncertainties in the timing indicators, we use a Monte Carlo approach centered about the initial fit with 1000 perturbations. To illustrate the range of uncertainties for the rate of change in

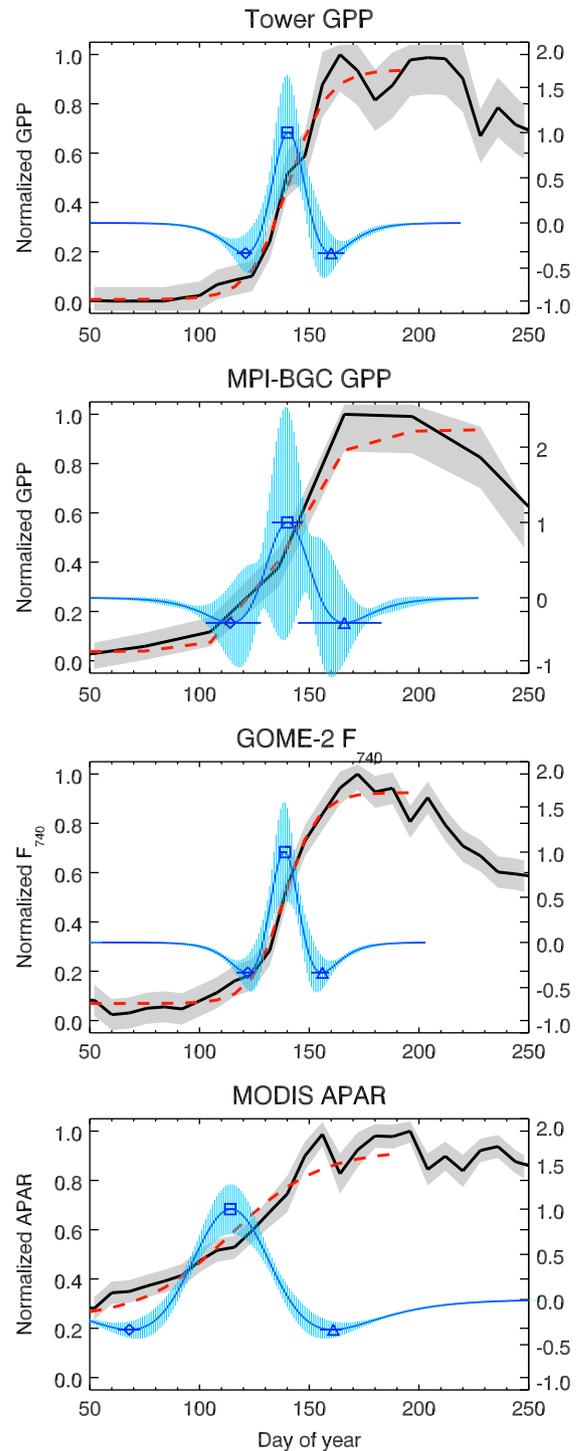


Fig. 5. Example of how timing indicators are computed at US-Bar tower; black solid line with gray shading: Normalized curves corresponding to left axes with associated uncertainties; blue solid with vertical bar shading: computed rate of change in the curvature from the fitting logistical function with computed error standard deviations along with timing indicators (symbols) and corresponding uncertainties (1σ , horizontal line) from the Monte Carlo simulation corresponding to right-side axes. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

curvature shown in Fig. 5, we use standard linear error analysis to propagate observation errors through the fitting procedure. Specifically, we compute the Jacobian of Eq. (6), K , and assume that the observation error covariance matrix, S_y , is a diagonal matrix (i.e., errors are assumed

to be unbiased and uncorrelated with respect to each other). The estimated error covariance for the fitted parameters in Eq. (6), S_f , is given by

$$S_f = \left(K^t (S_y)^{-1} K \right)^{-1} \quad (7)$$

S_f is then further propagated linearly using Eq. (7) with the analytically computed Jacobian of the rate of change of curvature function (see Zhang et al., 2003, for formulation of the rate of change of curvature). This provides a full error covariance for the rate of change of curvature. We show the error standard deviations for reference in Fig. 5 (note that errors are correlated with respect to each other). The errors from the Monte Carlo simulation for the timing parameters are also shown in Fig. 5.

The computed timing indicators and associated uncertainties are shown in Figs. 6–7 for tower and upscaled GPP, GOME-2 F_{740} , MODIS APAR, and the multi-model mean (results from both DD and Prog models are averaged together here). Note that the indicators for the multi-model means are available only for Ameriflux sites. Bias and χ^2 statistics with respect to the tower GPP (considered as the standard) are computed and averaged for each vegetation type and summarized in Table 2. Again, note that the multi-model mean uses only the available Ameriflux sites to compute these statistics.

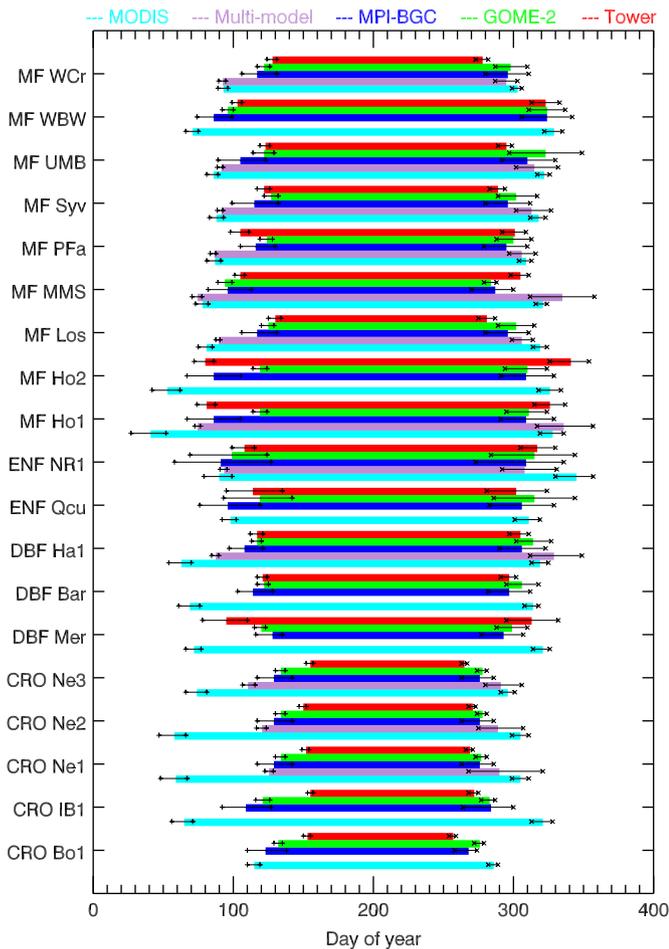


Fig. 6. Summary of the duration of photosynthesis from the photosynthetic onset (left end of horizontal bars with uncertainties indicated) to the dormancy onset (right end of horizontal bars) (see text for details) for various forest and cropland sites and data sets. The site name and majority IGBP vegetation type are indicated on the left. Timing indicators derived from the multi-model mean data are only available for Ameriflux sites. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

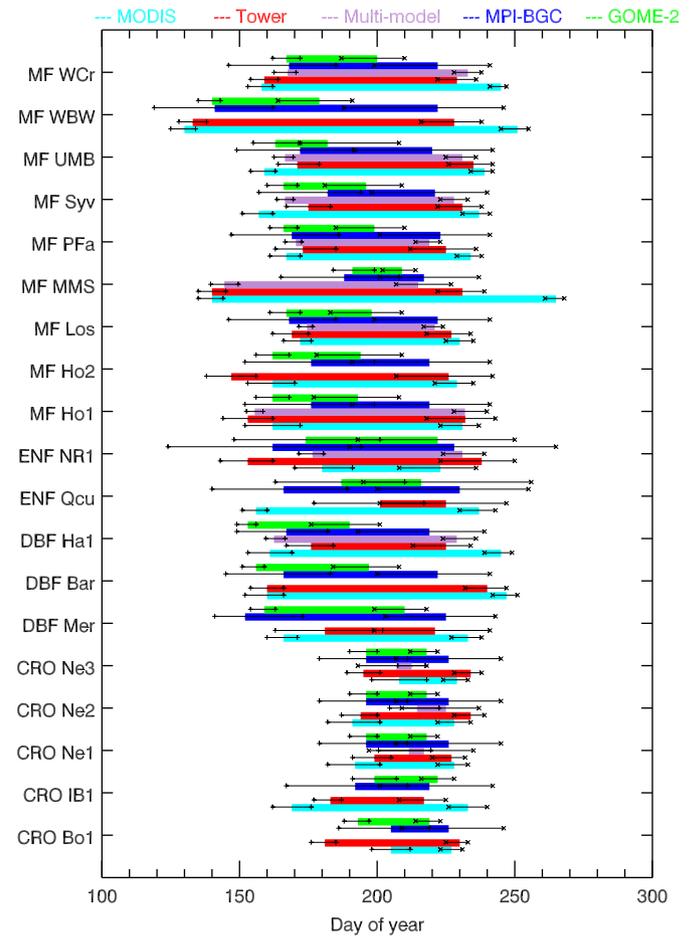


Fig. 7. Similar to Fig. 6 but showing the duration of maximum photosynthesis from onset of maximum photosynthesis (left end of horizontal bars) to the senescence onset (right end of horizontal bars).

Fig. 6 shows the duration of photosynthesis (similar to the carbon uptake period), from the onset of photosynthesis (the left edge of the various colored bars with corresponding uncertainties) to the onset of dormancy on the right edge of the bars. For MF and DBF sites in the northeast and northern midwest US, the photosynthesis onset according to the tower-based data occurs between about days 70 and 130. For these sites, both the MPI-BGC GPP and GOME-2 F_{740} track the tower onset reasonably well, while MODIS-based APAR shows a substantially earlier rise ranging from ~days 60–90. The multi-model mean shows a similar early onset of photosynthesis for many of these sites. Photosynthetic onset from MODIS APAR compares better with the tower data for the ENF-dominated sites.

For the midwest cropland sites, the onset of photosynthesis occurs much later, generally around day 150 according to the tower estimates. The larger scale GOME-2 F_{740} and MPI-BGC GPP detects photosynthetic onset somewhat earlier, around days 110–135, likely due to a mixture of other vegetation types within their averaging area. Despite the fact that the MODIS data are averaged over a much smaller area near the tower site, the MODIS APAR results again show a substantially earlier photosynthesis onset between days 50 and 80 for all agricultural sites except US-Bo1 where the onset was near day 115. The multi-model mean onset of photosynthesis is generally comparable to the MPI-BGC GPP results for the US-NE1–3 cropland sites.

Similarly, for the onset of dormancy in Fig. 6 (the end of the colored bars), MODIS APAR is somewhat late with respect to the tower data for croplands. The MPI-BGC GPP and GOME-2 F_{740} dormancy onset estimates are closer to the tower data and also closer to each other for croplands. For most of the MF and DBF sites, GOME-2 F_{740} provides

Table 2

Statistics for various timing indicators versus the standard (tower GPP). Significant differences in terms of the χ^2 statistic (>2.0) are shown in bold. The units of bias are days.

Type	Onset		Onset		Inflection		Inflection		Onset max.		Onset	
	Photosyn.		Dormancy		Spring		Autumn		Photosyn.		Senesce.	
	χ^2	Bias	χ^2	Bias	χ^2	Bias	χ^2	Bias	χ^2	Bias	χ^2	Bias
<i>MODIS APAR vs. tower GPP</i>												
CRO	71.9	−78.8	30.3	35.8	60.9	−38.0	16.7	18.6	2.3	2.6	0.6	0.6
DBF	21.0	−43.0	2.0	13.0	22.0	−26.3	5.1	12.7	0.7	−10.0	1.0	13.0
ENF	1.1	−17.0	1.1	18.5	1.4	−13.0	0.3	8.0	3.3	−9.0	0.4	−1.5
MF	21.2	−33.2	7.5	15.1	20.1	−17.1	11.5	12.9	0.8	−1.4	2.2	10.8
<i>MPI BGC GPP vs. tower GPP</i>												
CRO	3.9	−29.2	0.5	9.2	1.1	−11.0	0.1	2.6	0.3	6.6	0.1	−3.8
DBF	0.9	5.7	0.2	−6.3	0.2	−2.3	0.3	−6.7	0.4	−10.7	0.2	−6.7
ENF	0.3	−17.5	0.0	−2.0	0.7	−15.0	0.1	−3.0	0.5	−13.0	0.0	−2.5
MF	0.5	−5.9	0.7	−1.9	0.6	3.9	0.4	−5.3	0.6	13.3	0.1	−8.8
<i>GOME-2 F₇₄₀ vs. tower GPP</i>												
CRO	19.6	−22.0	5.9	11.6	3.2	−8.0	0.9	1.0	1.0	5.6	2.1	−9.4
DBF	0.5	8.7	0.4	1.3	1.4	−3.7	3.7	−14.3	1.5	−16.3	3.9	−29.7
ENF	0.0	−2.0	0.1	5.5	0.1	0.5	0.3	11.0	0.3	3.5	0.1	−12.5
MF	2.6	7.9	1.6	1.7	5.3	7.7	5.7	−16.4	2.4	7.1	3.5	−34.9
<i>Multi-model mean vs. tower GPP</i>												
CRO	47.3	−33.5	1.5	21.7	0.6	−6.2	0.2	3.0	3.0	16.8	1.2	−15.3
DBF	11.9	−29.5	1.2	23.9	14.5	−20.5	1.0	13.9	1.1	−13.5	0.1	3.9
ENF	1.2	−14.5	0.1	−9.0	0.5	4.5	0.4	−8.0	2.2	23.5	0.2	−7.0
MF	19.9	−27.6	2.1	18.6	9.7	−13.3	1.5	7.2	0.4	0.8	0.3	−4.5

dormancy onset estimates that are generally within uncertainty ranges of both MPI-BGC and tower-based GPP. The MODIS APAR and multi-model mean dormancy onset results are somewhat late with respect to the tower data for several sites but still fall within the uncertainty ranges for other sites. The dormancy onset results for the ENF sites from all estimates agree relatively well with each other to within the uncertainties.

Fig. 7 shows the duration of maximum photosynthesis from the onset of maximum photosynthesis and senescence onset; uncertainties tend to be larger for these estimates. The onset of maximum photosynthesis derived from the various datasets is in general agreement to within the relatively large uncertainties.

In contrast with the onset of dormancy, GOME-2 F_{740} shows consistently early onset of senescence for MF and DBF sites, although the error bars are quite large for some sites. This was similarly shown in Section 3.1 in the seasonal plots for representative sites. Again, this could be an indication that θ_F starts to decline slightly earlier than LUE, although errors bars for GOME-2 F_{740} and MPI-BGC generally overlap. Additional ground-based fluorescence and other measurements would be helpful to sort out this issue.

Table 2 highlights the cases of statistically significant differences in the timing indicators with respect to the tower GPP (considered to be the standard) and reinforces conclusions drawn from the barplots. For example, MODIS-based APAR and the multi-model mean show an early onset of photosynthesis for croplands, DBF, and MF in general as compared with the tower estimates. This early onset is also reflected in the multi-model mean for the same IGBP types. The early rise in MODIS APAR continues to the spring inflection point for these biomes which is not the case for the multi-model mean.

GOME-2 F_{740} and MPI-BGC GPP show an early onset of photosynthesis for croplands; this could be related to their larger spatial footprints. GOME-2 F_{740} has a significant early bias in the onset of senescence for croplands, DBF, and MF sites even with the relatively large error bars. MODIS APAR also shows later dates for dormancy onset and the autumn inflection point for some vegetation types. GOME-2 F_{740} shows a late bias in dormancy onset in croplands that again could be related to the spatial footprint. MPI-BGC GPP similarly shows a late bias, but it is not statistically significant given the estimated errors. Both MPI-BGC GPP

and GOME-2 F_{740} show early biases in the autumn inflection point for DBF and MF sites, though the biases are significant only for GOME-2 F_{740} .

Tables 3–5 summarize the results of the timing indicators for representative cropland and forested sites. The results are divided by majority biome type within the satellite averaging area and are ordered

Table 3

Summary of duration of photosynthesis, growing season (length between inflection points), and duration of maximum photosynthesis as described in the text with uncertainties in parentheses for majority agricultural sites.

Estimate	Duration of photosyn.	Duration of growing season	Duration of max. photosyn.
<i>US-Bo1 40.01°N –88.29°E</i>			
MODIS	171 (4.0)	97 (2.1)	22 (5.7)
Tower	104 (2.5)	76 (2.3)	49 (4.3)
MPI-BGC	145 (11.4)	83 (10.9)	21 (17.5)
GOME-2	144 (3.3)	85 (1.8)	26 (4.5)
<i>US-Ne1 41.17°N –96.48°E</i>			
MODIS	246 (7.9)	142 (3.0)	36 (7.8)
Tower	117 (2.5)	73 (3.5)	28 (6.5)
MPI-BGC	147 (12.0)	88 (9.0)	30 (17.6)
GOME-2	143 (3.8)	82 (2.0)	22 (5.0)
Multi-model	165 (18.9)	85 (9.7)	6 (15.0)
<i>US-Ne2 41.16°N –96.47°E</i>			
MODIS	247 (7.9)	142 (3.0)	37 (7.9)
Tower	121 (2.5)	80 (3.0)	40 (6.0)
MPI-BGC	147 (12.0)	88 (9.0)	30 (17.6)
GOME-2	144 (3.5)	83 (2.0)	22 (5.0)
Multi-model	169 (11.6)	90 (5.8)	11 (11.8)
<i>US-Ne3 41.18°N –96.44°E</i>			
MODIS	222 (6.4)	122 (3.2)	21 (7.8)
Tower	110 (2.3)	75 (2.3)	39 (5.5)
MPI-BGC	147 (12.0)	88 (9.0)	30 (17.6)
GOME-2	144 (3.5)	83 (2.0)	22 (5.0)
Multi-model	181 (9.7)	82 (7.2)	6 (9.5)
<i>US-IB1 41.86°N –88.22°E</i>			
MODIS	256 (7.5)	160 (3.0)	64 (7.0)
Tower	117 (2.9)	76 (4.0)	34 (7.0)
MPI-BGC	175 (17.8)	101 (13.8)	27 (21.3)
GOME-2	162 (5.0)	92 (2.5)	23 (7.1)

Table 4

Similar to Table 3 but for deciduous broadleaf forest (DBF) and evergreen needleleaf forest (ENF) sites as indicated.

Estimate	Duration of photosyn.	Duration of growing season	Duration of max. photosyn.
<i>US-Ha1 (DBF) 42.54°N – 72.17°E</i>			
MODIS	256 (7.1)	170 (3.0)	84 (6.7)
Tower	188 (5.9)	119 (3.8)	49 (9.6)
MPI-BGC	198 (14.4)	125 (10.3)	52 (20.0)
GOME-2	197 (9.2)	117 (3.7)	37 (9.2)
Multi-model	241 (13.2)	153 (8.2)	66 (4.9)
<i>US-Bar (DBF) 44.06°N – 71.29°E</i>			
MODIS	245 (6.4)	166 (2.9)	87 (5.9)
Tower	176 (4.6)	129 (2.8)	80 (6.8)
MPI-BGC	183 (13.8)	120 (8.1)	56 (19.8)
GOME-2	184 (8.6)	113 (3.4)	41 (8.9)
<i>CA-Mer (DBF) 45.41°N – 75.52°E</i>			
MODIS	249 (5.8)	158 (2.5)	67 (5.5)
Tower	218 (17.3)	129 (9.8)	40 (20.3)
MPI-BGC	165 (12.6)	119 (6.9)	73 (18.1)
GOME-2	179 (8.3)	115 (3.2)	51 (7.4)
<i>US-NR1 (ENF) 40.03°N – 105.55°E</i>			
MODIS	255 (11.9)	149 (5.9)	43 (12.4)
Tower	209 (10.5)	148 (4.5)	85 (11.7)
MPI-BGC	218 (33.0)	141 (29.6)	66 (36.3)
GOME-2	216 (28.8)	132 (19.8)	48 (27.5)
Multi-model	215 (13.9)	136 (7.2)	55 (6.2)
<i>CA-Qcu (ENF) 49.27°N – 74.04°E</i>			
MODIS	213 (7.3)	147 (3.5)	81 (5.6)
Tower	188 (20.8)	106 (16.3)	24 (21.6)
MPI-BGC	210 (22.3)	137 (14.9)	64 (26.0)
GOME-2	196 (26.8)	143 (23.2)	29 (27.2)

by latitude. These tables highlight that there is significantly more variability in the timing indicators for the ENF and MF sites that cover a larger range of latitudes. For example, the southern-most MF site (US-WBW) has a significantly longer duration of photosynthesis than most of the more northern sites as determined from tower and upscaled GPP as well as GOME-2 F_{740} . Some of the MF sites at similar latitudes also show significant differences; the northern midwestern sites, US-UMB and US-WCr (as well as other sites located nearby and not shown in the table), have significantly shorter durations of photosynthesis as compared with the US-Ho1 site located in the northeast US at a similar latitude, and US-UMB has a longer duration of photosynthesis as compared with US-WCr. Again, this is shown by tower and upscaled GPP as well as GOME-2 F_{740} . While MODIS and multi-model mean data produce significantly larger estimates of duration of photosynthesis, they generally show the same spatial variability.

We attempted to compare individual yearly estimates of the timing parameters from GOME-2 F_{740} , MPI-BGC GPP, and available flux tower measurements. In general, the interannual variability is smaller than the estimated uncertainties. To reduce uncertainties in the current data sets, we would need to average data over larger (regional) scales. We intend to pursue this in more detail in future studies.

4. Conclusions and ongoing work

Our direct comparisons of GOME-2 F_{740} with tower-based and upscaled GPP indicate that GOME-2 F_{740} tracks the spring onset and autumn decline of photosynthesis for several different biomes. Moderate to high values of MODIS-derived fPAR (>0.2–0.5) are maintained throughout the year at many sites for which green vegetation may absorb light but not utilize the energy for photosynthesis, particularly in winter. Our study suggests that GOME-2 F_{740} may be used to better constrain this aspect of GPP simulated by data-driven models and improve parameterizations in process-based models. We acknowledge the inherent difficulties in comparing the relatively small spatial scale tower-based GPP estimates with those of the

Table 5

Similar to Table 3 but for representative mixed forest sites.

Estimate	Duration of photosyn.	Duration of growing season	Duration of max. photosyn.
<i>US-WBW 35.96°N – 84.29°E</i>			
MODIS	258 (5.6)	189 (2.3)	121 (4.8)
Tower	220 (7.5)	158 (3.2)	95 (8.5)
MPI-BGC	238 (15.5)	159 (11.3)	81 (25.5)
GOME-2	228 (9.6)	134 (3.7)	39 (10.0)
<i>US-MMS 39.32°N – 86.41°E</i>			
MODIS	243 (4.3)	184 (1.8)	125 (4.0)
Tower	200 (5.2)	145 (3.0)	91 (7.0)
MPI-BGC	191 (15.3)	110 (12.3)	29 (19.8)
GOME-2	190 (4.8)	103 (2.5)	18 (6.8)
Multi-model	260 (16.5)	165 (10.7)	70 (7.9)
<i>US-Ho1 45.20°N – 68.74°E</i>			
MODIS	287 (10.7)	177 (4.1)	69 (8.6)
Tower	245 (9.0)	162 (4.3)	79 (10.9)
MPI-BGC	223 (19.0)	133 (13.8)	43 (24.3)
GOME-2	192 (10.8)	111 (5.9)	31 (11.8)
Multi-model	261 (14.2)	168 (9.6)	76 (4.7)
<i>US-UMB 45.56°N – 84.71°E</i>			
MODIS	236 (4.3)	157 (2.0)	80 (4.3)
Tower	172 (4.3)	118 (3.3)	64 (7.8)
MPI-BGC	205 (18.0)	127 (12.3)	48 (23.1)
GOME-2	201 (19.1)	112 (14.4)	19 (14.1)
Multi-model	223 (10.7)	144 (5.1)	64 (4.6)
<i>US-WCr 45.81°N – 90.08°E</i>			
MODIS	210 (3.5)	149 (1.8)	87 (3.8)
Tower	150 (4.0)	111 (2.5)	70 (6.1)
MPI-BGC	179 (14.1)	116 (8.3)	54 (20.3)
GOME-2	176 (8.7)	105 (3.8)	33 (8.9)
Multi-model	202 (5.9)	134 (2.4)	65 (4.5)

larger-footprint GOME-2 data that were produced for different sets of years. The use of the MPI-BGC upscaled GPP estimates for the same time periods as the GOME-2 data has provided a means of assessing potential differences arising from the differing spatial scales and temporal periods of tower- and satellite-based data.

Ecosystem models and reflectance-based data products from Earth-orbiting satellites (e.g., NDVI, EVI, LAI) are currently used to predict or monitor the seasonal dynamics of vegetated ecosystems that correspond with the growing season and carbon uptake period. However, as noted above, these models and satellite observations often do a poor job of describing the length of the growing season, as found in our current study and by others (e.g., Garrity et al., 2011; Richardson et al., 2012). Over- and under-estimation of the growing season and related carbon uptake period can lead to errors in predicting interannual variability in ecosystem-atmosphere carbon exchange and can negatively impact our ability to assess long term trends in ecosystem response to climate change (Garrity et al., 2011). Reflectance-based satellite products are typically linked to seasonal morphological development of plant canopies (e.g., LAI). Time lags between morphological and physiological development can lead to significant error in estimating seasonal carbon flux (Morecroft, Stokes, & Morison, 2003; Richardson et al., 2009, 2010). In contrast, our results show very good agreement between GPP and fluorescence for several important vegetation types (croplands and several forest types); this suggests that GOME-2 F_{740} may better capture seasonal dynamics of canopy physiology relevant to carbon flux in some ecosystems as compared with existing models and satellite data products.

Following the recent launch of a second GOME-2 instrument on the MetOp-B platform, the MetOp-A GOME-2 is now operating in a smaller pixel mode (since day 196 of 2013); ground pixels are now 40 × 40 km² with a 960 km wide swath. The MetOp-B operates in the standard wider swath mode as described above. This enables smaller pixel fluorescence observations of similar quality although with less frequent overpasses. Use of the two GOME-2 instruments should lead to improved

fluorescence data sets for further studies in the future. In addition, the upcoming launches of the Orbiting Carbon Observatory-2 (OCO-2) (Frankenberg, Butz, & Toon, 2011; Frankenberg et al., 2014) and the Sentinel-5 precursor TROPOMI (Veeffkind et al., 2012) will enable additional measurements near the O₂-A band at higher spatial resolution. The Fluorescence EXplorer (FLEX) (Rascher, 2007), an ESA Explorer 8 Mission selected for Phase A/B1 in early 2011, is designed specifically to make chlorophyll fluorescence measurements (Guanter et al., 2010) and would provide additional spectral information across the visible-NIR spectrum.

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Appendix A. Supplementary data

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