Estimation of vegetation photosynthetic capacity from space-based measurements of chlorophyll fluorescence for terrestrial biosphere models

Yongguang Zhang  
*Free University of Berlin*

Luis Guanter  
*Free University of Berlin*

Joseph A. Berry  
*Department of Global Ecology, Carnegie Institution for Science, Stanford, CA*

Joanna Joiner  
*NASA Goddard Space Flight Center, Greenbelt, MD*

Christiaan van der Tol  
*International Institute for Geo-Information Science and Earth Observation, PO. Box 6, 7500 AA, Enschede, The Netherlands*

*See next page for additional authors*

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Authors
Yongguang Zhang, Luis Guanter, Joseph A. Berry, Joanna Joiner, Christiaan van der Tol, Alfredo Huete, Anatoly Gitelson, Maximilian Voigt, and Philipp Köhler
Estimation of vegetation photosynthetic capacity from space-based measurements of chlorophyll fluorescence for terrestrial biosphere models

YONGGUANG ZHANG1, LUIS GUANTER2, JOSEPH A. BERRY2, JOANNA JOINER3, CHRISTIAAN VAN DER TOL4, ALFREDO HUETE5, ANATOLY GITELSON6, MAXIMILIAN VOIGT1 and PHILIPP KÖHLER1

1Institute for Space Sciences, Free University of Berlin, Berlin 12165, Germany, 2Department of Global Ecology, Carnegie Institution for Science, Stanford, CA 94305, USA, 3NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA, 4International Institute for Geo-Information Science and Earth Observation, P.O. Box 6, 7500 AA, Enschede, The Netherlands, 5Plant Functional Biology and Climate Change Cluster, University of Technology Sydney, Sydney, NSW 2007, Australia, 6School of Natural Resources, University of Nebraska – Lincoln, Lincoln, NE 68583, USA

Abstract

Photosynthesis simulations by terrestrial biosphere models are usually based on the Farquhar’s model, in which the maximum rate of carboxylation ($V_{\text{cmax}}$) is a key control parameter of photosynthetic capacity. Even though $V_{\text{cmax}}$ is known to vary substantially in space and time in response to environmental controls, it is typically parameterized in models with tabulated values associated to plant functional types. Remote sensing can be used to produce a spatially continuous and temporally resolved view on photosynthetic efficiency, but traditional vegetation observations based on spectral reflectance lack a direct link to plant photochemical processes. Alternatively, recent space-borne measurements of sun-induced chlorophyll fluorescence (SIF) can offer an observational constraint on photosynthesis simulations. Here, we show that top-of-canopy SIF measurements from space are sensitive to $V_{\text{cmax}}$ at the ecosystem level, and present an approach to invert $V_{\text{cmax}}$ from SIF data. We use the Soil-Canopy Observation of Photosynthesis and Energy (SCOPE) balance model to derive empirical relationships between seasonal $V_{\text{cmax}}$ and SIF which are used to solve the inverse problem. We evaluate our $V_{\text{cmax}}$ estimation method at six agricultural flux tower sites in the midwestern US using spaced-based SIF retrievals. Our $V_{\text{cmax}}$ estimates agree well with literature values for corn and soybean plants (average values of 37 and 101 $\mu$mol m$^{-2}$ s$^{-1}$, respectively) and show plausible seasonal patterns. The effect of the updated seasonally varying $V_{\text{cmax}}$ parameterization on simulated gross primary productivity (GPP) is tested by comparing to simulations with fixed $V_{\text{cmax}}$ values. Validation against flux tower observations demonstrate that simulations of GPP and light use efficiency improve significantly when our time-resolved $V_{\text{cmax}}$ estimates from SIF are used, with $R^2$ for GPP comparisons increasing from 0.85 to 0.93, and for light use efficiency from 0.44 to 0.83. Our results support the use of space-based SIF data as a proxy for photosynthetic capacity and suggest the potential for global, time-resolved estimates of $V_{\text{cmax}}$.

Keywords: Farquhar model, Cropland, GPP, photosynthesis, SCOPE, Solar-induced fluorescence, $V_{\text{cmax}}$

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Introduction

Accurately quantifying global and regional terrestrial gross primary productivity (GPP) is considered of great importance due to its key role in the atmosphere-biosphere interactions. For several decades, state-of-the-art terrestrial biosphere models (TBM) have been used to quantify the variability of GPP at different temporal and spatial scales (Dickinson, 1983; Sellers et al., 1997). Most of these models are based on C3 and C4 photosynthesis models developed by Farquhar et al. (1980) and Collatz et al. (1992) to calculate GPP, which are particularly sensitive to photosynthetic capacity, expressed as the maximum carboxylation capacity ($V_{\text{cmax}}$). $V_{\text{cmax}}$ is one of the key biochemical parameters in these photosynthesis models as it controls the carbon fixation process (Farquhar et al., 1980). There are large spreads in GPP estimates in space and time across models (Schaefer et al., 2012) owing to combinations of model structural error and parameter uncertainties (Bonan et al., 2011). The latter case most notably relates to the uncertainty in $V_{\text{cmax}}$ that has a magnitude comparable to model structural errors with an offsetting sign (Bonan et al., 2011). Thus, accurate estimations of $V_{\text{cmax}}$ are needed to simulate ecosystem GPP because...
Despite its importance, large-scale estimates of $V_{cmax}$ remain challenging. As a leaf-level parameter, $V_{cmax}$ cannot be measured directly, but only be inferred indirectly from leaf-level measurements of gas exchange (Wullschleger, 1993). However, making such observations is labor-intensive and can only focus on measurements at leaf or plant scale. On the other hand, eddy covariance flux measurements together with meteorological observations provide another way to make ecosystem-level estimates of $V_{cmax}$ through inverse modeling from CO$_2$ and water fluxes (Wolf et al., 2006; Wang et al., 2007). However, the parameterization of $V_{cmax}$ in a global, spatially continuous and time-resolved manner remains an unsolved problem.

Several studies have recently shown that $V_{cmax}$ varies seasonally (Wilson et al., 2001; Xu & Baldocchi, 2003; Grassi et al., 2005), and that photoperiod may regulate seasonal patterns of photosynthetic capacity as shown by Bauerle et al. (2012), with $V_{cmax}$ approaching a maximum around the summer solstice and then declining synchronously with the photoperiod. However, only a few terrestrial biosphere models have incorporated such seasonal variations in photosynthetic capacity (Medvigy et al., 2009; Oleson et al., 2010). Most of the models either assume a constant $V_{cmax}$ over time or derive it from more easily measurable parameters (Grassi et al., 2005) due to the limitations of available spatial and temporal information from relevant proxies. For example, in the widely used Community Land Model (CLM) (Oleson et al., 2010) $V_{cmax}$ is assigned a specific value for each broadly defined plant functional type (PFT) and then adjusted with day length. There is increasing evidence that the assumption of time-invariant photosynthetic parameters can cause significant errors if large seasonal variability in photosynthetic capacity occurs (Wilson et al., 2001; Kosugi et al., 2003; Medvigy et al., 2013). As a consequence, the broad implications of seasonal variations of $V_{cmax}$ on the carbon cycle are not well understood.

Remote sensing provides a unique opportunity to parameterize spatially explicit plant physiological information on local, regional and global scales, and thus improve simulations of carbon fluxes of terrestrial ecosystems (Hilker et al., 2008). Many efforts have been made to estimate the functional attributes of plant canopies with remote sensing data. Classical reflectance-based vegetation indices (VI) (Tucker, 1979), such as Normalized Difference Vegetation Index (NDVI), have substantially improved our understanding of the global biosphere by providing estimates of potential photosynthesis from greenness estimates (Turner et al., 2003; Running et al., 2004). Some VIs like photochemical reflectance index (PRI) can be successfully used to derive light use efficiency (LUE) from multi-angle satellite data (Hilker et al., 2011). However, reflectance-based measurements like NDVI are not directly linked to instantaneous photosynthetic processes and cannot alone quantify actual photosynthesis or its down-regulation due to environmental stresses. Therefore, the direct estimations of photosynthetic capacity ($V_{cmax}$) through space-based proxies have not yet been achieved.

As a complement to reflectance-based vegetation indices, solar-induced fluorescence (SIF) offers new possibilities to monitor photosynthesis from space (Baker, 2008). Solar-induced fluorescence is an electromagnetic emission in the 650–800 nm range originating at the core of the photosynthetic machinery. It has been used in leaf-scale studies of photosynthesis under laboratory conditions for several decades (Baker, 2008) and has also been shown to be an excellent proxy for GPP at canopy and ecosystem scales (Frankenberg et al., 2011; Guanter et al., 2012). Global data of SIF have recently been retrieved from a series of spaceborne instruments providing high resolution spectra, such as the GOSAT’s Fourier Transform Spectrometer (Frankenberg et al., 2011; Joiner et al., 2011; Guanter et al., 2012), ENVISAT/SCIAMACHY (Joiner et al., 2012) and MetOp-A/GOME-2 (Joiner et al., 2013). The new global retrievals of chlorophyll fluorescence enable the establishment of a direct link between a remotely sensed vegetation parameter related to photosynthetic capacity and actual terrestrial photosynthetic activity. In particular, the empirical study by Guanter et al. (2014) demonstrated that space-borne SIF is more sensitive to the high photosynthetic rates of cropland than other remotely sensed vegetation parameters.

In this work, we have used an integrated photosynthesis-fluorescence model, the Soil-Canopy Observation of Photochemistry and Energy fluxes (SCOPE) model, to invert $V_{cmax}$ from SIF retrievals obtained from GOME-2 data. Specifically, a key objective of this study is to investigate the utility of SIF as a proxy for photosynthetic capacity and to propose a new approach for spatially continuous and time-resolved estimation of $V_{cmax}$ from space-based SIF measurements.

**Materials and methods**

**SIF retrievals from GOME-2**

SIF (in radiance units) was derived from measurements by the GOME-2 instrument onboard Eumetsat’s MetOp-A platform launched in October 2006. Details of the retrieval of SIF from GOME-2 measurements can be found in Joiner et al. (2013).
GOME-2 measures in the 240–790 nm spectral range with a spectral resolution between 0.2 and 0.5 nm and a nominal footprint of 40 × 80 km². SIF retrievals are based on the inversion of the top-of-atmosphere measurements in the 715–758 nm windows overlapping the second peak of the SIF emission. The retrieval method disentangles the contribution of atmospheric absorption and scattering, surface reflectance and fluorescence to the measured top-of-atmosphere radiance spectra. The retrievals are quality-filtered and binned in 0.5° latitude-longitude grid boxes (Joiner et al., 2013). GOME-2 data between 2007 and 2011 have been used in this work. GOME-2 SIF retrievals were aggregated into biweekly periods to improve the signal-to-noise ratio of the SIF data.

**Flux sites and data**

We used six crop flux tower sites located in the corn belt in the midwestern US (Table 1). Sites have been selected on the basis of landscape homogeneity within the GOME-2 grid and on data availability in the period of interest (2007–2011). To determine landscape homogeneity, we used the MODIS products for land cover type (MCD12C1, Friedl et al., 2010), and Enhance Vegetation Index (EVI, MOD13C2, Huete et al., 2002) with spatial resolution of 0.05 degree. We selected those sites for which more than 90% of the GOME-2 pixel area around the flux tower sites corresponds to croplands and EVI standard deviation is <0.10 (Table 1).

We obtained the Level 2 flux data products for the 6 US crop sites from the AmeriFlux website (http://amerifluxornl.gov/). Half-hourly or hourly data of CO₂ flux and associated meteorological variables were extracted. Gap-filling and flux-partitioning were all processed by the online tool available at http://www.bgc-jena.mpg.de/~MDIwork/eddyproc/ from Max Planck Institute for Biogeochemistry (MPI-BGC). GPP was estimated by partitioning the observed net flux into GPP and ecosystem respiration as described in Reichstein et al. (2005) and Papale et al. (2006). Hourly absorbed photosynthetic active radiation (APAR) and fraction absorbed photosynthetic active radiation (FPAR) data was obtained from the flux data. Site-level leaf area index (LAI) and canopy height (hₖ) measurements were available for each site every 2 weeks during the growing season.

For each site, SIF values were extracted based on the coordinates of the flux tower, and averaged to biweekly means when at least 5 SIF retrievals were available within each biweekly period. To avoid signal contamination from urban areas, we extracted SIF from nearby homogeneous pixels for those sites in which urban areas fell inside the GOME-2 pixel. Given that in homogeneous landscapes flux measurements are usually representative of a large area, (i.e., US-IB1 is representative of central Illinois), we assumed that SIF from nearby grid pixels can represent that at the flux sites. The SIF measurement error in each biweekly period is estimated as the standard error of the mean (SE) and a nominal constant error of 0.2 W m⁻² μm⁻³ sr⁻¹ (Joiner et al., 2013). The standard error alone appear to underestimate the uncertainties as the large numbers of samples used in the averaging process lead to relatively small standard errors. The constant error is introduced to account for other error sources such as cloud contamination and variability. We used the maximum values of the constant error and the standard error of the mean in each biweekly period.

**The SCOPE model and input parameters**

SCOPE is a vertical (1-D) integrated radiative transfer and energy balance model (van der Tol et al., 2009a). The model calculates radiation transport in a multilayer canopy as a function of the solar zenith angle and leaf orientation to simulate fluorescence in the observation direction. The biochemical component has recently been updated on Collatz et al. (1991, 1992) for C3 and C4 plants, respectively. It calculates the illumination and net radiation of leaves with respect to their position (distance from the top of canopy in units of leaf area) and orientation (leaf inclination and azimuth angle), and the spectra of reflected and emitted radiation as observed above the canopy in the specified satellite observation geometry. The spectral range (0.4–50 μm) includes the visible, near and shortwave infrared and the thermal domain, with respectively, 1, 1, 100 and 1000 nm resolution. The geometry of the vegetation is

<table>
<thead>
<tr>
<th>Site ID</th>
<th>Latitude</th>
<th>Longitude</th>
<th>Study period</th>
<th>Max (LC)</th>
<th>Mean EVI</th>
<th>sd EVI</th>
<th>Crop rotations</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>USBo1</td>
<td>40.0062</td>
<td>-88.2904</td>
<td>2007</td>
<td>98%</td>
<td>0.5562</td>
<td>0.0399</td>
<td>Corn</td>
<td>Ryu et al. (2011)</td>
</tr>
<tr>
<td>USB1</td>
<td>41.8593</td>
<td>-88.2227</td>
<td>2007–2008</td>
<td>98%</td>
<td>0.4431</td>
<td>0.0780</td>
<td>Corn at even years and soybean at odd years</td>
<td>Allison et al. (2004)</td>
</tr>
<tr>
<td>USNe1</td>
<td>41.1651</td>
<td>-96.4766</td>
<td>2007–2011</td>
<td>95%</td>
<td>0.5641</td>
<td>0.0627</td>
<td>Continuous corn</td>
<td>Suyker et al. (2005)</td>
</tr>
<tr>
<td>USNe2</td>
<td>41.1649</td>
<td>-96.4701</td>
<td>2007–2011</td>
<td>95%</td>
<td>0.5608</td>
<td>0.0704</td>
<td>Corn except in 2008</td>
<td>Suyker et al. (2005)</td>
</tr>
<tr>
<td>USNe3</td>
<td>41.1797</td>
<td>-96.4397</td>
<td>2007–2011</td>
<td>95%</td>
<td>0.5731</td>
<td>0.0719</td>
<td>Corn at odd years and soybean at even years</td>
<td>Suyker et al. (2005)</td>
</tr>
<tr>
<td>USRo1</td>
<td>44.7143</td>
<td>-93.0898</td>
<td>2007–2010</td>
<td>98%</td>
<td>0.4912</td>
<td>0.0953</td>
<td>Corn at odd year and soybean at even year</td>
<td></td>
</tr>
</tbody>
</table>

*LC stands for Land Cover class; EVI is the MODIS Enhanced Vegetation Index; max(LC) stands for the percent of dominant vegetation cover within the GOME-2 pixel; sdEVI for standard deviation of EVI within the GOME-2 pixel.*
treated in a stochastic way with 60 elementary layers, 13 discrete leaf zenith inclination and 36 leaf azimuth classes. The azimuthal distribution is uniform, while the zenith angle distribution is provided as input. It describes the sun-canopy-observer geometry and leaf orientation, so that the different biophysical processes for sunlit and shaded components can be considered. Radiative transfer of chlorophyll fluorescence is calculated using a module similar to the FluorSAIL model (Miller et al., 2005), but allowing leaf fluorescence to vary depending on position and orientation in the canopy. A leaf-level biochemical model calculates GPP, stomatal resistance, and the energy balance of the leaf together with fluorescence from the absorbed flux of PAR, canopy temperature, and ambient vapor, CO₂ and O₂ concentrations (van der Tol et al., 2009b). In a recent update, the stomatal conductance model in SCOPE has been replaced by that of Ball et al. (1991), and the relationship between photochemical and fluorescence yield is based on the Genty equation (Genty et al., 1989) and has been calibrated to observations from leaf-scale fluorescence and gas exchange experiments with C3 and C4 crops. The model calculates radiation transport in a multilayer canopy as a function of the solar zenith angle and leaf orientation to simulate fluorescence in the observation direction. Other significant updates were: the FLUSPECT module replaced PROSPECT model, the leaf-level biochemical model for fluorescence was changed, the within canopy gradient in Vcmax parallels the extinction of light following Sellers et al. (1992), and the way of programming was changed by organizing variables in structures. In this work, we used the recent version of SCOPE (V. 1.52).

To simulate photosynthesis and fluorescence, SCOPE requires inputs of meteorological forcing (incoming shortwave and long-wave radiation, air temperature, humidity, wind speed, and CO₂ concentration) and four kinds of parameters: (1) vegetation structure parameters, such as canopy height, leaf size, leaf angle distribution, and LAI; (2) leaf biophysical parameters: leaf chlorophyll content (Cab), dry matter content (Cdm), leaf equivalent water thickness (Cw), senescent material (Cw), and leaf structure (N); (3) optical parameters: reflectance of soil in the visible, near infrared and thermal bands, and vegetation (thermal) emissivity; (4) plant physiological parameters: stomatal conductance parameter (m), and maximum carboxylation capacity, Vcmax of a top leaf standardized to a reference temperature at 25 °C (parameter Vcmax in the model).

Meteorological inputs to constrain SCOPE were available from flux tower measurements. Values or sources of some other important input parameters required for the SCOPE model are listed in Table 2. Leaf angle distribution is assumed to be spherical, which is a good approximation in crops such as soybean and corn (Table 2) (Lemeur & Blad, 1974; Verhoef & Bach, 2007). Estimates of LAI and canopy height and their seasonal variations were derived from the Ameriflux website. Based on soil texture classification from site-specific websites, soil reflectance spectra were derived from ASTER soil spectral library available at www.specilb.jpl.nasa.gov. Initial soil temperatures were set equal to the corresponding air temperatures.

Vcmax is a key parameter for biochemical modeling of CO₂ assimilation in SCOPE. It is a leaf-scale photosynthetic parameter, assumed to decrease exponentially with the depth in a canopy. The parameter Vcmax varies largely with different biomes (Wullschlegel, 1993; Sellers et al., 1997), and with day of the year (Mäkelä et al., 2004). As stated in the objective of this study, this parameter was chosen to be inverted from SIF (section ‘Inversion of Vcmax during the growing season from SCOPE simulations and SIF data’).

A rough estimation of Cab, Cw, Cdm, and N controlling the leaf and canopy radiative transfer was obtained from vegetation indices (VIs). Three VIs were used including NDVI and EVI (Huete et al., 2002), both extracted from the MOD13C2 product, and the MERIS terrestrial chlorophyll index (MTCI) (Dash & Curran, 2004). These indices provide indirect information on canopy structure and chlorophyll content. Many studies have shown the feasibility of inverting radiative transfer models using VIs to derive Cab, Cw, Cdm and N (Jacquemoud et al., 1996; Combal et al., 2003; Maire et al., 2004). We

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Symbol</th>
<th>Units</th>
<th>Range</th>
<th>Values or sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chlorophyll a + b content</td>
<td>Cab</td>
<td>µg cm⁻²</td>
<td>10–70</td>
<td>Inverted from VIs</td>
</tr>
<tr>
<td>Dry matter content</td>
<td>Cdm</td>
<td>g cm⁻²</td>
<td>0.001–0.02</td>
<td>Inverted from VIs</td>
</tr>
<tr>
<td>Leaf equivalent water thickness</td>
<td>Cw</td>
<td>cm</td>
<td>0.001–0.05</td>
<td>Inverted from VIs</td>
</tr>
<tr>
<td>Senescent material</td>
<td>Cw</td>
<td>/</td>
<td>/</td>
<td>0.0</td>
</tr>
<tr>
<td>Leaf structure</td>
<td>N</td>
<td>/</td>
<td>1.3–2.0</td>
<td>Inverted from VIs</td>
</tr>
<tr>
<td>Leaf angle distribution parameter a</td>
<td>LIDFₐ</td>
<td>/</td>
<td>/</td>
<td>−0.35</td>
</tr>
<tr>
<td>Leaf angle distribution parameter b</td>
<td>LIDFₐ</td>
<td>/</td>
<td>/</td>
<td>−0.15</td>
</tr>
<tr>
<td>Leaf width</td>
<td>w</td>
<td>m</td>
<td>/</td>
<td>0.1</td>
</tr>
<tr>
<td>Ball-Berry stomatal conductance parameter</td>
<td>m</td>
<td>/</td>
<td>/</td>
<td>Corn: 4; Soybean: 9</td>
</tr>
<tr>
<td>Dark respiration rate at 25 °C as fraction of Vcmax</td>
<td>Rd</td>
<td>/</td>
<td>/</td>
<td>0.015</td>
</tr>
<tr>
<td>Cowan’s water use efficiency parameter</td>
<td>αc</td>
<td>/</td>
<td>/</td>
<td>700</td>
</tr>
<tr>
<td>Leaf thermal reflectance</td>
<td>ρ (thermal)</td>
<td>/</td>
<td>/</td>
<td>0.01</td>
</tr>
<tr>
<td>Leaf thermal transmittance</td>
<td>τ (thermal)</td>
<td>/</td>
<td>/</td>
<td>0.01</td>
</tr>
<tr>
<td>Soil thermal reflectance</td>
<td>ρs (thermal)</td>
<td>/</td>
<td>/</td>
<td>0.06</td>
</tr>
<tr>
<td>Leaf area index</td>
<td>LAI</td>
<td>/</td>
<td>/</td>
<td>Field measurement</td>
</tr>
<tr>
<td>Canopy height</td>
<td>hₜ</td>
<td>m</td>
<td>/</td>
<td>Field measurement</td>
</tr>
</tbody>
</table>

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use a look-up table approach to solve the inversion problem which requires less computing time and generally performs well. The leaf reflectance model PROSPECT (Jacquemoud & Baret, 1990) was used for the inversion, which was also integrated into the SCOPE model. We built a database composed of hundreds of thousands of simulated leaf reflectance spectra with the PROSPECT model with a 1 nm resolution in forward mode. The ranges of the $C_{ab}$, $C_{uv}$, $C_{mn}$, and $N$ parameters are chosen from observed data (the LOPEX data set, Hosgood et al., 1994). The values of each parameter are given in Table 2. The space of model input variables was sampled by randomly drawing values by assuming uniform distribution function of each variable. The generated database contains a total of 280,000 simulations representing a wide range of leaves. A simple cost function was used to find the solution to the inverse problem, which minimizes the root mean squared error (RMSE) between measured and simulated vegetation inverse problem, which minimizes the root mean squared error (RMSE) between measured and simulated vegetation.

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Inversion of $V_{cmax}$ during the growing season from SCOPE simulations and SIF data

A schematic diagram of SIF-based $V_{cmax}$ retrieval scheme is given in Fig. 1. With the meteorological and other input parameters stated above, SCOPE was first run with a LUT of $V_{cmax}$ at half-hourly or hourly time steps at the flux tower sites for the 2007–2011 period. Based on the published literature (Wullschleger, 1993; Kattge et al., 2009; Lokupitiya et al., 2009), the ranges of $V_{cmax}$ were set to 10–70 $\mu$mol m$^{-2}$ s$^{-1}$ with a step of 5 $\mu$mol m$^{-2}$ s$^{-1}$ for corn and 10–200 $\mu$mol m$^{-2}$ s$^{-1}$ with a step 10 $\mu$mol m$^{-2}$ s$^{-1}$ for soybean, respectively. We also tested a smaller step; this showed no significant differences (data not shown). The resulting seasonal variables of $C_{ab}$, $C_{uv}$, $C_{mn}$, and $N$ were used as input biophysical parameters for SCOPE at each site.

Fig. 1: Overview flowchart of the Soil-Canopy Observation of Photosynthesis and Energy simulations and inversions of $V_{cmax}$ from solar-induced fluorescence.

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Relationships between $V_{cmax}$ and canopy fluorescence were established by running the SCOPE model in forward mode. The relationships were derived separately for different vegetative growth periods during the growing season for each year and each site as shown in the section ‘Relationship between $V_{cmax}$ and SIF during the growing season from SCOPE simulations’. To match the biweekly GOME-2 SIF retrievals, we derived the relationship for each biweekly period during the growing season. This implies that for each biweekly period, a unique linear relationship was established for the inverse retrieval of $V_{cmax}$ from GOME-2 SIF at each site. Then, using corresponding GOME-2 SIF biweekly retrievals, seasonal $V_{cmax}$ was inverted from the derived relationships for corn and soybean during the growing season for each year and each site, respectively. We estimated the uncertainties in each biweekly period from the measurement error of SIF which was propagated to $V_{cmax}$ through the linear models between $V_{cmax}$ and SIF.

It should be noted that, due to the coarse resolution of GOME-2, we applied this inversion approach on a mixture of corn and soybean canopies assuming similar intrinsic light use efficiency of fluorescence and a similar intrinsic FPAR for them. Although FPAR and the canopy light use efficiency of fluorescence vary with chlorophyll content $C_{ab}$ and leaf area (Gitelson et al., 2012), the intrinsic light use efficiency of fluorescence at photosystem level is assumed to be equal for both crops. This means that the two crops produce similar canopy fluorescence and electron transport rates (ETR) (Weis & Berry, 1987; Genty et al., 1989; Baker, 2008). Actual ETR is similar (Fig. 2) for soybean and corn despite large differences in their rates of CO2 assimilation related to the difference in photosynthetic pathways. In Fig. 2, actual ETR for corn and soybean was calculated according to von Caemmerer & Farquhar (1981) from CO2 assimilation rate (GPP) estimated from flux tower measurements for the year 2007 (corn, C4) and 2008 (soybean, C3) at the site of U5-Ne3. We compare the daily cycles of actual ETR for the peak month for corn (July) and soybean (August), respectively. The mean ratio of ETR corn/soybean is 1.09 (±0.12) from flux tower measurements. This comparison demonstrates the similar actual ETR of these two crops which supports our assumption that the two crops produce similar canopy fluorescence. Previous work (Edwards & Baker, 1993) showed that the coupling of fluorescence to ETR is similar for C3 and C4 species. We conclude that while the area is a mixture of soybean and corn, we can use the observed fluorescence properties of the mixture as if it were all soybean or all corn and solve for the respective values of $V_{cmax}$ that are consistent with the observations.

After the $V_{cmax}$ inversion, we performed time-series simulations of GPP and canopy fluorescence at half-hourly or hourly steps using SCOPE with parameters stated above (Table 2) for each site. SCOPE was run with two different configurations to evaluate the effect of $V_{cmax}$ parameterizations on simulated SIF and GPP. The following SCOPE simulations were conducted:

1. Fixed $V_{cmax}$ simulations with a constant PFT-specific $V_{cmax}$ values: 54 $\mu$mol m$^{-2}$ s$^{-1}$ for corn, and 100 $\mu$mol m$^{-2}$ s$^{-1}$ for soybean (Wullschleger, 1993; Kattge et al., 2009;
Lokupitiya et al., 2009) which are commonly used in the TBM community.

2. \( V_{\text{cmax}} = f(\text{SIF}) \): simulations with \( V_{\text{cmax}} \) as a function of SIF from GOME-2 retrievals. For seasonal \( V_{\text{cmax}} \), we used an arbitrary value of 10 \( \mu \text{mol m}^{-2} \text{s}^{-1} \) for the non-growing season periods.

Analysis of SCOPE simulations with different \( V_{\text{cmax}} \)

configurations

GOME-2 has a sun-synchronous orbit and samples near 9:30 hours local time. We used data only under mostly clear-sky condition up to cloud fraction of 40% or less. From SCOPE model results, we defined midday values of fluorescence as average values between 09:00 and 12:00 hours. To match the window of inversion of GOME-2 SIF, we determined the model values of fluorescence of that at the 740 nm wavelengths. We also integrated the half-hourly or hourly simulations to biweekly to compare with GOME-2 SIF retrievals. For GPP, we used the average of 24-hour values of each day for both flux tower estimates and model results, and then aggregated to biweekly values for comparisons. The results of GPP generated from the SCOPE model were similarly aggregated and validated against flux tower observations at each site. To show the feasibility of modeling SIF with SCOPE, we compared the SIF simulations with PFT-fixed \( V_{\text{cmax}} \) with GOME-2 SIF retrievals. Due to the spatial mismatch between GOME-2 grid cell and flux tower footprint, we also compared the SIF simulations with seasonal variable \( V_{\text{cmax}} \) with satellite retrievals for corn and soybean to validate our inversion process. In addition to SIF and GPP comparisons with different \( V_{\text{cmax}} \) parameterizations, we also compared the two light use efficiencies: LUEp and LUEf. LUEp represents photosynthetic light use efficiency, defined as GPP/APAR. LUEf represents light use efficiency for SIF (i.e., the fraction of absorbed PAR photons that are re-emitted from the canopy as SIF photons); this is also known as fluorescence quantum yield (Govindjee, 2004), and is obtained by dividing SIF by APAR.

The performance of inversions of \( V_{\text{cmax}} \) from SIF was evaluated against the data by different validation statistics including the mean absolute error (MAE) and the root mean squared error (RMSE):

\[
\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} \text{abs}(\text{RES}_i)
\]

\[
\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \text{RES}_i^2}
\]

RESi denotes the residual at the ith observations, i.e., OBSi – SIMi, where OBSi and SIMi are the corresponding observed and simulated values.

Results

Relationship between \( V_{\text{cmax}} \) and SIF during the growing season from SCOPE simulations

SCOPE simulations have shown strong linear relationships between \( V_{\text{cmax}} \) and canopy fluorescence at biweekly steps during the growing season for corn and soybean, respectively (Fig. 3). Figure 3 illustrates these relationships for one example (the site of US-Ne3 at Mead, Nebraska in 2007 and 2008). This site has the longest period of data after 2007 and longest rotations of corn and soybean (Table 1). The top panel is for soybean in 2008, and the bottom is for corn in 2007. The other years and sites had similar patterns so they are not shown. Chlorophyll fluorescence increased linearly with \( V_{\text{cmax}} \) within the range of our look-up tables. This suggests that \( V_{\text{cmax}} \) has a significantly positive impact on simulations of SIF when other parameters, such as radiation, LAI, and Cab, remain unchanged using ancillary observations.

The slope of the linear relationship between \( V_{\text{cmax}} \) and SIF varies for different biweekly periods (Fig. 3). The variations were substantial between the mid-growing season and early or end of the growing season. The slopes of fits between \( V_{\text{cmax}} \) and SIF decreased from start to the mid-growing season, and then increased to the end of the growing season (Fig. 3b, d). The reason for such seasonal shifts may be due to seasonal variations of APAR. Figure 3a, d show that the slopes of fits have significantly negative correlation with APAR for both corn and soybean (Pearson correlation, \( r > 0.9, \))
In addition, the slopes are rather high in the very early or end of the growing season (e.g., June 18 for soybean in Fig. 3a, b), implying that larger increases in $V_{\text{cmax}}$ would only result in smaller increases in canopy SIF and that plant carboxylation rates may not be Rubisco-limited and $V_{\text{cmax}}$ may be non-limiting during this period. However, much more work is needed in the future to investigate this underlying mechanism of growing season shifts between $V_{\text{cmax}}$ and SIF. In this study, we focused on the utilization of this linear relationship to retrieve $V_{\text{cmax}}$ from space measurements of GOME-2.

### Seasonal variability of $V_{\text{cmax}}$ from SIF

With the derived linear relationships shown above, seasonal values of $V_{\text{cmax}}$ were retrieved using the GOME-2 biweekly retrievals for each year and each site. Figure 4 shows the temporal evolution of $V_{\text{cmax}}$ and its uncertainties derived from SIF over the growing season for all the six sites during 2007–2011. The values of $V_{\text{cmax}}$ for soybean are higher than those for corn and both are in good agreement with published values (Wullschleger, 1993). During the growing season, our estimates for $V_{\text{cmax}}$ of corn at 25 °C varied from 11 to 75 µmol m$^{-2}$ s$^{-1}$ with an average of 37 µmol m$^{-2}$ s$^{-1}$ for all the years and sites, while the soybean $V_{\text{cmax}}$ ranged from 17 to 190 µmol m$^{-2}$ s$^{-1}$ with an average 101 µmol m$^{-2}$ s$^{-1}$. The uncertainties of $V_{\text{cmax}}$ due to the uncertainties in SIF are approximately 4.3 ± 1.2 and 10.9 ± 4.4 µmol m$^{-2}$ s$^{-1}$ for corn and soybean, or approximately 13.2 ± 6.5% of mean $V_{\text{cmax}}$ for corn and 12.3 ± 6.3% of mean $V_{\text{cmax}}$ for soybean for all site-years together (Fig. 4).

As expected, there were strong seasonal variations in $V_{\text{cmax}}$ (Fig. 4). During the growing season, $V_{\text{cmax}}$ increased rapidly with time and reached maximum values at early-mid-growing season for all the years and sites except the year 2007 at the Mead site (US Ne1-3) which had peak values in later growing season of late July or early August. Thereafter, there was a rapid decline in $V_{\text{cmax}}$ toward the end of the growing season as leaves started to senesce. Due to different planting dates and lengths of growing season for corn and soybean, $V_{\text{cmax}}$ generally peaked later for soybean than for corn (Fig. 4). This suggests that both the timing and amplitude of the seasonally varying $V_{\text{cmax}}$ was associated with the onset of leaf growth difference between the two crops.
SIF simulations with different $V_{\text{cmax}}$ parameterizations

Here, for the first time, we evaluate SCOPE SIF simulations with GOME-2 space retrievals. To show that the inversion scheme is working properly, we compared the SIF simulations with constant and seasonally varying $V_{\text{cmax}}$ parameterizations. As an example, Fig. 5 demonstrates the seasonal impact of using different $V_{\text{cmax}}$ parameterizations on modeled canopy fluorescence for the crop flux site of US Ne3 at Mead, Nebraska. Figure 5a compares the biweekly time-series of GOME-2 SIF retrievals with its standard error to SCOPE simulations using a fixed $V_{\text{cmax}}$ of 54 and 100 $\mu$mol m$^{-2}$ s$^{-1}$ for corn and soybean, respectively, and $V_{\text{cmax}}$ derived from biweekly GOME-2 SIF time-series record. Figure 5b, c show the same data as scatter plots. Figure 6 present this comparison between observed and modeled SIF for all site-years together. Table 3 lists the $R^2$ values and bias error between observations and model predictions for each of the sites. Generally, there are good agreements between model predictions and measurements for both simulations and we also observe an improvement in the SIF simulations when seasonal $V_{\text{cmax}}$ is used. Figure 5 also shows that there are similar canopy SIF for corn and soybean from SCOPE simulations. The similar SIF simulations from SCOPE again prove our assumption of similar fluorescence yield for both crops even though they have different photosynthesis rate (or GPP, Gitelson et al., 2012). In these simulations, the results from seasonally varying $V_{\text{cmax}}$ generally tracked the observations a little more closely, especially for soybean. The use of seasonal $V_{\text{cmax}}$ reduces bias error (MAE from 0.59 to 0.36 $\mu$mol m$^{-2}$ s$^{-1}$, Fig. 6) and the correlation coefficient ($R^2$) increases from 0.80 to 0.88. However, some high values of SIF were not captured by either type of simulation (Fig. 5). In addition, the model was unable to simulate the earlier onset (late May and early June) of crop growth for soybean in years 2008 and 2010 (Fig. 5a). This is possibly due to the spatial mismatch between GOME-2 and the flux tower footprint. Obviously, GOME-2 pixels contain more than one crop, resulting in what is often referred to as mixed pixels. There was a much greater portion of corn crop area within the GOME-2 pixels than soybean area, and soybean is usually planted later (USDA, 2010; USDA National Agricultural Statistics Service Cropland Data Layer, 2013).

GPP simulations with different $V_{\text{cmax}}$ parameterizations

We compare flux tower-based GPP estimates with SCOPE simulations. We first present the comparisons on an hourly time scale for an example site. Figure 7 compares predicted and observed hourly values of GPP for the US Ne3 site during the period of 2007–2011. Generally, hourly GPP is substantially overestimated for corn and underestimated for soybean when a constant $V_{\text{cmax}}$ is assumed (Fig. 7a). Clearly, the use of $V_{\text{cmax}}$ as a function of biweekly GOME-2 SIF improved...
hourly GPP modeling, which is evidenced by an increase of the correlation coefficient ($R^2$) from 0.82 to 0.92 and a reduction of bias error (MAE) from 6.1 to 4.0 l mol m$^{-2}$ C$^0$ s$^{-1}$ (Fig. 7b). The simulations underestimate high GPP values for soybean, but the underestimation is substantially reduced with seasonal $V_{cmax}$ (Fig. 7b). The results for other sites show similar improvements in GPP modeling with seasonally varying $V_{cmax}$ from SIF.

On a seasonal time scale, the use of seasonal variable $V_{cmax}$ also improves the correlation between observed and modeled values for biweekly GPP and reduces the bias, especially for soybean. The overall performance of the seasonal impact of using different $V_{cmax}$ parameterizations on modeled bi-weekly GPP for all site-years is presented in Figs 8 and 9; Table 3. The time-series of modeled and observed GPP shows that the SCOPE model can track the seasonal variability of
photosynthesis fairly well with both constant and seasonally varying $V_{c_{\text{max}}}$ (Fig. 8). However, SCOPE generally overestimates GPP for corn during the mid-late growing season, and underestimates GPP for soybean during the mid-growing season when a fixed $V_{c_{\text{max}}}$ is used (Fig. 8). When the seasonality of $V_{c_{\text{max}}}$ inverted from SIF is incorporated into the model, SCOPE more accurately simulates the seasonal variations of GPP (Fig. 8), with $R^2$ values $>0.94$ for all the sites (Table 3), and a reduction of bias by more than 40% for all sites together (Fig. 9). For example, the mid-late growing season GPP is better captured for corn for all the site-years (Fig. 8). The regression of observed vs. modeled GPP is closer to the 1 : 1 line with seasonally varying $V_{c_{\text{max}}}$ with slopes between 0.95 and 1.08 for corn and soybean, respectively (Fig. 9).

To further evaluate the performance of our derived seasonally varying $V_{c_{\text{max}}}$ from GOME-2 data and also to evaluate its effect on photosynthesis modeling, we compare flux tower data with simulations of the canopy-level light use efficiency of photosynthesis ($\text{LUE}_p$) and fluorescence yield (LUE$_f$) before and after implementing retrieved seasonal $V_{c_{\text{max}}}$ (Figures 10 and 11). The correlation coefficient ($R^2$), RMSE, and MAE are reduced from 0.75 to 0.40 for all site-years together, while Table 3 lists some statistical information ($R^2$, RMSE, and MAE) for corn and soybean for each of the sites. It should be noted that we only calculate daytime $\text{LUE}_p$ and LUE$_f$ during the growing season because of unrealistic values during night and the non-growing season. We observe that modeling $V_{c_{\text{max}}}$ as a function of SIF improved the simulations of $\text{LUE}_p$ and LUE$_f$ as compared with constant $V_{c_{\text{max}}}$ parameterizations, providing a closer match with observations during the growing season (Figs 10 and 11; Table 3). The correlation coefficient ($R^2$) increases from 0.44 to 0.83, and the bias (MAE) is reduced from 0.75 to 0.40 for $\text{LUE}_p$ for all sites together (Fig. 11). For LUE$_f$, the improvement is much larger with an increase of $R^2$ from 0.1 to 0.73, and a reduction of bias error (MAE) from 0.18 to 0.10 (Fig. 10). With constant $V_{c_{\text{max}}}$, there

| Table 3 Model-observed data comparisons statistics for biweekly SIF, GPP, LUE$_p$, and LUE$_f$ at the six sites* |
|--------------------------------------------------|--------------------------------------------------|--------------------------------------------------|--------------------------------------------------|--------------------------------------------------|
| **Statistic** | **USBo1** | **USIB1** | **USNe1** | **USNe2** | **USNe3** | **USRo1** | **USBo1** | **USIB1** | **USNe1** | **USNe2** | **USNe3** | **USRo1** |
| **SIF-C3** | $R^2$ | 0.555 | 0.873 | 0.810 | 0.699 | 0.804 | 0.927 | 0.882 | 0.836 |
| | RMSE | 1.174 | 0.499 | 0.537 | 0.737 | 0.779 | 0.378 | 0.422 | 0.544 |
| | MAE | 0.698 | 0.378 | 0.400 | 0.500 | 0.479 | 0.277 | 0.291 | 0.379 |
| **SIF-C4** | $R^2$ | 0.815 | 0.827 | 0.856 | 0.903 | 0.925 | 0.954 | 0.946 | 0.911 | 0.949 | 0.957 | 0.961 | 0.957 |
| | RMSE | 0.808 | 0.590 | 0.560 | 0.438 | 0.400 | 0.315 | 0.441 | 0.424 | 0.333 | 0.291 | 0.288 | 0.305 |
| | MAE | 0.730 | 0.416 | 0.368 | 0.308 | 0.209 | 0.226 | 0.287 | 0.300 | 0.241 | 0.209 | 0.208 | 0.221 |
| **GPP-C3** | $R^2$ | 0.712 | 0.869 | 0.945 | 0.898 | 0.980 | 0.936 | 0.964 | 0.978 |
| | RMSE | 2.415 | 1.410 | 1.005 | 1.597 | 0.640 | 0.990 | 0.813 | 0.739 |
| | MAE | 2.031 | 0.723 | 0.620 | 0.689 | 0.372 | 0.500 | 0.355 | 0.419 |
| **GPP-C4** | $R^2$ | 0.752 | 0.976 | 0.865 | 0.960 | 0.945 | 0.969 | 0.904 | 0.950 | 0.953 | 0.986 | 0.977 | 0.987 |
| | RMSE | 2.788 | 1.005 | 2.353 | 1.518 | 1.789 | 1.282 | 1.732 | 1.447 | 1.387 | 0.890 | 1.169 | 0.826 |
| | MAE | 2.051 | 0.675 | 1.322 | 0.904 | 1.020 | 0.788 | 1.172 | 0.795 | 0.798 | 0.495 | 0.603 | 0.447 |
| **LUE$_p$-C3** | $R^2$ | 0.591 | 0.552 | 0.421 | 0.485 | 0.619 | 0.836 | 0.809 | 0.647 |
| | RMSE | 0.704 | 0.381 | 0.612 | 0.776 | 0.635 | 0.396 | 0.351 | 0.642 |
| | MAE | 0.457 | 0.305 | 0.464 | 0.585 | 0.486 | 0.295 | 0.252 | 0.499 |
| **LUE$_p$-C4** | $R^2$ | 0.294 | 0.373 | 0.236 | 0.515 | 0.694 | 0.790 | 0.939 | 0.543 | 0.761 | 0.773 | 0.939 | 0.963 |
| | RMSE | 0.578 | 0.988 | 1.213 | 0.625 | 0.743 | 0.789 | 0.170 | 0.444 | 0.678 | 0.427 | 0.332 | 0.332 |
| | MAE | 0.424 | 0.660 | 0.924 | 0.471 | 0.555 | 0.583 | 0.128 | 0.727 | 0.474 | 0.283 | 0.258 | 0.241 |
| **LUE$_f$-C3** | $R^2$ | 0.426 | 0.570 | 0.408 | 0.000 | 0.686 | 0.932 | 0.779 | 0.687 |
| | RMSE | 0.253 | 0.148 | 0.347 | 0.284 | 0.187 | 0.062 | 0.212 | 0.235 |
| | MAE | 0.181 | 0.112 | 0.234 | 0.200 | 0.114 | 0.044 | 0.148 | 0.130 |
| **LUE$_f$-C3** | $R^2$ | 0.465 | 0.560 | 0.151 | 0.089 | 0.003 | 0.073 | 0.852 | 0.287 | 0.728 | 0.723 | 0.834 | 0.854 |
| | RMSE | 0.165 | 0.104 | 0.237 | 0.173 | 0.242 | 0.264 | 0.087 | 0.087 | 0.134 | 0.096 | 0.099 | 0.105 |
| | MAE | 0.115 | 0.071 | 0.162 | 0.126 | 0.063 | 0.201 | 0.058 | 0.058 | 0.089 | 0.063 | 0.053 | 0.079 |

* $\text{LUE}_p$ represent photosynthesis light use efficiency; $\text{LUE}_f$ represent light use efficiency for SIF which is fluorescence yield (i.e. the fraction of absorbed PAR photons that are re-emitted from the canopy as SIF photons); RMSE, root mean squared error; MAE, mean absolute error.
are poor correlations between simulated and observed LUE$_p$ and LUE$_f$ and disagreement with the 1 : 1 line. After optimization with seasonally varying $V_{cmax}$ derived from SIF, the regression of observed vs. modeled LUE$_p$ and LUE$_f$ is closer to the 1 : 1 line (slopes of 0.93 and 1.28 for LUE$_p$ and LUE$_f$, respectively, in Figs 10 and 11). At site level, the mean bias error (MAE) is reduced from 0.54 to 0.36 and 0.15 to 0.08 LUE$_p$ and LUE$_f$, respectively, leading to a decrease in bias of 40% on average (Table 3).
Previous studies showed that chlorophyll fluorescence is a powerful technique to quantify photosynthetic efficiency and monitor vegetation dynamics (Flexas et al., 2002; Meroni et al., 2008; Damm et al., 2010). With recent retrievals of SIF (Joiner et al., 2013), Guanter et al. (2014) first showed the feasibility to monitor crop photosynthesis at regional to global scale, and capture the high photosynthetic rate of the corn belt of midwestern US. Following that work, our study shows that we are also able to derive sensible space-based estimates of seasonal \( V_{cmax} \) by combining space-based retrievals of SIF and a photochemistry and radiative transfer model (SCOPE).

**Comparison of obtained \( V_{cmax} \) in corn and soybean with literature values**

In this study, the estimates of \( V_{cmax} \) (Fig. 3) are within the range of those reported in the literature for corn and soybean except for several of the higher values (Wullschleger, 1993; Kattge & Knorr, 2007; Kattge et al., 2009; Houborg et al., 2013). Houborg et al. (2013), for example, reported \( V_{cmax} \) at 25 \(^\circ\)C of 11 to 48 \( \mu \text{mol m}^{-2} \text{s}^{-1} \) for corn during the growing season derived from leaf chlorophyll (Chl) content. For comparison, most of our estimations range from 11 to 64 \( \mu \text{mol m}^{-2} \text{s}^{-1} \) for \( V_{cmax} \) of corn. For soybean, our retrieved values of \( V_{cmax} \) are between 95 and 134 \( \mu \text{mol m}^{-2} \text{s}^{-1} \) during the mid-growing season, which is in good agreement with literature values (Kattge et al., 2009; Houborg et al., 2013).
agreement with field estimates from gas exchange measurements during mid-August near Champaign, IL, USA (Ainsworth et al., 2014). They reported values of $V_{cmax}$ at 25°C ranging from 76 to 136 l mol m$^{-2}$ s$^{-1}$ for soybean. On the other hand, we estimate slightly higher values of $V_{cmax}$ for soybean during the early growing season, varying between 160 and 190 l mol m$^{-2}$ s$^{-1}$.

This larger $V_{cmax}$ during the early growing season may be due to two combined reasons: (1) larger slopes between $V_{cmax}$ and SIF due to this period being not Rubisco-limited (Fig. 3); and (2) spatial mismatch between GOME-2 pixel and flux tower footprint. This suggests the limitations that are primarily due to the current data availability of SIF. We assumed relatively homogeneous landscape for GOME-2 pixel, but there is obviously spatial variability within such a footprint, especially the mosaic of soybean and corn. In addition, there are different seasonal patterns of soybean and corn. As shown in Fig. 5, an earlier onset of the growing season was observed for soybean year through SIF from satellite while measurements were later from the flux tower. Hence, the assumption that it can be represented equally well for soybean and corn is tenuous in the early seasons (early to mid-June). The future reevals of SIF with higher spatial resolution from the Sentinel-5 Precursor (TROPOMI, Veefkind et al., 2012) would address this issue.

**Effects of seasonal variability in $V_{cmax}$**

Including the seasonal patterns of $V_{cmax}$ in photosynthesis simulations significantly improved the agreement between independently modeled and measured estimates of GPP over the growing season for croplands (Figs 7–9). This result is in good agreement with other studies that found better modeling of CO$_2$ exchange between terrestrial ecosystems and the atmosphere by considering seasonal variations of $V_{cmax}$ (Wilson et al., 2001; Houborg et al., 2013; Medvigy et al., 2013). In addition, the substantial improvements between modeled and flux tower derived estimates of LUE$_p$ and LUE$_f$ further increase our confidence that space reevals of SIF can be used to invert seasonally varying $V_{cmax}$ and improve modeling of GPP and LUE (Figs 10 and 11). Assuming a constant value of $V_{cmax}$ in the simulations with SCOPE over the growing season results in overestimating GPP for corn but underestimating that for soybean. Yet, this approach of parameterizing $V_{cmax}$ with constant values is widely implemented in most of terrestrial biosphere models due to the difficulties of measuring in the field and to prescribe values on a global scale (Kattge et al., 2009). This study addresses the need to consider seasonal variability in photosynthetic capacity for croplands and provides an approach to derive sensible space-based estimates of seasonal $V_{cmax}$ with space-based measurements of SIF.

**Implications for biophysical models**

Our results suggest that measurements of SIF provide a new indicator of the magnitude and seasonality in $V_{cmax}$. Recently, spectroscopic data has been used to estimate various leaf or canopy-level biophysical parameters (Gillon et al., 1999; Asner & Martin, 2008). However, there are only a few studies that have related

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**Fig. 11** Scatter plots of flux tower measured light use efficiency of photosynthesis (LUE$_p$) against Soil-Canopy Observation of Photosynthesis and Energy simulations at biweekly step during the growing season with (a) constant $V_{cmax}$ and (b) seasonal variable $V_{cmax}$ at biweekly step for all site-years during 2007–2011.
spectral data to photosynthetic capacity parameters ($V_{cmax}$) in the literature (Doughty et al., 2011; Serbin et al., 2011; Ainsworth et al., 2014). In these studies, $V_{cmax}$ values were estimated for short-term periods using full-spectrum leaf optical properties from ground measurements. To our knowledge, there is only one other study that explored this potential relationship with satellite data (Houborg et al., 2013), in which they quantified the seasonal variability in $V_{cmax}$ over a corn growing season based on Landsat-derived leaf chlorophyll estimates and a generalized indirect $V_{cmax} -$ Chl relationship for leaf nitrogen. On an operational basis, however, the required hyperspectral instruments are not currently available from space and satellite retrievals of Chl remain complex and uncertain. In this case, chlorophyll fluorescence, which has a much more direct link to vegetation photosynthetic activity, can provide an alternative way to more accurately assess key biophysical properties of vegetation compared to traditional reflectance-based measures.

The mechanistic relationship between SIF and $V_{cmax}$ shown in this study, offers the advantage of directly integrating SIF information into TBMs that rely on the C3 and C4 photosynthesis model developed by Farquhar et al. (1980) and Collatz et al. (1992). To more accurately quantify global and regional terrestrial GPP, information is needed on the seasonal variability of $V_{cmax}$ (Wilson et al., 2001; Medvigy et al., 2013). As Bonan et al. (2011) has pointed out, it is important to parameterize $V_{cmax}$ for simulating GPP because model structural errors can be partially compensated for by adjusting this parameter. In many modeling exercises, however, $V_{cmax}$ was assumed to be constant for each broadly defined PFT over time. It has long been sought to estimate the photosynthetic capacity of plant canopies from remote sensing data in space and time. The highly correlated relationship between $V_{cmax}$ and canopy-level chlorophyll fluorescence can be used to derive seasonal $V_{cmax}$ from space retrievals of SIF provided that other parameters, such as LAI and $C_{ab}$, are available from ancillary observations.

It should be pointed out that other parameters especially LAI may have similar effects to $V_{cmax}$ on the simulations of chlorophyll fluorescence. Systematic errors in LAI may lead to compensating errors in the inversion of $V_{cmax}$. In this study we have used in situ field measurements of LAI from the sites and hence this should not be important problem in our inversion of $V_{cmax}$. However, some sensitivity analyses need to be done in the future especially if LAI data is used from ancillary satellite-based measurements. Another point should be noted that, SCOPE is based on Collatz et al. (1991, 1992) for photosynthesis which assumes that the proximal cause of the decrease in photosynthetic capacity at elevated leaf temperature is incomplete activation of Rubisco. In the original Farquhar et al. model, this control is attributed to potential rate of electron transport ($I_{max}$). This parameter is used in several land surface models (e.g., CLM) and is generally assumed to be a constant ratio with $V_{cmax}$ across species (Wullschleger, 1993). Variations of this ratio have been found for different species (Medly et al., 2002; Onoda et al., 2005). However, we don’t anticipate that this difference in model structure would have any significant effect on the inversions for $V_{cmax}$ reported here.

To conclude, we demonstrated that the magnitude and seasonal variability of $V_{cmax}$ can be estimated with chlorophyll fluorescence, and that the consideration of seasonally varying $V_{cmax}$ improves the modeling of GPP and LUE for both C3 and C4 crops. We evaluated the performance of our methods using six AmeriFlux eddy covariance flux sites in the midwestern US. A high correlation (linear relationship) was found between $V_{cmax}$ and SIF using SCOPE simulations for different vegetative growth stages during the growing season when other parameters in the model are specified using ancillary data. The resulting relationships were utilized to determine the magnitude and seasonal variability of $V_{cmax}$ from GOME-2 SIF retrievals at biweekly time steps. This study indicates that the use of seasonally varied $V_{cmax}$ derived from SIF, rather than a fixed PFT-specific value, significantly improves the agreement of simulated GPP and LUE with the observed tower fluxes.

Our approach provides the basis for regional or even global estimation of key photosynthetic capacity parameters like $V_{cmax}$ from the state-of-the-art remote sensing instruments. These estimates may represent a unique data for the constraint and benchmarking of TBMs in which global vegetation is typically classified by biome, and LUTs are used to estimate model parameters for each biome (Sellers et al., 1997), especially for the key parameter of $V_{cmax}$. There are now two GOME-2 instruments on the MetOp-A and MetOp-B (launched in 2006 and 2013, respectively), and the MetOp-A is now providing data at a higher spatial resolution ($40 \times 40 \text{ km}^2$). This will lead to improved fluorescence data sets for further studies. In addition, several future instruments, such as the Orbiting Carbon Observatory-2 (OCO-2) (Frankenberg et al., 2014) and the Sentinel-5 Precursor (TROPOMI, Vreekind et al., 2012) satellite missions to be launched in 2014–2016 will provide data with an up to 100-time improvement in spatial resolution and total number of observations. This will especially benefit the applications over the fragmented agricultural areas such as in Europe and China, and improve the application of our approach. With these
high spectral and spatial resolution instruments, we could have not only the ability to derive the seasonal variability of leaf photosynthetic capacity, but also the potential to map $V_{\text{cmax}}$ on a broad scale over fragmented areas. This would provide large-scale observations of $V_{\text{cmax}}$ that could further facilitate the parameterization improvements for the dynamic global vegetation models.

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Conflicts of interest

The authors declare no conflict of interest.

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