Optimizing a remote sensing production efficiency model for macro-scale GPP and yield estimation in agroecosystems

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ABSTRACT

Earth observation data are increasingly used to provide consistent eco-physiological information over large areas through time. Production efficiency models (PEMs) estimate Gross Primary Production (GPP) as a function of the fraction of photosynthetically active radiation absorbed by the canopy, which is derived from Earth observation. GPP can be summed over the growing season and adjusted by a crop-specific harvest index to estimate yield. Although PEMs have many advantages over other crop yield models, they are not widely used, because performance is relatively poor. Here, a new PEM is presented that addresses deficiencies for macro-scale application: Production Efficiency Model Optimized for Crops (PEMOC). It was developed by optimizing functions from the literature with GPP estimated by eddy covariance flux towers in the United States. The model was evaluated using newly developed Earth observation products and county-level yield statistics for major crops. PEMOC generally performed better at the field and county level than another commonly used PEM, the Moderate Resolution Imaging Spectroradiometer GPP (MOD17). PEMOC and MOD17 estimates of GPP had an R² and root mean squared error (RMSE) over the growing season of 0.71–0.89 (9.87–17.47 g CO₂ d⁻¹) and 0.59–0.83 (6.86–22.20 g CO₂ d⁻¹) with flux tower GPP. PEMOC produced R²s and RMSE of 0.70 (0.52), 0.60 (0.61), and 0.62 (0.59), while MOD17 produced R²s and RMSE of 0.65 (0.57), 0.53 (0.66), and 0.65 (0.57) with corn, soybean, and winter wheat crop yield anomalies. The sample size of rice was small, so yields were compared directly. PEMOC and MOD17 produced R²s and RMSE of 0.53 (3.42 t ha⁻¹) and 0.40 (4.89 t ha⁻¹). The most sizeable model improvements were seen for C₃ and C₄ crops during emergence/senescence and peak season, respectively. These improvements were attributed to C₃ and C₄ partitioning, optimized temperature and moisture constraints, and an evapotranspiration-based soil moisture index.

1. Introduction

Global warming is projected to drive crop yield losses over much of the globe in the second half of the 21st century (Challinor et al., 2014). These losses are expected to increase world food prices, affect the trade balance in favor of net exporters of agricultural products, and reduce the real income of those lacking sufficient coping mechanisms (Hertel et al., 2010). From a supply-side perspective, management practices could be implemented to reduce the impact of climate-driven yield loss. These include: changing or engineering new crop varieties; adjusting planting dates; expanding irrigation or transferring cultivation to cooler climates; and improving crop residue management (Lobell et al., 2011). Crop yield models quantify plant-climate-soil interactions in order to identify management practices that improve crop yield. Large-area crop yield models (LACMs) are crop models that are intended to inform decision-making at the macro-scale under various climate change trajectories (Challinor et al., 2004). Earth observation is increasingly used for the macro-scale approach, because it provides spatially consistent eco-physiological information over large areas and a long time frame (Doraiswamy et al., 2003). Although Earth observation has advantages over other techniques, bias and uncertainties must be reduced, before macro-scale research questions are addressed.

Moulin et al. (1997) and Lobell (2013) review crop yield models utilizing Earth observation. The models typically estimate total crop biomass or the amount of aboveground dry matter generated over the growing season, which is then converted to seed or crop yield using the harvest index (Hay, 1995).

Models for estimating biomass from remote sensing can be empirical, semi-empirical, or mechanistic. Empirical models consist of statistical relationships between biomass and the Normalized

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Difference Vegetation Index (NDVI) (Tucker, 1979) or other vegetation index derived from red and near infrared (NIR) reflectance. Photosynthetically active canopies preferentially absorb in the red and scatter in the NIR due to the composition and size of leaves and stems (Ollinger, 2011). Although NDVI has been widely used to estimate biomass, it tends to saturate for dense canopies and is sensitive to soil wetness (Huete et al., 2002). As remote sensing platforms improved and included more spectral information, new broadband indices (e.g. Enhanced Vegetation Index: EVI) were developed to overcome these limitations. Data mining techniques, such as singular value decomposition and stepwise regression, were later used to develop indices more sensitive to biomass when hyperspectral data became available (Mariotto et al., 2013; Marshall and Thenkabail, 2015). Empirical models are typically developed and tuned to biomass estimates in a particular area. These models are prone to over-fitting and often must be recalibrated or may not produce reliable results at all when applied in other areas.

Semi-empirical models, also known as light-use efficiency or Production Efficiency Models (PEMs), rely on the conservative and positive response of carbon assimilation to increased solar radiation (Monteith, 1972; Monteith and Moss, 1977). This makes transferability to other regions less of an issue. In addition, the models are relatively easy to parameterize and can be run efficiently over large areas. They estimate Gross Primary Production (GPP) from Photosynthetically Active Radiation (PAR) weighted by the fraction of photosynthetically active radiation absorbed by the canopy (F_{PAR}) and energy to dry matter or quantum conversion efficiency (\( \varepsilon \)). F_{PAR} is derived from remote sensing. Climate constraints are typically used to further down-regulate GPP. GPP is integrated over the growing season to estimate Net Primary Production (NPP). Growth and maintenance respiration costs for NPP are either accounted for indirectly, e.g. Carnegie-Ames-Stanford Approach (CASA: Potter et al., 1993) and the Moderate Resolution Imaging Spectroradiometer GPP/NPP product (MOD17A2 hereafter MOD17: Running et al., 2004; Zhao et al., 2005) or directly, e.g. GLOPEM2 (Goetz et al., 1999). PEMs do not directly account for non-climatic constraints, such as management practices or nutrient availability (Grassini et al., 2015), but assume these effects are captured by F_{PAR} (Garcia et al., 1988; Squire et al., 1986; Field, 1991). Further, they tend to underperform in agroecosystems and other non-forested ecosystems, because eco-physiological constraints on GPP are more complex and phenological changes are subtler (Yuan et al., 2014; Schaefer et al., 2012).

Mechanistic models can be driven by light adaptive crop growth, but also include several interactive modules that deal with crop type and variety, soil moisture, soil carbon and nitrogen, and management practices such as inter-cropping. Remote sensing is primarily used for re-initialization or re-calibration, i.e. crop model initial conditions or parameters are adjusted until they match a remote sensing biophysical parameter, such as the leaf area index (de Wit et al., 2012; Dente et al., 2008; Li et al., 2015; Wang et al., 2013). Fully mechanistic approaches can be very accurate, provided they are properly calibrated, but are the most computationally demanding, making their use for macro-scale applications difficult unless several simplifying assumptions are made (Grassini et al., 2015).

LACMs have been used to inform a wide range of climate-related decisions in the 20th century, but improved accessibility and reliability is needed to address the challenges of the 21st century (Rotter et al., 2011). Challinor et al. (2009) recommends that model improvement should involve three synergistic activities given the large number of models and range of strengths and weaknesses of each. These include:

![Fig. 1. Workflow illustrating major inputs (●), intermediary processes (■), and final outputs (○) with site-level and macro-scale data.](image-url)
1) quantification of impacts uncertainty via sensitivity analysis or ensemble modeling; 2) coupling eco-physiological constraints or modeling approaches to account for non-linear interactions; and 3) rigorous model calibration/optimization and validation to achieve parsimony and prevent over-fitting.

This paper presents a new PEM (Production Efficiency Model Optimized for Crops –PEMOC) to improve crop yield estimation at the macro-scale using Earth observation data. The PEM approach was selected over empirical or fully mechanistic approaches, given its simplicity, direct use of Earth observation, and compatibility with remote sensing models that compute the moisture counterpart to GPP, evapotranspiration (ET) (see Cleugh et al., 2007; Fisher et al., 2008; Mu et al., 2007a, 2007b, 2011 for examples). PEMOC was developed from the ground up using the activities suggested by Challinor et al. (2009). A diagram of the complete workflow is shown in Fig. 1. First, eco-physiological functions taken from the remote sensing-based crop biomass/yield and ET model literature were integrated. Second, the function constraints were optimized with site-level eddy-covariance flux tower GPP and micrometeorological data. Third, a sensitivity analysis was performed on the optimized model. Finally, the model was driven by recently developed Earth observation products and geospatial climate data across the Contiguous United States (CONUS) to evaluate model performance with coarser spatial resolution and county-level crop yield data. PEMOC was evaluated alongside the MOD17 formulation, which was used to estimate yield for important field crops across CONUS (Xin et al., 2013; Johnson, 2016).

2. Data and processing

2.1. Site-level data

Micrometeorological data were acquired for model development and site-level evaluation. The dataset consisted of eight eddy-covariance flux towers in croplands of CONUS that are part of the AmeriFlux network (http://amerifluxornl.gov/) (Table 1). Sites were selected if GPP was available or could be derived over a period of three or more years during the MODIS era. The stations yielded 66 years of daily station data. The sites consisted of rainfed and irrigated fields that were often rotated between C3 (canola, cowpeas, rice, soybean, and winter wheat) and C4 (corn) crops. With the exception of US-TWT, the stations were in the interior of the country and had a continental climate. US-TWT was near the Pacific coast and experienced a Mediterranean climate. The interior sites had higher annual rainfall and lower but more variable average daily temperatures than US-TWT. Rainfall at the interior sites occurred during May–October when most crops are grown in the U.S. Conditions at US-TWT were generally dry during the primary growing season. The stations either recorded data at hourly or half-hourly intervals, which were aggregated to a daily time step. GPP in \( \mu \text{mol CO}_2 \text{ m}^{-2} \text{s}^{-1} \) was derived using the Marginal Distribution Sampling method (Reichstein et al., 2005). It was provided by the principle investigators for US-Ne1, US-Ne2, US-Ne3, and US-Twt. For the remaining stations, GPP was estimated using the Marginal Distribution Sampling method. Shortwave incoming radiation (W m\(^{-2}\)), temperature (°C), and the vapor pressure deficit (VPD: kPa) were also collected for model-building. Shortwave incoming radiation was masked for daytime values outside the range of instrument error (> 5 W m\(^{-2}\)) and converted to PAR (\( \mu \text{mol m}^{-2} \text{d}^{-1} \)) using the sw.to.par function in R (Britton and Dodd, 1976).

Maximum daytime VPD and temperature were used for model-building instead of daily averages, because plant-atmosphere coupling is strongest at midday when eddy formation is highest (Fisher et al., 2008). Other PEMs typically assume the plant response to eco-physiological factors is instantaneous, but in reality, plants take several days to acclimate to new conditions (Field, 1991; Pearcy and Sims, 1994; Thornley, 1998). The climate data were therefore smoothed using a 5-day exponential moving average filter to account for the time lag. Surface reflectance was not available for all the sites, so Moderate Resolution Imaging Spectroradiometer (MODIS) Terra 16-day 250 m NDVI (MOD13Q1) was used instead. NDVI was estimated by averaging 3 × 3 MOD13Q1 grid cells selected with the MODIS subset tool (http://daac.ornl.gov/) over the fetch of each tower. The fetch is defined here as the upwind area that contributes to eddy formation during daylight hours in the growing season. Poor quality MODIS data were masked and filled using an adaptive Savitsky-Golay filter (Chen et al., 2004). In some cases, the boundary of the 3 × 3 window included areas outside the fetch. These pixels were omitted from the average to avoid mixed pixel effects. Finally, the data were masked for the primary growing season. Start and end of season dates were provided by growers or farm managers.

2.2. Macro-scale data

County-level crop yield and pixel-based crop area for corn, rice, soybean, and winter wheat were used to evaluate the model at the macro-scale. County-level crop yield was collected on an annual basis and downloaded from the U.S. Department of Agriculture National Agriculture (USDA) Statistics Service (NASS https://www.nass.usda.gov/). Following Lobell et al. (2002), counties where cropped area of a given crop were < 25% of the total county area were omitted from the analysis to avoid over-fitting sparsely cropped counties. Only NASS data from 2010 to 2015 were analyzed, because high quality pixel-based crop-specific area mosaics for CONUS were available over the period through the USDA Cropland Data Layer (CDL: http://nassgeodata.gmu.edu/). CDL is created on an annual basis using decision-tree classification and surface reflectance retrieved from several sources (Landsat, MODIS, IRS RESOURCESAT-1 Advanced Wide Field Sensor) (Boryan et al., 2011). Post 2011, CDL was generated exclusively with Landsat and the new Disaster Monitoring Constellation (Deimos-1 and UK2). The maps are trained and validated with extensive ground surveys collected by the Farm Service Agency. On a pixel-by-pixel basis, CDL is 80% accurate, but is generally more accurate (mid-90%) for...
crops that have high national coverage such as corn, rice, soybean, and winter wheat. CDL is projected in Albers Conical Equal Area projection (North American Datum of 1983) at 30 m resolution. The mosaics were resampled to 250 m resolution where each new grid cell represented the proportion of 30-meter pixels classified as a particular crop type. PEMOC and MOD17 crop yield estimates were weighted by the mosaics and then averaged over each county to compare with NASS crop yield. The final dataset consisted of NASS-predicted pairs for 316, 5, 306, and 18 corn, rice, soybean, and winter wheat counties, respectively.

MOD17 is typically driven by MODIS 8-day 1 km FPAR (MOD15A2) and surface reanalysis data from the NASA Global Modeling and Assimilation Office (GMAO). In this study, the MOD17 formulation was driven instead with the same FPAR and climate data as PEMOC for consistency. This means that our use of the MOD17 term refers solely to the formulation and not the product. FPAR and climate inputs were derived from the U.S. Geological Survey (USGS) Earth Resources Observation and Science Center (EROS) expedition MODIS-based NDVI product (eMODIS) (Brown, 2018; Brown et al., 2015; Jenkinson et al., 2010); and MOD17 daily gridded surface climate data Version 2 (Thornton et al., 2014). eMODIS is a MODIS product for near real-time applications and mosaicked for CONUS. MODIS Terra and Aqua daily surface reflectance (level 2-MOD09.L2) data are converted to NDVI and provided in a user-friendly format. The data include a daily cloud mask (MOD35.L2) and are produced as a daily seven-day composite in the USGS EROS eMODIS system. For this study, we used the archived CONUS mosaics of MODIS Terra NDVI projected in Lambert Azimuthal Equal Area at 250 m horizontal resolution. eMODIS includes a data quality band, which was used together with a weighted least squares regression temporal time-series smoother to estimate NDVI. The USGS also produces estimates of the start and length of the primary growing season derived from eMODIS NDVI and a curve-fit approach (Brown, 2016). These data were used to sum MOD17 and PEMOC GPP over the growing season.

Daymet consists of continuous layers of weather data required for plant growth modeling (day length, shortwave incoming radiation, maximum daily temperature, minimum daily temperature, and average daily water vapor pressure). The layers are interpolated from weather station data distributed by the National Climate Data Center and Natural Resources Conservation Service. Temperature and precipitation estimates are interpolated using an inverse-distance algorithm, assuming a truncated Gaussian distribution and weighted by a digital elevation model (Thornton et al., 1997). Shortwave incoming radiation and vapor pressure are derived from the diurnal temperature range and dew-point temperature, respectively. The algorithms for shortwave incoming radiation and vapor pressure have since been improved from version one to account for variable solar geometry and lapse rates in complex terrain (Thornton et al., 2000). Daymet is available on a daily basis as CONUS mosaics projected in Lambert Conformal Conic (Datum = WGS-84) at 1 km horizontal resolution. Daymet was resampled to 250 m resolution using nearest neighbor. 250 m resolution was selected, because we assumed that the resolution of NDVI was driving spatial heterogeneity in GPP and crop yield. The assumption is reasonable, because row crops in CONUS are grown primarily on flat terrain and therefore tend to have gentle climate gradients. Daily average VPD was used instead VPDx for the macro-scale assessment.

### 3. Methods

#### 3.1. Model descriptions

**3.1.1. Production Efficiency Model Optimized for Crops (PEMOC)**

PEMOC assumes maximum GPP (g CO₂ m⁻² d⁻¹) from the utilizable absorbed PAR under “ideal” conditions. Sims et al. (2005) and Owen et al. (2007) showed strong linearity between gross and maximum daily GPP across multiple ecosystems. Based on their results, the model estimates gross daily GPP as a conservative fraction (63%) of maximum daily GPP. The utilizable absorbed PAR is defined by two components: FPAR and εMAX (Table 2).

$$\text{f_{MAX} = f_{MAX}(mol mol^{-1})}$$

is the ratio of carbon assimilated to the amount of light absorbed by the canopy. It is defined in this case separately for the two pathways of carbon metabolization: C₃ and C₄. C₃ metabolism is more common than C₄ metabolism, because the latter is better adapted to hot moist or dry climates (Chapin et al., 2011). C₃ metabolism is catalyzed by the Rubisco enzyme, which is temperature dependent, while C₄ metabolism is catalyzed first by PEP carboxylase to concentrate CO₂ for Rubisco catalysis. The concentration has the effect of minimizing the temperature dependency of Rubisco partitioning (Collatz et al., 1992). Based on Collatz et al. (1991), the temperature dependency for C₃ metabolism was defined in terms of available CO₂ (340 μmol mol⁻¹) and the ratio of oxygenase to carboxylase reactions for Rubisco. The ratio is partitioned according to temperature. Quantum conversion efficiency is “realized” after accounting for long-term or seasonal temperature (FL), short-term moisture (FS), and long-term or seasonal moisture (FQ) functions ranging from zero to one.

Some of the PEMOC functions have been used to estimate crop biomass/yield in previous studies, while others (Fₚ and Fₐ) were based on more recent and parallel studies. Fₚ and Fₐ are typically computed as a linear function of NDVI or EVI (Mu et al., 2007a, 2007b). Canopies that are more photosynthetically active have a higher NDVI or EVI (Fₚ → 1) than less photosynthetically active canopies or bare soils (Fₚ → 0). Fₚ is typically defined as a function of VPD, which is the difference between leaf and atmospheric moisture. As VPD increases, crops assimilate less CO₂ to prevent stress (Fₚ → 0). This decay can be defined using ramp (MOD17) or other concave functions (Fig. 2a). Alternatively, exponential (Potter et al., 1993) or other convex functions are used. Medlyn et al. (2011) provides the first theoretical basis for Fₚ and confirms several empirical studies that use the convex approach. Fₚ in PEMOC in line with Medlyn et al. (2011) assumes a logarithmic decay, which occurs when VPD exceeds 1 kPa when crops are more sensitive to changes in moisture. In reality, this threshold may vary under different moisture conditions and for different crop species (Zhou et al., 2013). Using the optimized constraints for C₃ and C₄ crops derived in

### Table 2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Equation</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>εMAX</td>
<td>Maximum quantum conversion efficiency</td>
<td></td>
<td>This study</td>
</tr>
<tr>
<td>FPAR</td>
<td>Fraction of photosynthetically active radiation</td>
<td>a₀ NDVI + a₁</td>
<td>Potter et al., 1993</td>
</tr>
<tr>
<td>Fₚ</td>
<td>Temperature stress</td>
<td>1.1814 / (1 + e⁻ᵃ⁽²⁽²⁻⁽ᵀₓ₋₁₀⁻₁₀⁾⁾) (1 + e⁻ᵃ⁽²⁽²⁻⁽ᵀₓ₋₁₀⁻₁₀⁾⁾)</td>
<td>Potter et al., 1993</td>
</tr>
<tr>
<td>Fₚ/Fₐ</td>
<td>Seasonal moisture stress</td>
<td>1 - a₄ ln (VPDₓ)</td>
<td>Medlyn et al., 2011</td>
</tr>
<tr>
<td>C3 crops</td>
<td>ε₀ = 0.08 + (Cₐ - 1)/(Cₐ + 2F)</td>
<td>Fisher et al., 2008</td>
<td></td>
</tr>
<tr>
<td>C4 crops</td>
<td>ε₀ = 0.06</td>
<td>Collatz et al., 1991</td>
<td></td>
</tr>
<tr>
<td>C4 crops</td>
<td>ε₀ = 0.06</td>
<td>Collatz et al., 1992</td>
<td></td>
</tr>
</tbody>
</table>
this study, the rate of decline in FM with VPD is much less than the Potter et al. (1993) formulation. FT is defined either as a ramp function (MOD17) or asymmetric curve (Potter et al., 1993) (Fig. 2b). In the case of the ramp function, as temperature increases, assimilation increases and saturates at 12 °C. FT in this case is used to capture the cold (nighttime) crop response. With the asymmetric formula, the response is more gradual and reverses after an optimal temperature (Topt). Unlike the ramp function, the inflection accounts for heat stress. The relationship is asymmetric, because the change is more rapid after Topt has been exceeded. The optimized FT derived in this study is much more asymmetric than the Potter et al. (1993) formulation. As one might expect, FT for C4 crops is virtually unaffected by temperatures exceeding Topt. Moisture stress can also occur when plants cannot adapt to changes in soil moisture over the growing season (FA). Although some PEMs include a seasonal soil moisture term, it was not used explicitly here, given the difficulty of acquiring calibration data and the goal of model parsimony. Instead, a simplification proposed in Fisher et al. (2008) was used that assumes the relative change in FPAR over the season responds primarily to changes in plant water status and is therefore indicative of soil moisture stress. With this approach, any moisture stress before peak light absorption is assumed negligible, meaning it responds primarily to extended dry spells.

The constraints (a0–a4) have been defined empirically in previous studies, but were estimated in this study via optimization with site-level data. The optimization was performed for each micrometeorological station using the Levenberg-Marquardt non-linear fitting algorithm available in the minipack.lm package in R (Elzhov et al., 2016). It returns the constraints after the sum of squared residuals between the simulated and observed GPP data is minimized. Seed and boundary conditions for each constraint were defined posteriori and a maximum of 1000 iterations was set to avoid fitting local optima (Table 3).

### Table 3

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Seed</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>a0</td>
<td>1.2</td>
<td>[0, 2]</td>
</tr>
<tr>
<td>a1</td>
<td>0.11</td>
<td>[0, 0.2]</td>
</tr>
<tr>
<td>a2</td>
<td>0.2</td>
<td>[0, 1]</td>
</tr>
<tr>
<td>a3</td>
<td>0.3</td>
<td>[0, 1]</td>
</tr>
<tr>
<td>a4</td>
<td>0.6</td>
<td>[0, 1]</td>
</tr>
</tbody>
</table>

### Table 4

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPPMAX</td>
<td>εMAX FPAR FT FM PAR</td>
</tr>
<tr>
<td>FPAR</td>
<td>MODIS FPAR</td>
</tr>
<tr>
<td>FM</td>
<td>1 – (VPD – VPD,MIN) / (VPD,MAX – VPD,MIN)</td>
</tr>
<tr>
<td>εMAX</td>
<td>Constant</td>
</tr>
</tbody>
</table>

#### 3.1.3. Crop yield

Gross primary production was converted to crop yield (t ha⁻¹) using the harvest index (Prince et al., 2001):

\[
Y = \sum_{i=SOS}^{n} Pn_i \times \frac{HI}{1 + RS} \times \frac{1}{1 - MC}
\]

The harvest index (HI) is the ratio of seed yield to the biological yield (Y) or total amount of dry matter the crop generates aboveground over the growing season (Hay, 1995). It is usually determined destructively, so estimates are generally assumed constant for a given crop or variety and area. The biological yield is the sum of net photosynthesis (Pn) over each day (i). Pn is summed from the start of season (SOS) and harvest (n). Net photosynthesis equals GPP after aboveground and belowground maintenance respiration costs (R) have been...
The dimensionless parameters (HI = harvest index, MC = grain moisture content, and RS = root to shoot ratio) converted total net photosynthesis (gross primary production minus respiration costs) to crop yield.

<table>
<thead>
<tr>
<th>Crop type</th>
<th>RS</th>
<th>MC</th>
<th>HI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Corn</td>
<td>0.18</td>
<td>0.11</td>
<td>0.50</td>
</tr>
<tr>
<td>Rice</td>
<td>0.10</td>
<td>0.09</td>
<td>0.40</td>
</tr>
<tr>
<td>Soybean</td>
<td>0.15</td>
<td>0.1</td>
<td>0.41</td>
</tr>
<tr>
<td>Winter wheat</td>
<td>0.20</td>
<td>0.11</td>
<td>0.37</td>
</tr>
</tbody>
</table>

The harvest index may vary between crop species and under different moisture regimes (Unkovich et al., 2010) however previous macro-scale studies (e.g. Lobell et al., 2002 and Xin et al., 2013) assumed it was constant, because it is difficult to obtain crop or location specific values. Further, the variation in HI is smaller than the variation in NPP, so its impact on crop yield is comparatively small. Two other crop-specific constraints shown in Eq. (1) were also assumed constant for each crop: the root to shoot ratio (RS) and harvest moisture content (MC). The values are shown in Table 5. The RS and HI values were taken from Prince et al. (2001). The MS values were taken from Lobell et al. (2002).

3.2. Analytical approach

3.2.1. Model optimization

Three levels of optimization (C3, C4, and both C3 and C4 crops) were performed for each station and compared using the coefficient of determination (R²) and cross-validated root mean square error (RMSE). The mean of the optimized coefficients for each level was used to estimate PEMOC GPP and compare to MOD17 GPP. Two additional performance metrics were also computed: systematic root mean square error (RMSEc) and unsystematic root mean square error (RMSEi). The former measures the correctable predicted error (bias), while the latter measures the random predicted error. The performance metrics were calculated only for the growing season.

3.2.2. Sensitivity analysis

A sensitivity analysis was performed after model optimization to identify the most important constraints and guide future model improvements. The sensitivity analysis was performed on the four primary inputs (NDVI, PAR, TX, and VPDX) using the one-parameter-at-a-time approach (Haan, 2002). The inputs at each station were varied randomly 10,000 times between ±2σ of each station’s mean, while the other inputs were kept at their mean. The impact of each input was then tested by relating it to PEMOC GPP. Since most of the functions are nonlinear, the non-linear fitting algorithm was used to define each relationship. The comparison was made in standard space to determine relative sensitivity. With this approach, inputs with a larger absolute slope were more sensitive than inputs with a lower absolute slope.

3.2.3. Macro-scale evaluation

PEMOC was compared to MOD17 across CONUS. The two models were compared against county-level crop yield using R² and RMSE. Yield data were converted to standardized anomalies to prevent serial autocorrelation and the effects of other inherent non-linearities. Additional statistics (long-term μ and σ) were computed to characterize general patterns across CONUS. To improve PEMOC efficiency, GPP was computed as a weighted average of C3 and C4 fixation pathways at each grid cell. The weights were derived from resampled 1° (~111 km at the equator) resolution proportion of C3 and C4 vegetation maps (Datum = WGS-84) developed by the International Satellite Land Surface Climatology Project Initiative II (Still et al., 2003).

4. Results

4.1. Model optimization and sensitivity analysis

The optimization produced high correlations and low-moderate error with site-level GPP (Table 6). The low-moderate errors were due to the underestimation of peak GPP. The highest correlations were for the corn-soybean sites and the lowest correlation was for the rice site. The optimizations were robust, since the maximum number of iterations in each case was ≤30, which is well below the maximum limit. The mean constraints when C3 and C4 crops were optimized together were a0 = 1.14, a1 = 0.12, a2 = 0.17, a3 = 0.66, and a4 = 0.09. These were used for the sensitivity analysis and model evaluation. The coefficient of variation was 0.10, 0.51, 0.28, 0.58, and 0.91, respectively. The coefficient of variation (μ/μ) expresses the variation of a coefficient relative to other coefficients. The high value for a4 indicates much variation among stations, while the small value for a1 indicates relatively little variation across stations. Compared to other linear FPAR functions (Myneni and Williams, 1994; Xiao et al., 2004; Potter et al., 1993), PEMOC FPAR changed at a similar rate, but was higher (e.g. FPAR = 0.12 when NDVI = 0.5) which controls the ascending (“cold”) arm of FPAR was closed to the seed value (0.2) taken from Potter et al. (1993) for both C3 and C4 crops, meaning crops had a fairly consistent response to temperatures below TOPT, a4 which controls the descending (“warm”) arm of FPAR was much higher than the seed value (0.3) taken from Potter et al. (1993). For many of the C3 crops, a2 was closer to the seed value, which may reflect that C3 crops are more sensitive to temperatures exceeding TOPT. For other C3 and C4 crops, a3 was much higher or one. These crops could be less sensitive to temperatures exceeding TOPT.

4.2. Micro-scale evaluation

The relative sensitivity of PEMOC to model inputs for each flux tower is shown in Table 7. The slope indicates the predicted positive or negative change in PEMOC GPP due to a standard deviation increase in a given model input (NDVI, PAR, TX, and VPDX). The model was most sensitive to PAR, because the absolute slope was the largest. The slope

<table>
<thead>
<tr>
<th>ID</th>
<th>a0</th>
<th>a1</th>
<th>a2</th>
<th>a3</th>
<th>a4</th>
<th>N</th>
<th>Iteration</th>
<th>R²</th>
<th>RMSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>US-Arm</td>
<td>1.36</td>
<td>0.20</td>
<td>0.11</td>
<td>0.05</td>
<td>0.18</td>
<td>2410</td>
<td>9</td>
<td>0.79</td>
<td>4.60</td>
</tr>
<tr>
<td>C3</td>
<td>1.34</td>
<td>0.20</td>
<td>0.11</td>
<td>0.05</td>
<td>0.13</td>
<td>2050</td>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C4</td>
<td>1.34</td>
<td>0.20</td>
<td>0.11</td>
<td>0.05</td>
<td>0.13</td>
<td>2050</td>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>US-Bo1</td>
<td>1.18</td>
<td>0.10</td>
<td>0.11</td>
<td>0.02</td>
<td>0.11</td>
<td>590</td>
<td>11</td>
<td>0.87</td>
<td>9.72</td>
</tr>
<tr>
<td>C3</td>
<td>1.06</td>
<td>0.06</td>
<td>0.20</td>
<td>0.10</td>
<td>0.27</td>
<td>174</td>
<td>10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C4</td>
<td>1.16</td>
<td>0.10</td>
<td>0.11</td>
<td>0.27</td>
<td>0.00</td>
<td>416</td>
<td>23</td>
<td></td>
<td></td>
</tr>
<tr>
<td>US-Ne1</td>
<td>1.08</td>
<td>0.08</td>
<td>0.16</td>
<td>0.04</td>
<td>0.00</td>
<td>448</td>
<td>26</td>
<td>0.82</td>
<td>9.67</td>
</tr>
<tr>
<td>US-Ne2</td>
<td>1.18</td>
<td>0.15</td>
<td>0.19</td>
<td>0.28</td>
<td>0.00</td>
<td>795</td>
<td>26</td>
<td>0.89</td>
<td>9.96</td>
</tr>
<tr>
<td>C3</td>
<td>1.11</td>
<td>0.10</td>
<td>0.06</td>
<td>0.85</td>
<td>0.00</td>
<td>347</td>
<td>30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C4</td>
<td>1.20</td>
<td>0.18</td>
<td>0.32</td>
<td>0.31</td>
<td>0.00</td>
<td>448</td>
<td>27</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Summary statistics (coefficient of determination - R² and cross validated root mean squared error-RMSE) for constraints (a0–a4) optimized to predict GPP (g CO₂ m⁻² d⁻¹) at each micrometeorological station. The optimization was performed for C3, C4, and both C3 and C4 portion of the time series.
was positive, meaning that as the amount of solar energy available to the canopy increased, GPP increased. The model was most sensitive to PAR at US-Crt whose signal was dominated by winter wheat. Winter wheat is planted well before the onset of the primary growing season so light is most abundant. After PAR, the model was most sensitive to NDVI, which is used to parameterize FPAR and FA. The slopes, with the exception of US-Arm were similar across sites. The low response at US-Arm could be due to the presence of canola and cowpeas, which are planted well before the onset of the primary growing season and have relatively low $F_{\text{PAR}}$. The model was least sensitive to VPD$_X$ and $T_X$, which are used to parameterize $F_{\text{SH}}$ and $F_T$. NDVI (VPD$_X$) is directly (inversely) proportional to GPP, meaning as photosynthetic activity in the canopy increases and atmospheric moisture demand decreases, GPP increases. $F_T$ had an inflection point at $T_{OPT}$. When $T_X$ was less than $T_{OPT}$, GPP increased with temperature and when $T_X$ was higher than $T_{OPT}$, GPP decreased with temperature. The asymmetry around $T_{OPT}$ led to a slightly negative slope for temperatures exceeded $T_{OPT}$.

### 4.2. Model evaluation (site-level)

In general, PEMOC produced higher correlations and lower error with the micrometeorological data than MOD17 (Figs. 3 and 4). MOD17 tended to under-predict peak GPP. From the time series of observed and predicted GPP (not shown), it was also apparent that MOD17 over-predicted periods of emergence and senescence. MOD17 was particularly poor at predicting peak GPP for corn, the only C$_4$ crop (US-Ne1, US-Ne2, and US-Ne3). Errors from MOD17 estimates were both unsystematic and systematic. PEMOC under-predicted peak GPP for corn, but not as severely as MOD17. It tended to over-predict peak GPP for C$_3$ crops. Predictions during emergence and senescence were more realistic. The error of PEMOC for most of the stations was largely systematic and therefore correctable. Two exceptions were at US-Crt and US-Twt where PEMOC had higher $R^2$, but higher RMSE as well. The higher error from PEMOC was due to larger spread and over-prediction of peak GPP, respectively.

### 4.3. Model evaluation (macro-scale)

There were regional differences between PEMOC and MOD17 GPP/NPP. Fig. 5 shows the $\mu$ and $\sigma$ of NPP for CONUS at 250 m resolution masked for cropped areas from 2001 to 2015. MOD17 tended to predict higher and more variable NPP than PEMOC using the eMODIS and Daymet data. Some notable exceptions include the most agriculturally intensive regions of the country: the corn-soybean dominant upper Midwest and rice dominant lower Mississippi River and upper Central Valley of California; winter-wheat dominant Colombia and Snake Rivers; and mixed crops in the lower Central Valley of California. In these regions, PEMOC tended to produce higher and more variable estimates of NPP.

The results of the macro-scale evaluation were fairly consistent with the site-level evaluation. PEMOC produced higher correlations and lower error with NASS county-level yield anomalies for corn and soybean, particularly for low to moderate producing counties (Fig. 6). MOD17 performed slightly better for winter wheat, particularly for moderate to high producing counties. PEMOC and MOD17 significantly under-predicted rice yield, which led to the poorest performance overall. Fig. 7 shows simulated versus NASS rice yield. The scatter plots do not show anomalies, because the sample size was small ($N = 11$). PEMOC showed an upward trend, while MOD17 showed a downward trend with rice yield, meaning PEMOC may be able to better capture anomalies if more data were available.

### 5. Discussion

PEMs represent an important class of remote-sensing based approaches for estimating biomass/yield. Unlike empirical approaches, which represent the other main remote-sensing approach, they can be used for macro-scale applications with sufficient calibration and validation. They were originally designed for forest ecosystems and tend to perform poorly for agroecosystems and grasslands. This study specifically addresses deficiencies in PEMs for estimating crop biomass/yield, but could easily be adapted to improve performance in other ecosystems. The results make three important contributions to remote-sensing based estimation of crop biomass/yield at the macro-scale. First, the largest improvements in crop yield estimation, particularly for corn and soybean, were made by simulating C$_3$ and C$_4$ pathways separately. Second, PEMOC was most sensitive to PAR and NDVI, followed by moisture and temperature. Options exist to reparameterize PAR and $F_{\text{PAR}}$ that could lead to further model improvements. Finally, the model was optimized with available eddy covariance flux tower data, but could easily be re-optimized when more data from agroecosystems become available. The means of optimized constraints were used in this study for comparison purposes, but resulted in a clear systematic bias. Performance was better when the model was optimized by crop type. Quality control issues, particularly with the macro-scale assessment need to be addressed, but in the meantime, the model could be used at the macro-scale with the mean constraints or more effectively with the constraints optimized to specific crops.

Maximum quantum efficiency is highly variable in space and time. It is considered the major source of MOD17 and other PEM uncertainty and bias (Zhang et al., 2008). It can be greatly reduced through $C_3$ and $C_4$ partitioning (Schaef er et al., 2012; Zhang et al., 2017). Unlike MOD17, which assumes that $e_{\text{MAX}}$ is constant for all crops, PEMOC assumes that $C_3$ $e_{\text{MAX}}$ is temperature-dependent and $C_4$ $e_{\text{MAX}}$ is constant. The $C_3$ and $C_4$ partitioning in PEMOC led to higher correlations and
lower error with micrometeorological GPP and county-level yield data. These improvements can be attributed mainly to lower bias in peak season GPP and secondly to more realistic estimates of GPP during emergence/senescence. MOD17 tended to underestimate peak season GPP, particularly for C4 crops. Over-estimation of MOD17 during emergence/senescence can be impacted by partitioning as well, but others have observed that poor parameterization of FM with VPD is the main culprit (Schaefer et al., 2012).

Further PEM improvements for agroecosystems could be achieved by improving PAR estimates and the functional relationships for FPAR, FM, and FT. The sensitivity analysis revealed that PEMOC was most sensitive to PAR and NDVI, meaning they govern most of the variability in GPP and should be the first terms addressed to improve model accuracy. PEMOC assumes that light use efficiency improves with PAR under clear sky conditions. Some studies have shown that light use efficiency is higher under diffuse sky (cloudy) conditions (Suyker and Verma, 2012). A cloud-adjusted PAR was recently implemented in a PEM with high success, $R^2 = 0.926$ and 0.909 for the calibration and validation datasets using US-Ne1, US-Ne-2, and US-Ne-3 simulated versus observed daily GPP (Nguy-Robertson and Xiao, 2015). NDVI is used to estimate FPAR and FA. The relationship between FPAR and NDVI was assumed linear. This assumption typically leads to overestimation of FPAR outside the primary growing season when canopy cover is low. Within the growing season, NDVI can saturate when crops reach peak productivity, which can lead to underestimation of FPAR. The MODIS FPAR product or another approach that applies a radiative transfer algorithm or a ratio-based EVI FPAR could be used to address non-linearity. The model showed the least variation among sites for the primary
control on FPAR, a0, so we expect re-optimization of FPAR will have little effect on improving model accuracy. Fₐ is used in ET models, but has not been adopted in PEMs. Fₐ tracks seasonal changes in temperature/light and may not relate to drought. High inter-correlation among PEM parameters has been observed in previous studies (Anav et al., 2015) and parameterizing Fₐ with NDVI gives added weight to this input that could amplify errors in the presence of uncertain data. Two other indices have been proposed that could be used to constrain soil moisture instead of Fₐ: thermal inertia (ATI) index (Garcia et al., 2013) and Land Surface Water Index (LSWI) (Xiao et al., 2004). ATI and LSWI utilize land surface temperature and shortwave infrared, respectively. Both are readily available in the MODIS-era, but for more historical analyses, NDVI-based Fₐ remains a good alternative.

The model was less sensitive to temperature and moisture constraints, but showed considerably more variation among sites. The greatest variation was with a₄, which controlled FM. Average a₄ was low (0.09) and zero for many of the sites. For PEMOC, an FM was selected based on a consensus reached on moisture limitations to stomatal conductance and GPP. FM is considered a poor indicator of soil moisture status, especially for irrigated crops (see Biggs et al., 2016 for an evaluation of VPD-based techniques), so authors have suggested introducing a suitable short-term soil moisture parameter to reduce over-estimation of GPP (Mu et al., 2007b). There are several alternatives that could be evaluated within the optimization workflow, since we ruled out omitting FM entirely. This could include an additional optimization constraint that replaces the 1 kPa threshold over which increases in VPD downregulate GPP selected for this study. The temperature function in PEMOC is widely used, but a few alternatives, such as the

![Fig. 4. Scatterplots of daily MOD17 predicted gross primary production (GPP) versus observed GPP and 1:1 line (canola = +, corn = ■, cowpea = x, rice = ▲, soybean = ●, and winter wheat = ♦). Summary statistics include the coefficient of determination-R², root mean squared error-RMSE, unsystematic root mean squared error-RMSE_u, and systematic root mean squared error-RMSE_s.](image-url)
MOD17 ramp function do exist that could also be evaluated. Perhaps the most interesting result of the $F_T$ optimization was with $a_3$, which controls the descending node when temperatures exceed $T_{OPT}$. For many of the sites, $a_3$ approached one, meaning GPP was independent of temperature fluctuations that do not co-vary with more important terms, such as $F_{PAR}$. Aside from $a_0$, $a_3$ was the highest on average (0.66) and well above the seed value taken from the literature (0.3). The results agree with other studies, such as Woodward and Smith (1994) who suggest a more asymptotic $F_T$ than Potter et al. (1993). PEMs should consider a much higher coefficient on the ascending arm of $F_T$.

FA is widely used by the ET modeling community to indicate seasonal soil moisture status and therefore should be considered along with the C3 and C4 partitioning to reduce PEM bias and uncertainty.

The PEM presented did not consider other factors that could be relatively easy to implement in the optimization work flow. Leaf age can also impact GPP, as emerging and senescing crops have lower light use efficiency than fully productive crops (Kallas et al., 2011). One could argue that $F_A$ presented in this study captures leaf age, but it was not considered explicitly.

It is difficult to compare the results of this study to others, given differing objectives and methods. The primary purpose of this study was to present a new work flow for developing remote sensing-based macroscale estimation of crop yield. Instead of simply plugging in and evaluating new functions, we integrated and optimized functions gleaned from an exhaustive literature review. The final model using mean constraints generally performed better than the MOD17 formulation. On an individual crop basis, performance was higher. Both models were highly correlated with eddy covariance flux tower data, but RMSE was higher than previous studies conducted in agroecosystems, e.g. 2.81 g CO$_2$ m$^{-2}$ d$^{-1}$ was reported for corn in Zhang et al. (2008). The higher PEMOC and MOD17 GPP error can be attributed to the period over which it was computed for this study. In other studies, RMSE was computed over the entire year and included several low GPP estimates outside the growing season. Including them would tend to lower RMSE. In this study, RMSE was only computed over the growing season when GPP is high. This was done because at some sites, data were not available outside the primary growing season. In addition, crop yield is computed over the primary growing season, so estimates outside the primary growing season are redundant, because they do not contribute to model performance. PEMOC performance was comparable to the “improved” MOD17 model proposed in Xin et al. (2013) for corn ($R^2 = 0.55–0.77$) and soybean ($R^2 = 0.50–0.73$. In Xin et al. (2013),
Fig. 6. Scatterplots of standardized crop yield anomalies from 2010 to 2015 as simulated by PEMOC and MOD17, respectively: A–B) corn and C–D) soybean, and winter wheat (E–F). The dashed line is a 1:1 relationship.
only county-level rainfed corn and soybean were evaluated and over a much smaller spatial domain (12 states in the Midwestern United States) than this study. They used a more liberal threshold of inclusion (5% versus 25% harvested area). This criterion introduced very low producing counties that acted as leverage points and introduced non-linearity that could have inflated the performance of the model. Further, Xin et al. (2013) was driven by different climate forcing than this study, which may prevent realistic comparison. Johnson (2016) compared the relationship between NDVI, GPP, and other MODIS-based vegetation products with NASS yield statistics for several crops across CONUS. Unlike previous studies, they considered timing as a factor for predictability. For corn and soybean, the highest correlations were during the middle of the growing season. NDVI showed the highest correlation with corn ($R^2 = 0.64$) and soybean ($R^2 = 0.49$) yield, which were lower than the PEMOC correlations with corn and soybean yield. Similarly, NDVI showed the highest correlation with wheat yields early in the primary growing season, but the results were still lower ($R^2 = 0.49$) than what was reported for PEMOC. For rice there was no relationship ($R^2 = 0.00$), because the sample size was small.

Other factors make the comparison of model performance with county-level yield difficult. Inherent in the PEM approach, the influence of non-biophysical influences on yield are subsumed in $F_{PAR}$, but may be better simulated separately. The CDL harvested area that was used to weight PEMOC yield for corn includes silage and grain yield. PEMOC however only predicted grain yield. The conversion between bushels to MT for corn and soybean was assumed constant because more detailed information was unavailable, but in reality these terms vary. The evaluation focused on winter wheat instead of all wheat varieties, because it is the dominant variety. This may have proved problematic however as winter wheat is grown outside the primary growing season when other crops with a stronger signal may be grown and could be influencing the phenology algorithm. PEMOC is spatially more variable than MOD17, meaning geo-location errors due to resampling could enhance errors in estimates over spatially smoother MODIS estimates, and PEMOC required an additional input (proportion of C3 and C4 photosynthesis) that was only available at coarse (1°) resolution. Finally, the conversion between GPP and NPP, harvest index, root to shoot ratio, and harvest moisture content, which were assumed constant, can all vary among crop varieties and under different climatic conditions (Sinclair and Muchow, 1999; Turner et al., 2003). Some of these uncertainties can easily be addressed in the near future. For example, the 1° C3-C4 proportion map could be replaced with the forthcoming 10 km resolution map for North America using the methodology proposed for South America in Powell et al. (2012). Other issues, particularly concerning yield uncertainties are more difficult and may be best addressed by comparing the approach to other spatially explicit approaches derived from observed data, such as machine learning (You et al., 2017) or solar-induced fluorescence (Guan et al., 2015).

This study did not directly address the impact of different forcing data on model results. The inputs were selected due in part because they are available near real-time and we wanted to demonstrate how crop yield could be monitored across CONUS with Earth observation for the first time. Daymet shows a high level of fidelity with other temperature and precipitation geospatial datasets (Huang et al., 2016), but like other geospatial datasets, shortwave radiation remains a leading source of bias and uncertainty due to the poor quantification of cloud, aerosol, and water vapor content (Zhao et al., 2013). Since PEMOC was most sensitive to PAR, reducing bias and uncertainty in shortwave radiation could lead to improvements in GPP and crop yield estimated by PEMOC.

6. Conclusions

Macro-scale crop yield models are an important tool used by practitioners and decision-makers to compare options and investments to support “best” policies and practices related to sustainable food security. Production efficiency models (PEMs) are an important class of remote sensing-based models that can be used to address questions in macro-scale climate change and food security analysis. PEMs still have large bias and uncertainties in agroecosystems that need to be addressed in order for best policies and practices to be properly identified and implemented. Here we developed a PEM that integrated eco-physiological functions taken from the Earth observation light-use efficiency and evapotranspiration model literature. The function constraints were optimized and a sensitivity analysis was performed using eddy covariance flux and other micrometerological data from agroecosystems. The model was evaluated with county-level crop yield statistics and compared against another commonly used PEM formulation used to develop the MOD17 product. Compared to the MOD17 formulation, improvements were seen via the integration of C3 and C4
photosynthesis partitioning, optimized moisture and temperature constraints, and a seasonal soil moisture index taken from the evapo-transpiration model literature. These improvements significantly reduced Gross Primary Production (GPP) bias and uncertainty during peak season for C4 crops and periods of emergence and senescence for C3 crops.

The model was purposely driven by new near real-time Earth observation products to illustrate how it could be used as a crop monitoring tool for CONUS in the future. It was calibrated with rainfed and irrigated crops widely grown in CONUS, but should be evaluated for other crops and optimized on a per crop basis, before the workflow is operationalized.

The model could also be used to conduct historical or projected (i.e. scenario-building) crop yield assessments in CONUS or other regions of the world. For example, the model will be optimized with historical rice yield estimates across Asia in the near future to evaluate the transition of C3 to C4 rice yields under climate change.

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University of Montana, Missoula, MT.


Aggregate Description of Land Atmosphere Interactions.


