Estimating Global GPP with SIF and a Data Assimilation System

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• Global GPP estimates vary widely (see review by Anav et al. 2015)
• Observations need to be better integrated with predictive models
• Linear relationship at monthly timescale
• Slope can vary with ecosystem type and environmental conditions
• Can use a simple linear scaling (e.g. Macbean et al. 2018):
  • This may omit some important non-linearities
  • Cause additional equifinality issues

• Can use a more complex model:
  • Better basis for prediction
  • Semi-empirical models e.g. Guan et al. (2015), Zhang et al. (2018)
  • More mechanistic models e.g. Koffi et al. (2015), Norton et al. (2018)

We use the SCOPE model embedded within the land surface model BETHY to simulate SIF and GPP globally.
• This provides a mechanistic relationship between SIF and GPP
• So, the relationship is described by processes, not linear scaling parameters
Our Data Assimilation Framework

- We use a variational data assimilation system:
  - Apply a quasi-Newton minimization algorithm (Tarantola, 2005)
  - It is iterative
  - The Jacobian (sensitivities) is re-calculated after each iteration to account for non-linearities (this has a large computational demand)

Minimizes a global cost function that describes the mismatch between the model and observations weighted by their uncertainties.
The BETHY-SCOPE Model

- Simulates SIF and GPP globally at 2° x 2°
- 13 PFTs (can have 3 PFTs per pixel)
- BETHY provides the infrastructure to simulate SCOPE globally.
  - It can also simulate prognostic LAI and provide it to SCOPE.
- SCOPE simulates SIF and GPP
  - It is 1D (i.e. no horizontal variation in canopy structure)
  - Not a full SVAT model, but it simulates SIF mechanistically
- Process parameters can be PFT-specific (e.g. $V_{\text{cmax}}$), PFT-grouped (e.g. LIDF) or global (e.g. Michaelis-Menten kinetic constants).
- Leaf Area Index (LAI) is prescribed
  - We use “MODIS Improved” dataset (Yuan et al., 2011)

For more information see: Rayner et al. (2005); Knorr et al. (2010); Koffi et al. (2015); Norton et al. (2018)
OCO-2 SIF

- Gridded to 2° x 2° and monthly scales
- We use:
  - 2015 for optimization/calibration
  - Sep-Dec 2014 for validation
- Calculated uncertainties:
  - We don’t use the standard error
  - Calculated uncertainties are between standard error and average of single measurement precision error
- Data over water (IGBP) are omitted
Model vs Observations: Prior

For calibration period (2015)

\[
SIF \text{ Residual} = \text{Model} - \text{Observed}
\]

\[
SIF \text{ Mismatch} = \frac{\text{Model} - \text{Observed}}{\text{Uncertainty}}
\]
Model vs Observations: Posterior

For calibration period (2015)

\[ SIF \text{ Residual} = \text{Model} - \text{Observed} \]

\[ SIF \text{ Mismatch} = \frac{\text{Model} - \text{Observed}}{\text{Uncertainty}} \]
Model vs Observations

Prior
(2015)

Posterior
(2015)
Model vs Observations: Validation

Prior
(Sep-Dec 2014)

Posterior
(Sep-Dec 2014)
An optimal fit, given the uncertainties, will give:

\[ \chi^2 = 1 \]

**Calibration period (2015):**

- Prior: \[ \chi^2 = 2.24 \]
- Posterior: \[ \chi^2 = 1.18 \]

**Validation period (Sep-Dec 2014):**

- Prior: \[ \chi^2 = 2.10 \]
- Posterior: \[ \chi^2 = 1.04 \]

We are fitting the data well and not overfitting!
Optimized Parameters

42 parameters are exposed to the optimization: each is represented by a Gaussian PDF.

Following the assimilation of SIF:

• Chlorophyll content decreases (except C3 grass):
  • Posterior estimates range from 1-13 μg cm\(^{-2}\)
  • Strong reduction of uncertainty (typically around 90%)

• \(V_{c_{\text{max}}}\) generally increases:
  • Posterior estimates range from 11-125 μmol m\(^{-2}\) s\(^{-1}\)
  • Weak reduction of uncertainty (typically < 10%)

• Little change in other physiology parameters (e.g. \(K_{c}\), \(K_{o}\))
• Varied changes to canopy structure (e.g. LIDFa, LIDFb)

Remember that LAI is prescribed and therefore fixed.
SIF-Optimized GPP (2015)

- Increase in extra-tropics.
- Decreases in dry tropics (forests + grasslands).
- Little change in wet tropical forests.

Overall increase in global annual GPP from
128 Pg C → 137 Pg C
SIF-Optimized GPP (2015)

The uncertainty in GPP due to uncertain parameters is reduced by 65% by the SIF observations.

- Global annual GPP:
  - Prior = 128 ± 17 Pg C
  - Posterior = 137 ± 6 Pg C
Overall the spatial patterns look reasonable. Compared to other GPP estimates, our SIF-optimized GPP is:

- Relatively high in the tropics and the temperate north
- Higher than FLUXCOM GPP almost everywhere (except north of 65° N)

Global GPP:

- Prior = 128 Pg C
- Posterior (SIF) = 137 Pg C
- TRENDY = 142 Pg C
- FLUXCOM = 103 Pg C
What causes the change in GPP following the SIF assimilation?

- APAR decreases globally
  - Due to decline in chlorophyll
- LUE increases globally
  - Due to decline in APAR
  - Due to increase in $V_{c_{\text{max}}}$
The model struggles to simultaneously fit low and high SIF values (> 1.0 W m\(^{-2}\)).

Remaining Challenges

- Ecosystems with a large seasonal cycle in OCO-2 SIF show the largest model-observed mismatch. Why?
  - Parameters (e.g. chlorophyll, \(V_{cmax}\), LIDF) probably vary seasonally, we keep them constant.
  - Issues with prescribed LAI?
  - Issues with spatial averaging differences between SIF, LAI, climate variables?
Remaining Challenges

• The model struggles to simultaneously fit low and high SIF values (> 1.0 W m⁻²).
  → Seasonal variation in parameters would help fit the data and be more realistic.
Remaining Challenges

- The model struggles to simultaneously fit low and high SIF values (> 1.0 W m\(^{-2}\)).
  - Seasonal cycle in LAI is vastly different to SIF in some regions
  - Shown here: SIF peaks in July-August but LAI peaks in November (LAI retrieval issues?)
Remaining Challenges

• Validating parameters (e.g. chlorophyll, $V_{c_{max}}$) and derived variables (e.g. APAR, LUE).
  → Very challenging at this scale!
  → We could evaluate against site-based data: issues with representativity
  → We could evaluate chlorophyll against the MERIS Terrestrial Chlorophyll Index
  → We’re open to suggestions!
Remaining Challenges

• Validating GPP

→ Also very challenging at this scale

→ Test: Does the SIF-optimized model improve our match with atmospheric CO$_2$ or COS?

→ Comparison with FLUXCOM GPP over North America and Europe (where density of flux towers is higher) suggest the general patterns are decent:
  • The correlation with FLUXCOM GPP improves following the SIF assimilation.
  • However, the SIF-optimized GPP magnitude is larger.
  • We wouldn’t do this for the tropics!

**North America**

$R^2$ (prior) = 0.80  \hspace{1cm} R^2$ (post.) = 0.86

**Europe**

$R^2$ (prior) = 0.77  \hspace{1cm} R^2$ (post.) = 0.83
Next Steps

- Interannual variability: can the optimized model capture IAV in SIF?
- Conduct a similar optimization at sites.
- Use complementary observations (e.g. FAPAR, NIRv): use these to constrain chlorophyll and/or LAI first.
Thank you!


