Introducing a mechanistic modelling of COS fluxes in the ORCHIDEE Land Surface Model

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In collaboration with:
L.M.J. Kooijmans, K.-M. Kohonen (Hyytiala observations)
R. Commane, N. Wehr (Harvard observations)
J. Ogée (soil modelling)

Objectives

Goal:

Improve the representation of the Gross Primary Production (GPP).

-> Use COS as a proxy to constrain GPP.

-> Need of a COS model for continental vegetation and soil fluxes.

This study:

Vegetation uptake

- Implement a mechanistic model for COS uptake.
- Study the model's behavior in terms of fluxes and conductances at site level.
- Compare to the former Leaf Relative Uptake (LRU) approach.

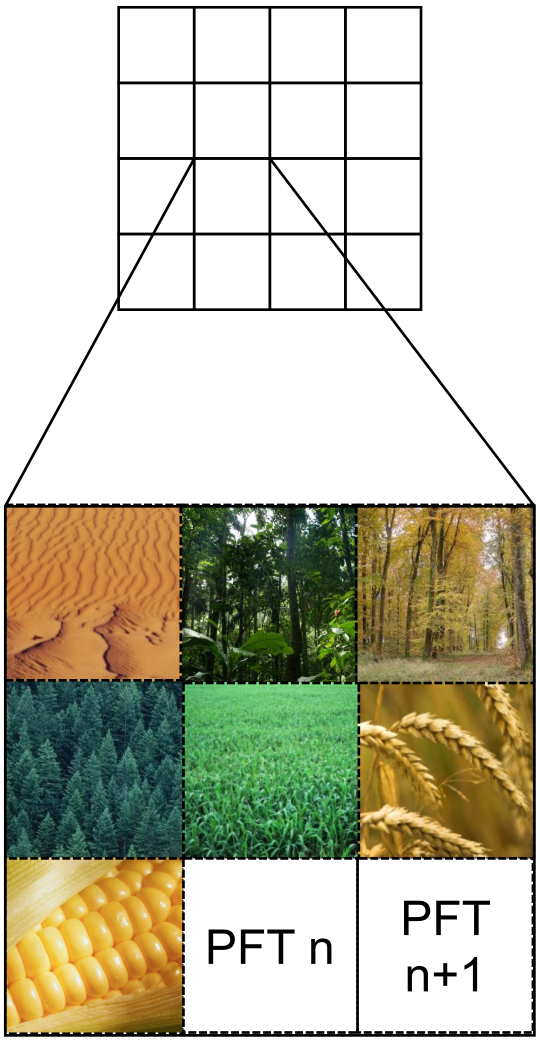
Soil fluxes

- Preliminary test of Berry and Ogée models.

Vegetation Uptake

Plant Functional Types

grid cells



Photosynthesis module

- Farquhar et al. (1980) for C3 plants
- Collatz at al. (1991) for C4 plants
- Ball et al. (1987) for stomatal conductance
- Kattge & Knorr (2007) for temperature dependences
- Yin & Struik (2009) for improvements and analytical resolution

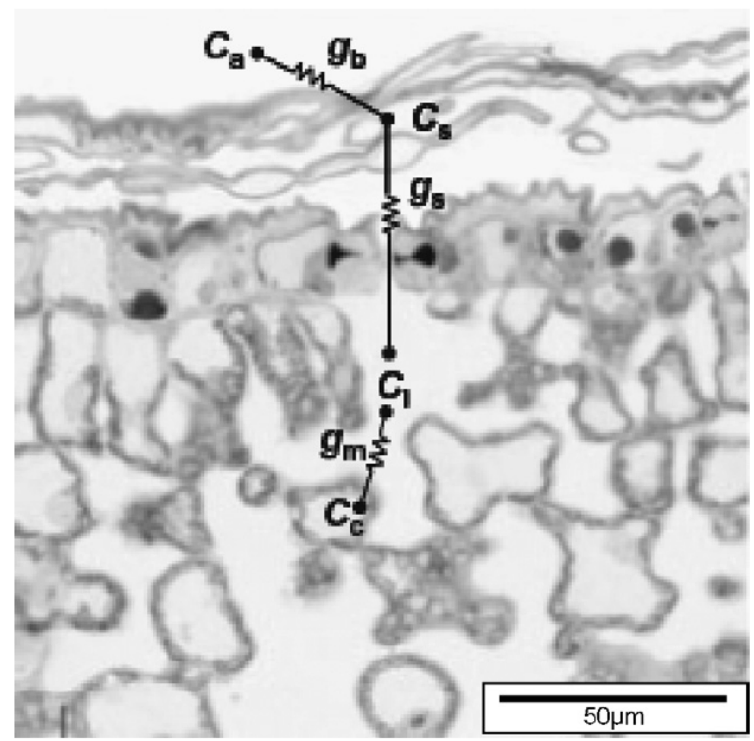


Fig. 4. Micrograph of the abaxial surface of a typical leaf, illustrating the pathway of CO_2 transfer from ambient air (C_a) through leaf surface (C_s) and intercellular air spaces (C_i) to the Rubisco carboxylation-sites in chloroplasts (C_c). Boundary-layer conductance (g_b), stomatal conductance (g_s), and mesophyll conductance (g_m) are indicated. Revised from Flexas et al. [39].

Yin & Struik (2009)

VEGETATION UPTAKE OF COS: THE BERRY ET AL. (2013) MODEL

$$\boxed{g_i = \alpha V_{cmax}}$$

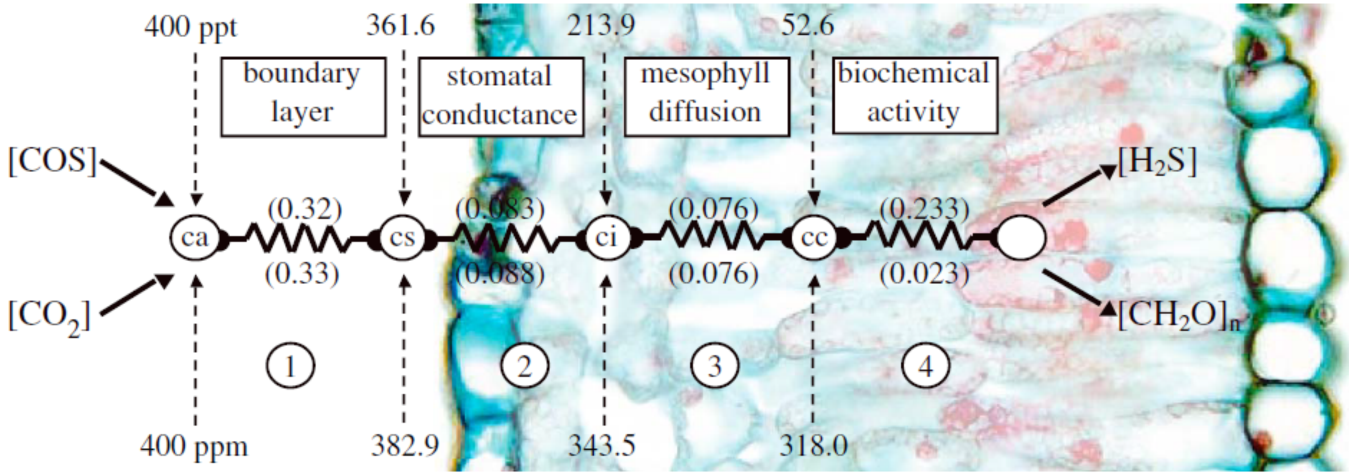
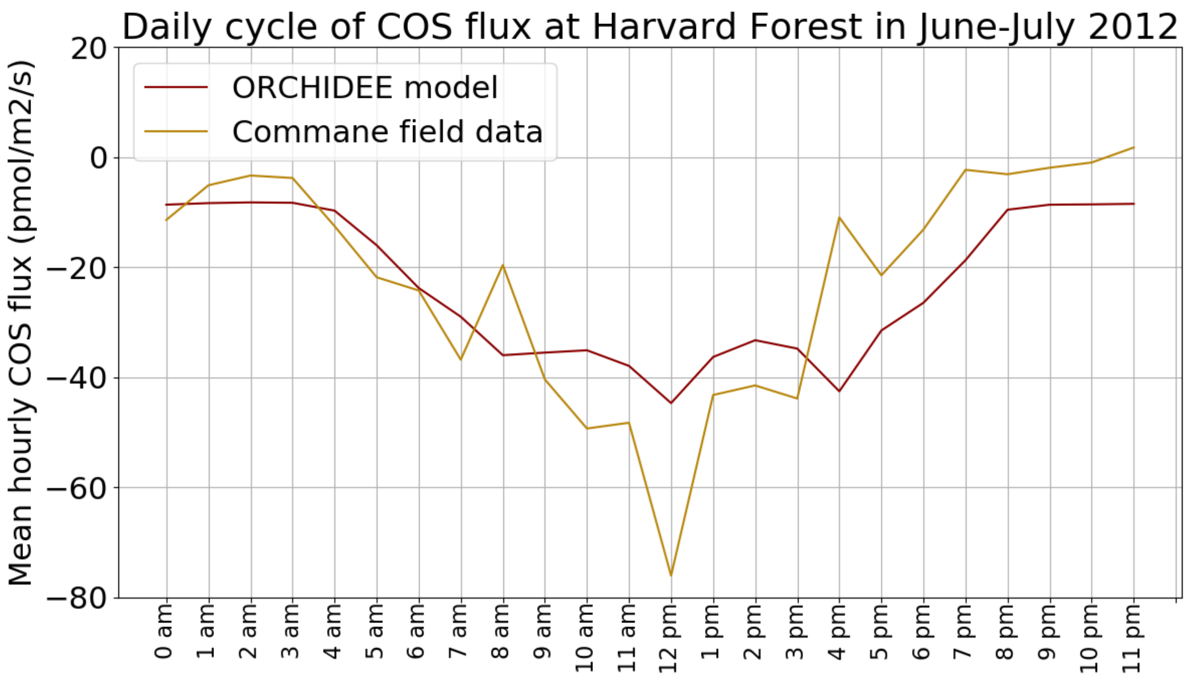


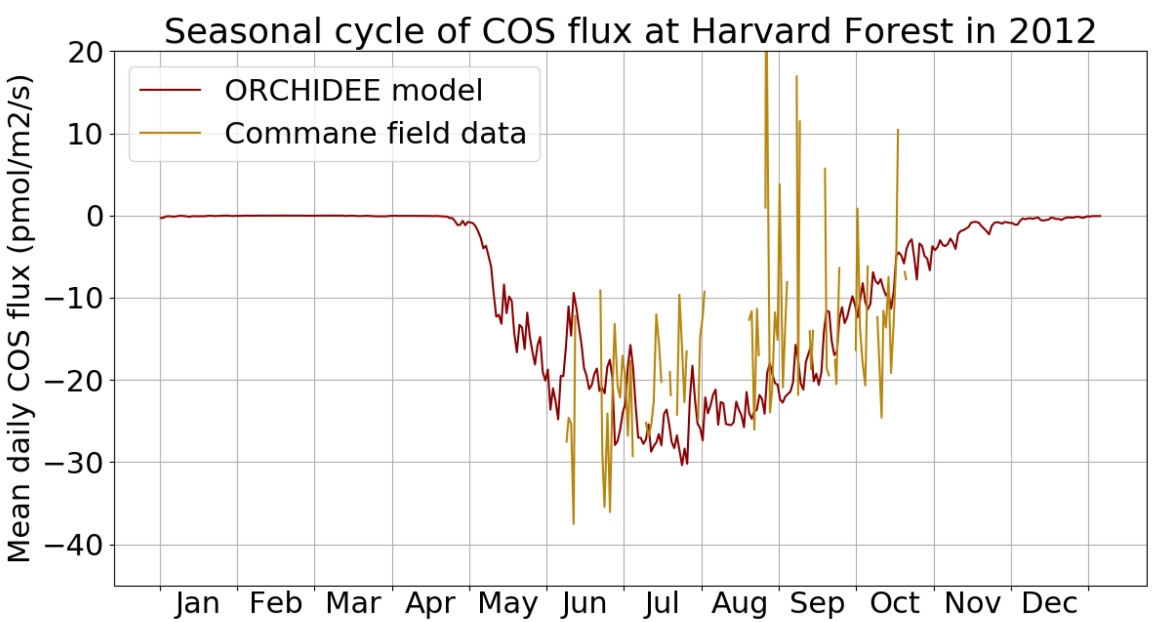
Figure 2. Resistance analog model of CO_2 and COS uptake. Numbers in parentheses are conductance values ($mol\,m^{-2}\,s^{-1}$) corresponding to the numbered key: (1) Boundary layer conductance, g_b. (2) Stomatal conductance, g_s. (3) Mesophyll conductance, g_i. (4) Biochemical rate constant used approximate photosynthetic CO_2 uptake by Rubisco or the reaction of COS with carbonic anhydrase as a linear function of c_c. In this case, COS uptake is 12.6 pmol $m^{-2}\,s^{-1}$ and that of CO_2 is 5.6 μmol $m^{-2}\,s^{-1}$.

Berry et al. (2013)

+ Implementation of night-time conductances

Results: Diel and seasonal cycles of COS fluxes

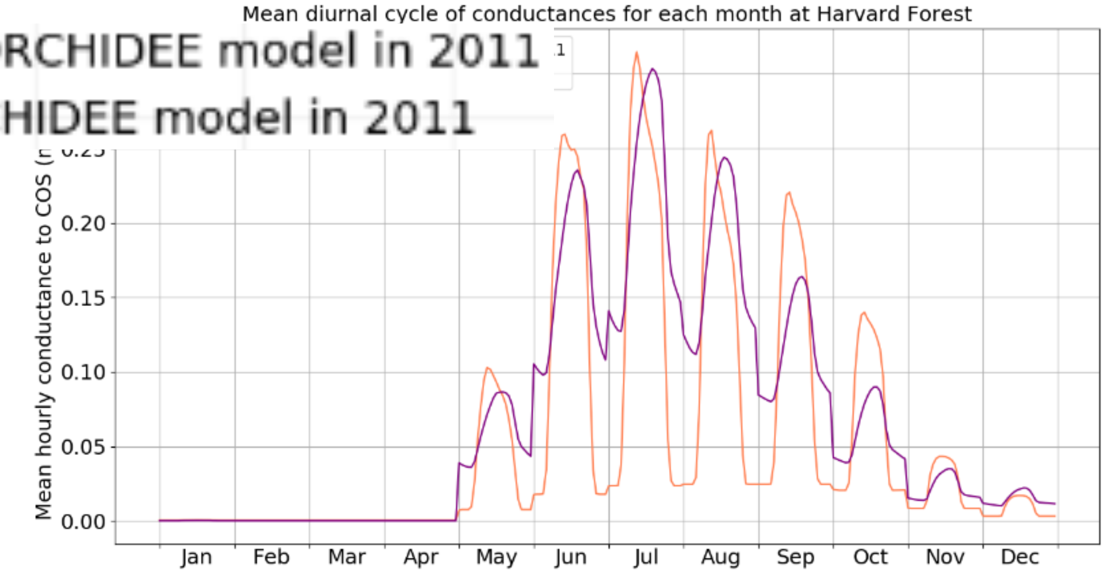




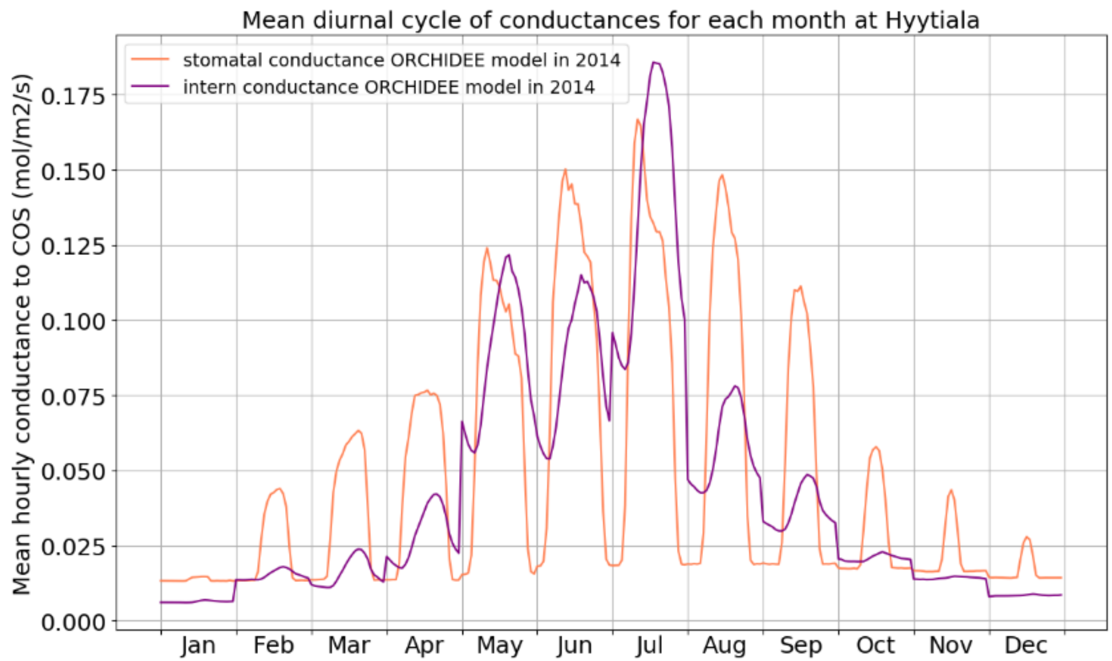
Harvard Forest site *in situ* data from Wehr et al. (2017)

Results: Conductances at sites - Mean daily cycle

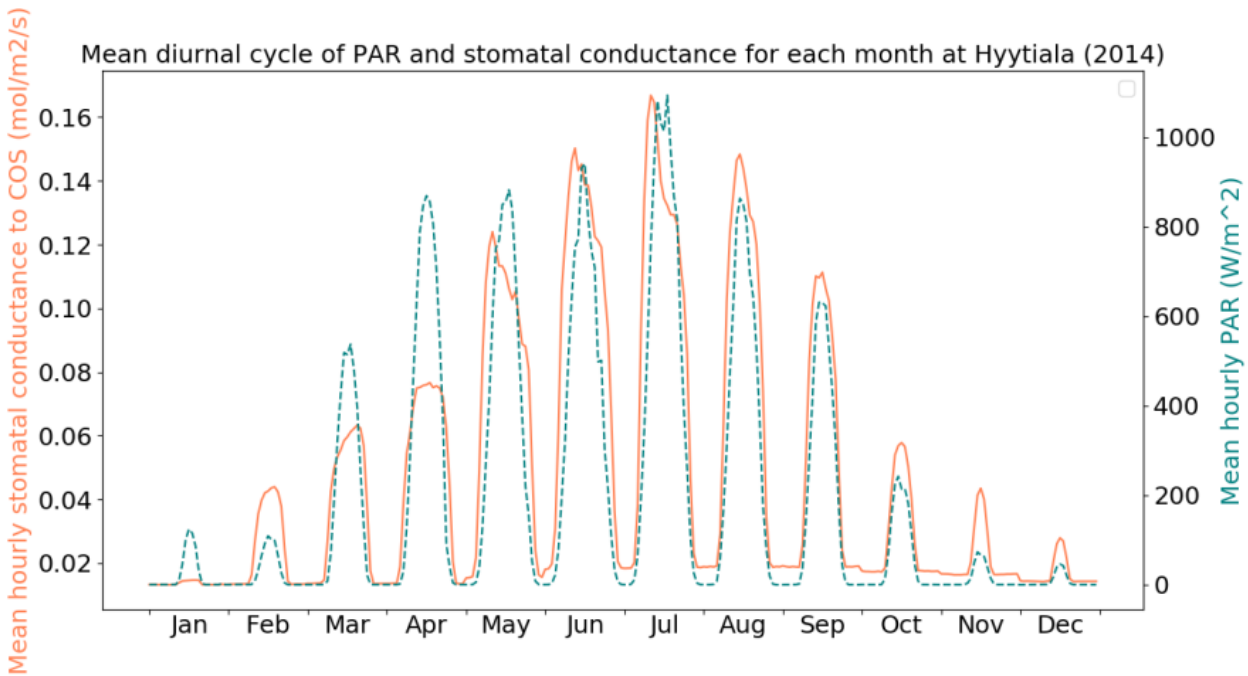
Harvard
2011

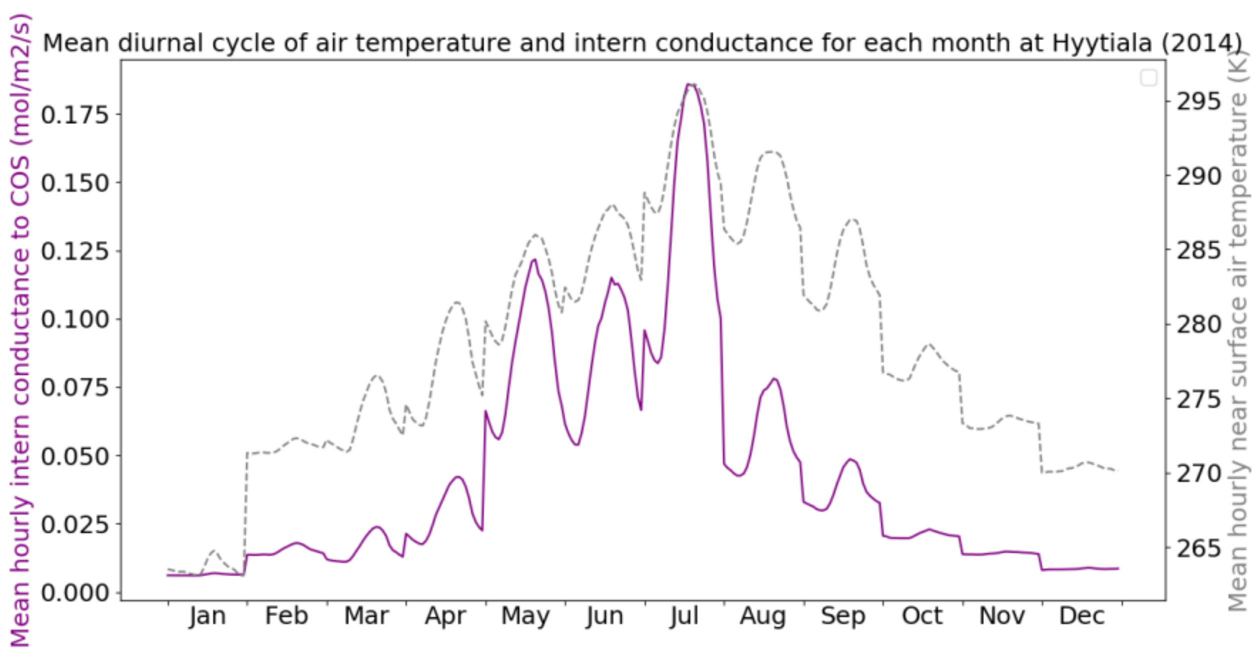


Hyytiala
2014



Results: Conductances at sites - Drivers





Hyytiala
2014

$R^2(g_s, PAR)=82\%$

$R^2(g_i, Tair)=72\%$

$R^2(g_i, VPD)=78\%$

RESULTS: COS VEGETATION FLUXES - LRU

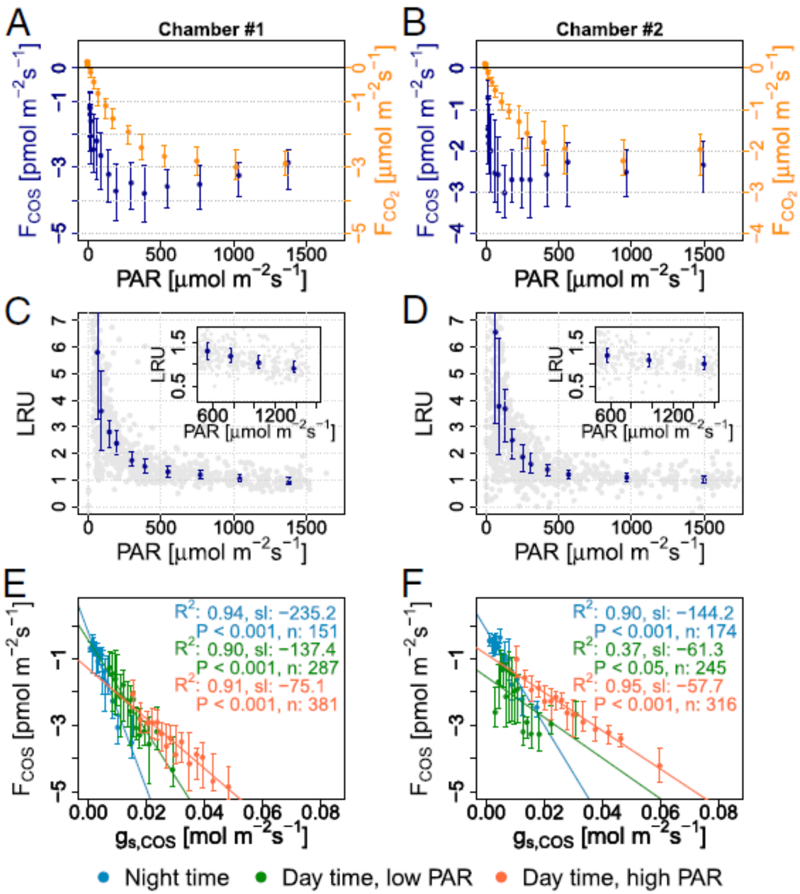
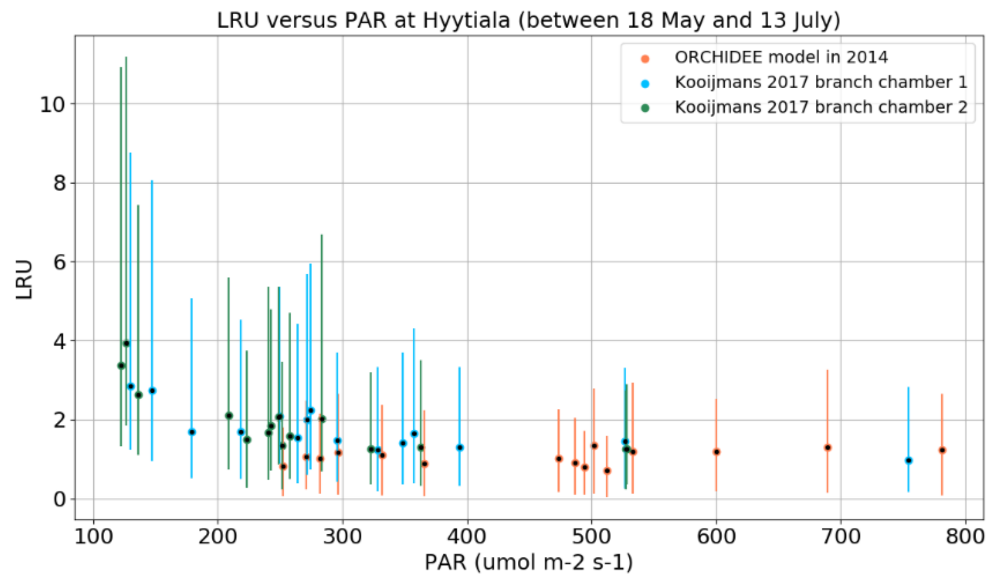
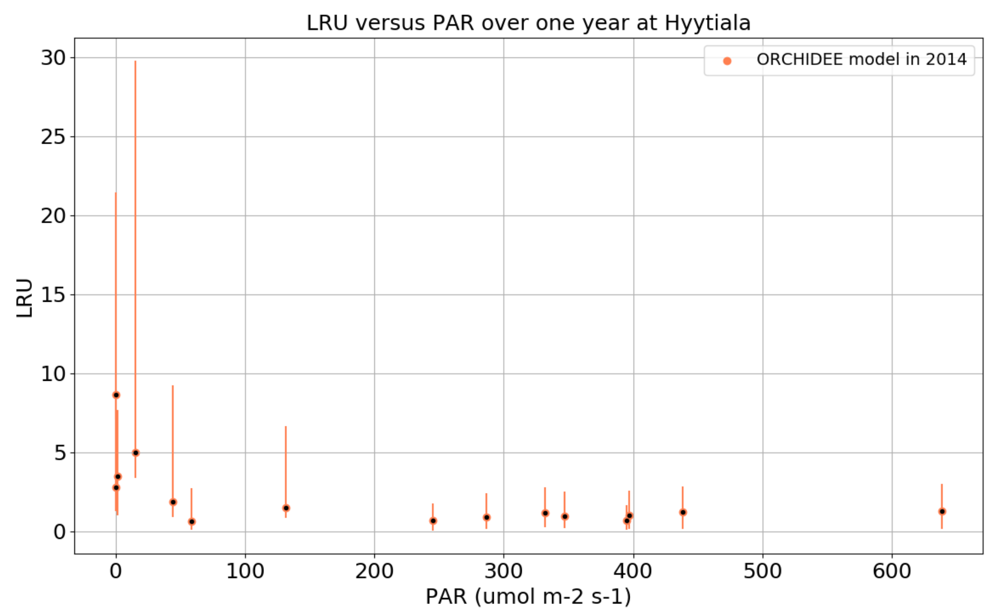


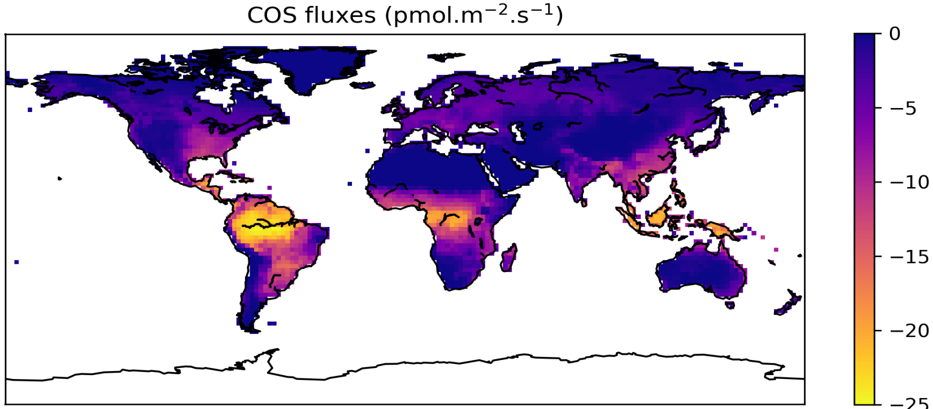
Fig. 2. Responses of F_{COS}, F_{CO2}, and LRU to light and of F_{COS} to $g_{s,COS}$. Average F_{COS}, F_{CO2} (*A* and *B*) and LRU (*C* and *D*) versus PAR, and F_{COS} versus $g_{s,COS}$ (*E* and *F*) from 18 May to 13 July for chambers 1 (*Left*) and 2 (*Right*). Data are plotted as the median of 15 equal-sized bins in the *x* range. The error bars represent the 25th and 75th percentiles of data in each bin. For the correlation of F_{COS} with $g_{s,COS}$ (*E* and *F*) the different colors represent different light conditions: nighttime (blue); daytime with low light conditions (PAR < 150 and 100 µmol $m^{-2} \cdot s^{-1}$ for chambers 1 and 2, respectively; green); daytime with high light conditions (PAR > 300 µmol $m^{-2} \cdot s^{-1}$; orange). A transition phase between low and high PAR values is neglected. The coefficient of determination (R^2), slope (sl), significance level (P), and number of data (n) are given for a linear regression through the median values (*E* and *F*).

Kooijmans et al. (2019)

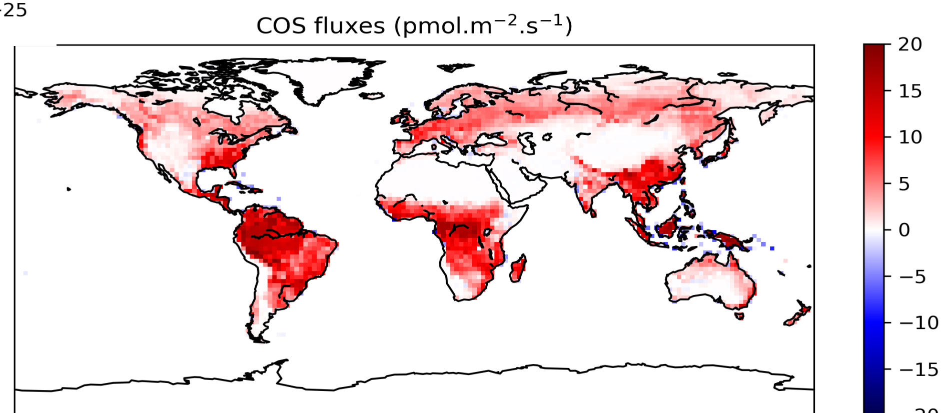




Results: COS fluxes - Global scale



Mechanistic model

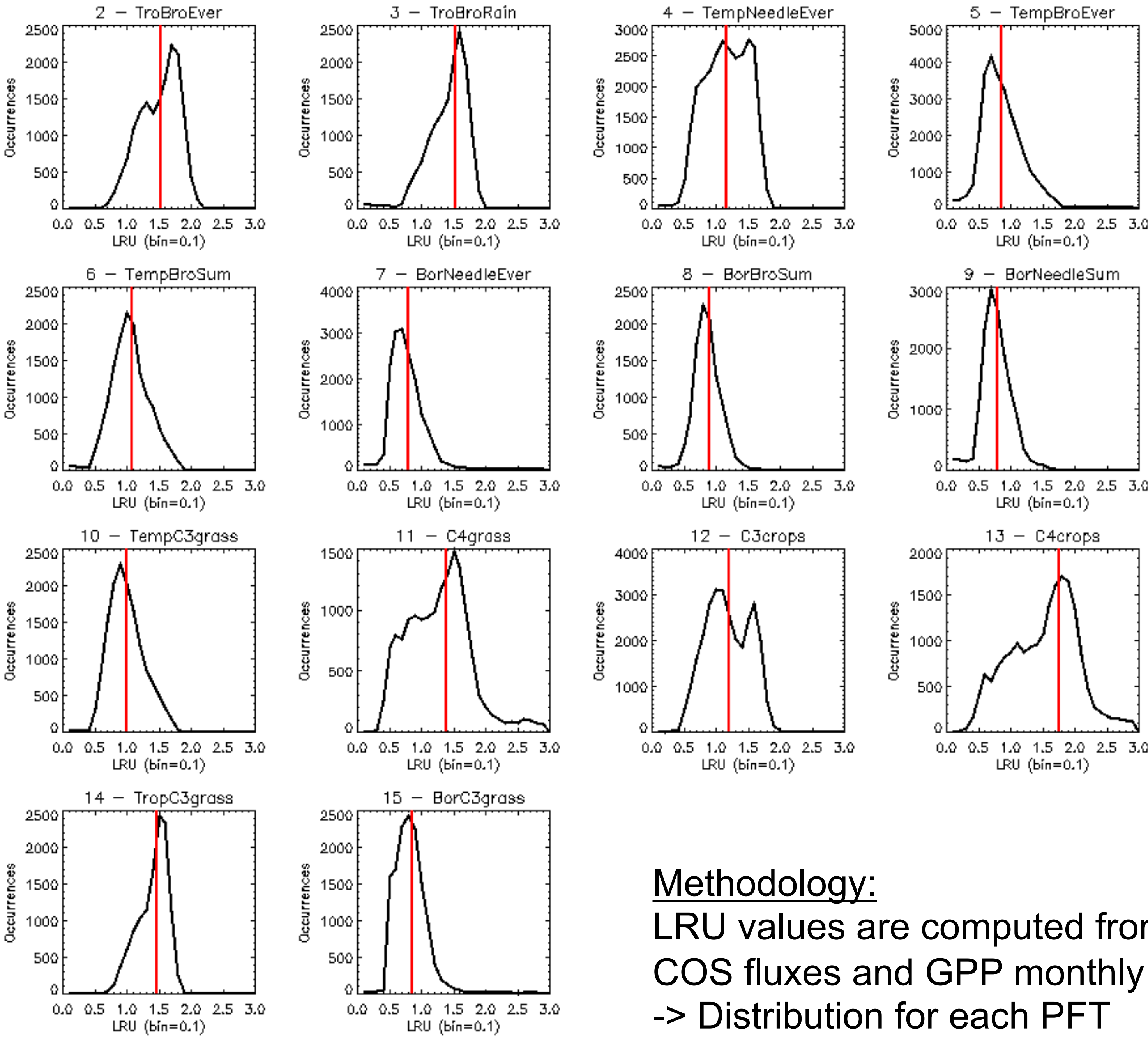


Mechanistic model minus Launois-LRU-Seibt model

Estimates of COS plant uptake per year (Gg S.yr^{-1})

	Kettle et al., 2002	Montzka et al., 2007	Suntharalingam et al., 2008	Berry et al., 2013	Launois et al., 2015			This study
					ORC	LPJ	CLM4	
Uptake by plants	-238	-730 to -1500	-490	-738	-1335	-1069	-930	-747

LRU distribution over space and time

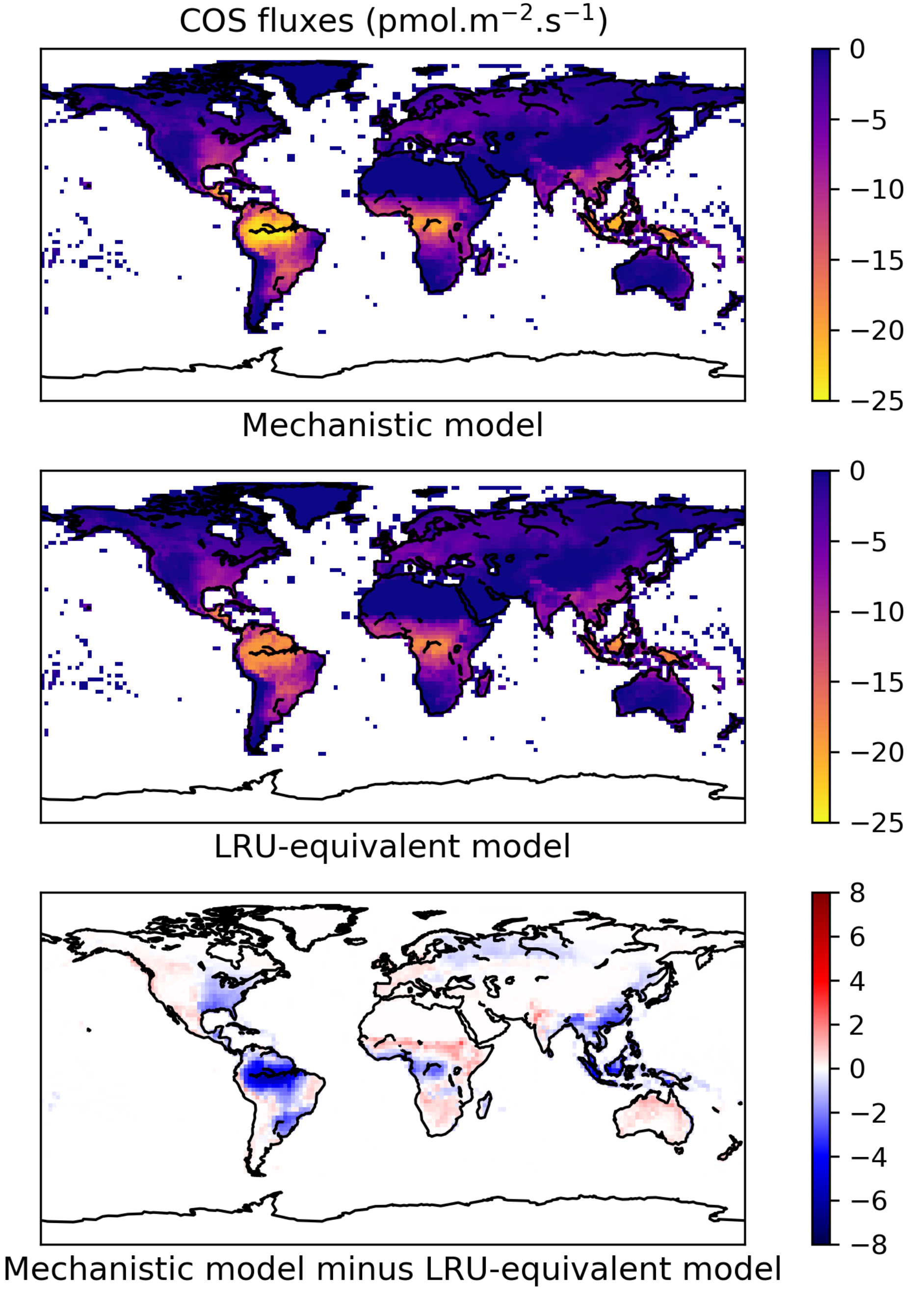


<u>Methodology:</u>

LRU values are computed from mechanistic COS fluxes and GPP monthly values

-> Distribution for each PFT

Spatial discrepancy introduced by the LRU approach

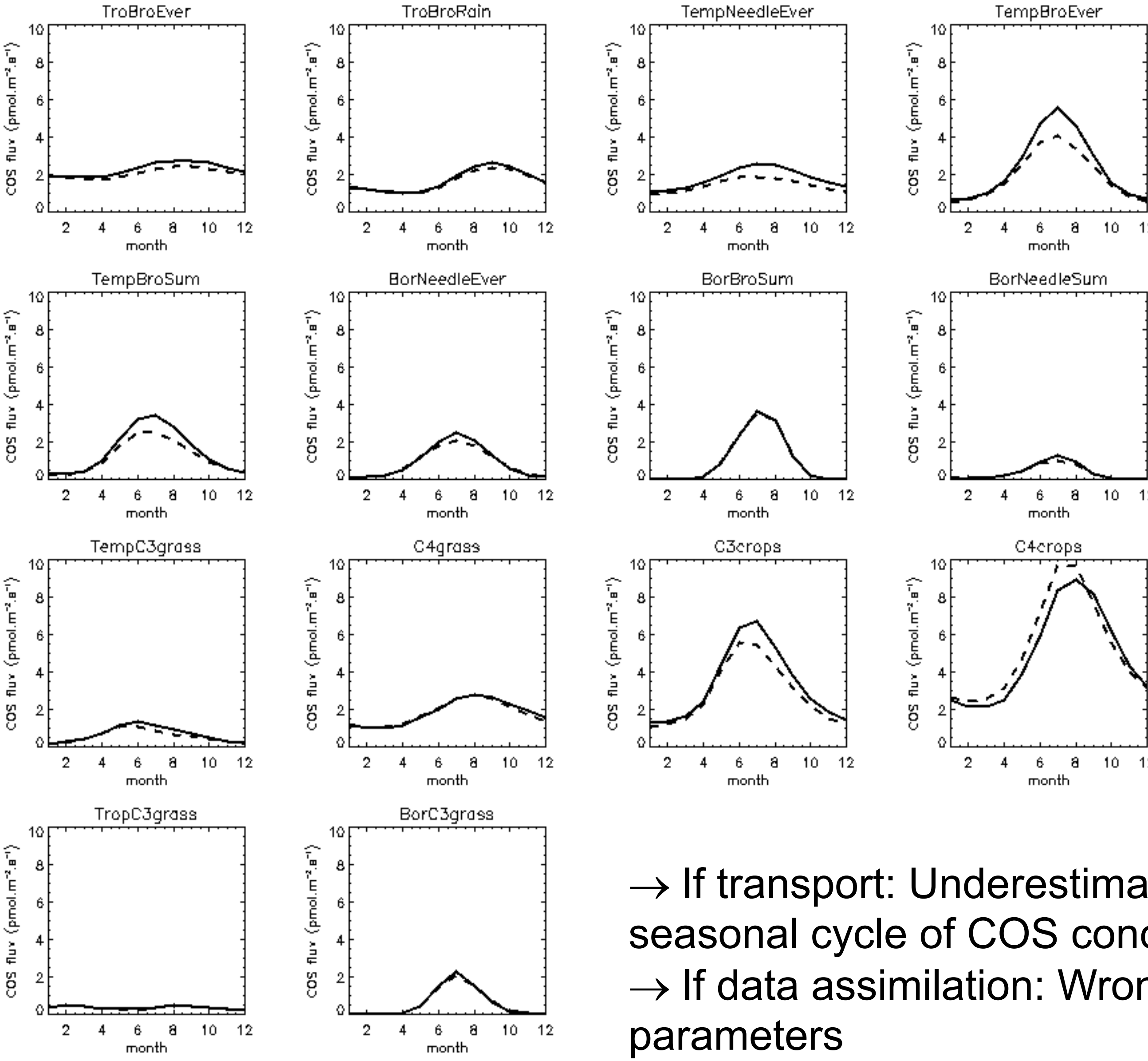


<u>Methodology:</u>
COS_LRU is computed from GPP and LRU median values.

TEMPORAL DISCREPANCY INTRODUCED BY THE LRU APPROACH

Methodology:

COS_LRU_seasonal is computed from monthly GPP and LRU median values.



Mechanistic

LRU

→ The amplitude based on LRU is often underestimated.

→ The cycle may be shifted.

→ If transport: Underestimation of the amplitude of the seasonal cycle of COS concentrations

→ If data assimilation: Wrong values of the optimized parameters

Soil Fluxes

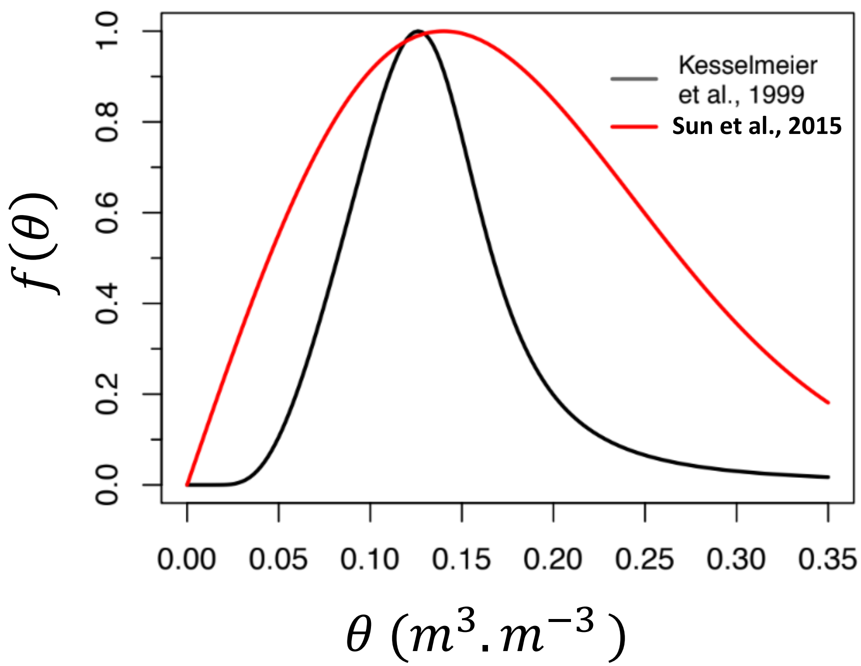
COS soil fluxes: The Berry et al. (2013) model

COS soil uptake is proportional to soil heterotrophic respiration R_h:

$$\boxed{F_{COS,\,soil} = -\,k_{soil} * f(\theta) * R_h}$$

Berry et al. (2013)

Moisture limitation function $f(\theta)$:



$$\boxed{f(\theta) = A_w * \frac{\theta}{\theta_{opt}^2} * \exp\left(-\frac{\theta^2}{\theta_{opt}^2}\right)}$$

Sun et al. (2015)

COS soil production is not represented in this model.

COS soil fluxes: The Ogée et al. (2016) model

Mechanistic approach based on the mass balance equation:

$$\boxed{\frac{\partial \varepsilon_{tot} C}{\partial t} = -\frac{\partial F_{diff}}{\partial z} + P - U}$$

Ogée et al. (2016)

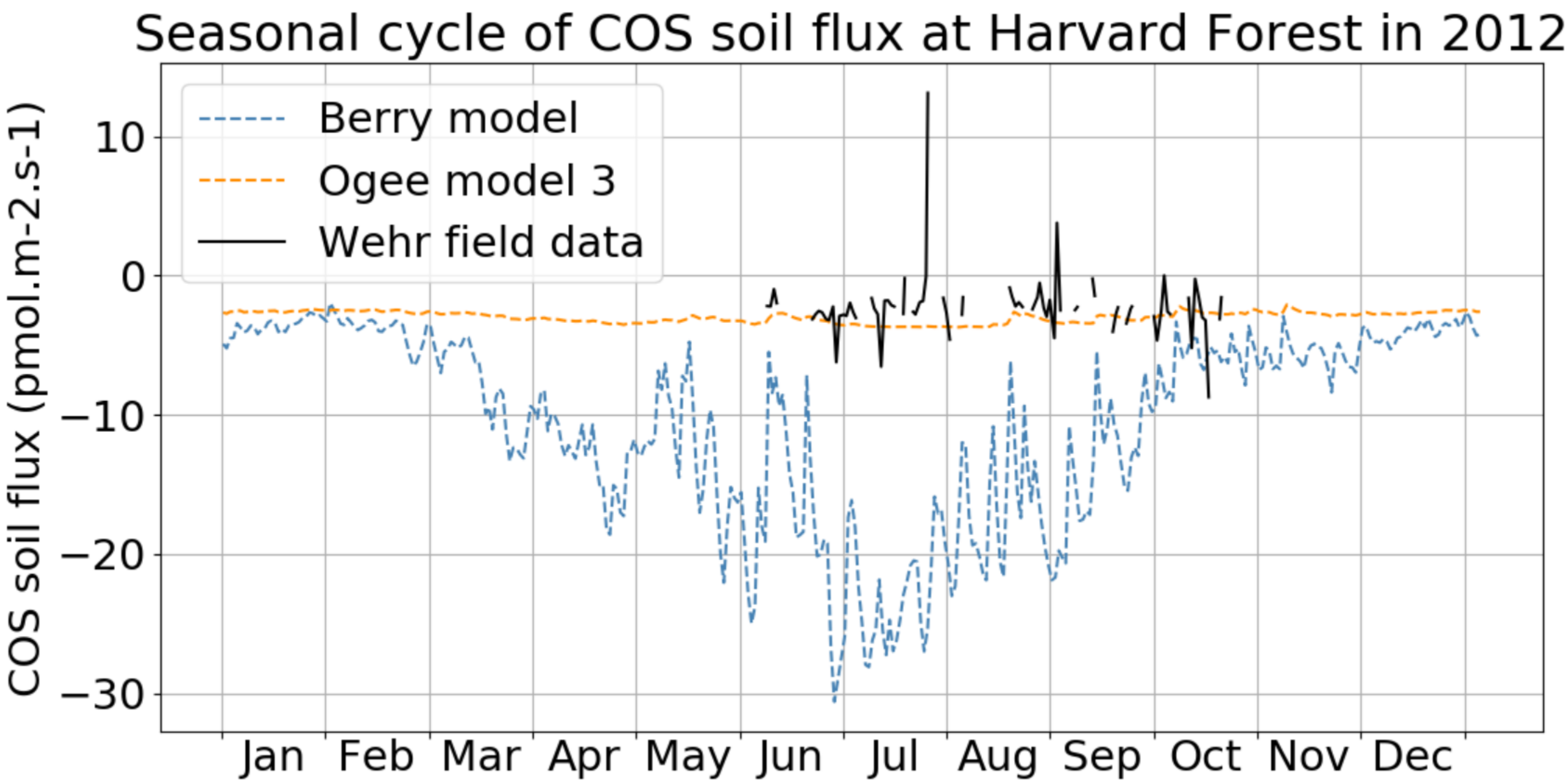
Mechanisms:

- COS diffusion (F_{diff}) through the soil matrix in the gaseous and liquid phases
- COS biotic and abiotic production (*P*)
- COS uptake (*U*) by soil microorganism hydrolysis and uncatalyzed hydrolysis

COS soil fluxes function of:

- Soil temperature
- Soil pressure
- Soil pH
- Soil water content
- Soil porosity
- Soil redox potential
- Carbonic anhydrase soil concentration

COS soil fluxes: Site simulations



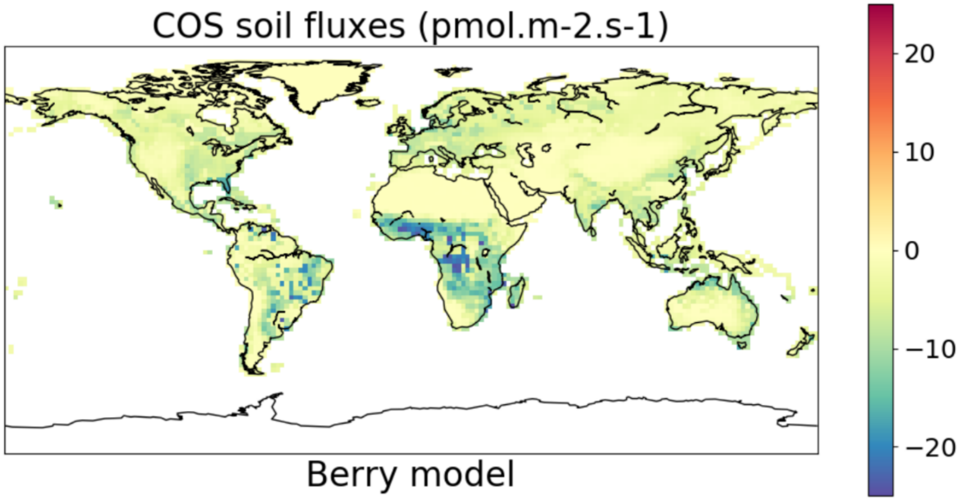
Harvard Forest site *in situ* data from Wehr et al. (2017)

Ogée model 3 → CA enhancement factor depends on biomes (values from Meredith et al., 2019)

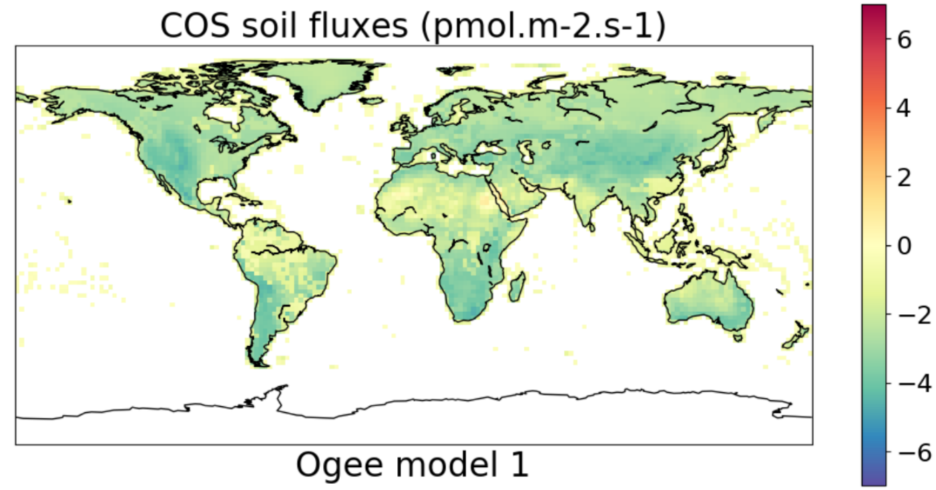
OCS soil fluxes: Global simulations

Model	Hypothesis
Berry et al., 2013	- Soil optimum water content is constant θ_{opt} = 15%
Ogée et al., 2016 version 1	- CA enhancement factor is constant fCA = 30 000 - Soil redox potential is constant
Ogée et al., 2016 version 2	- CA enhancement factor is constant at its median value fCA = 66 000 - Soil redox potential is constant
Ogée et al., 2016 version 3	- CA enhancement factor depends on biomes (Meredith et al., 2019) - Soil redox potential is constant

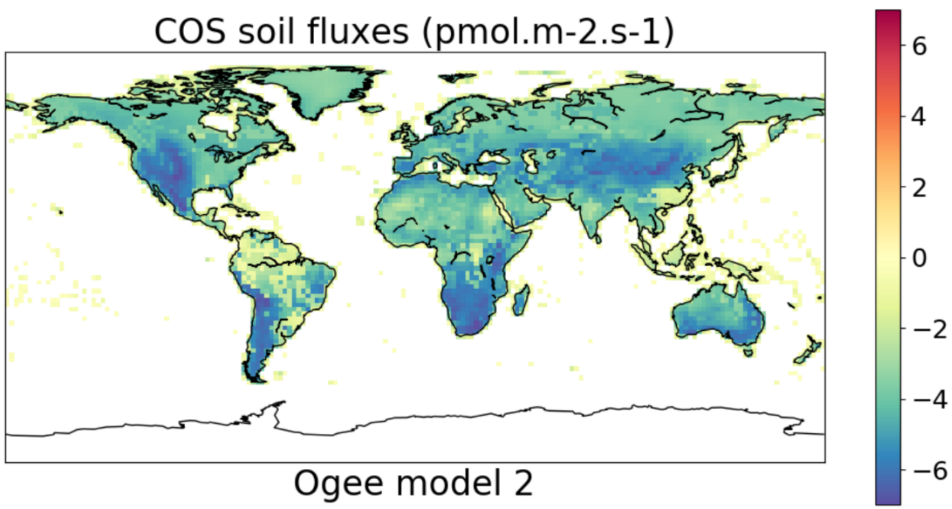
Spatial discrepancy between COS soil models



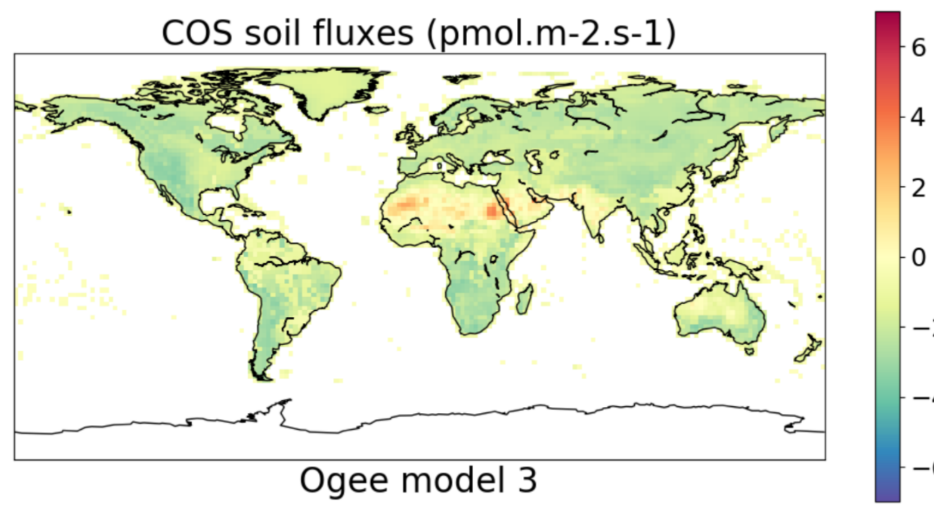
COS soil flux = [0;-25]



fCA = 30 000
COS soil flux = [-4;1]



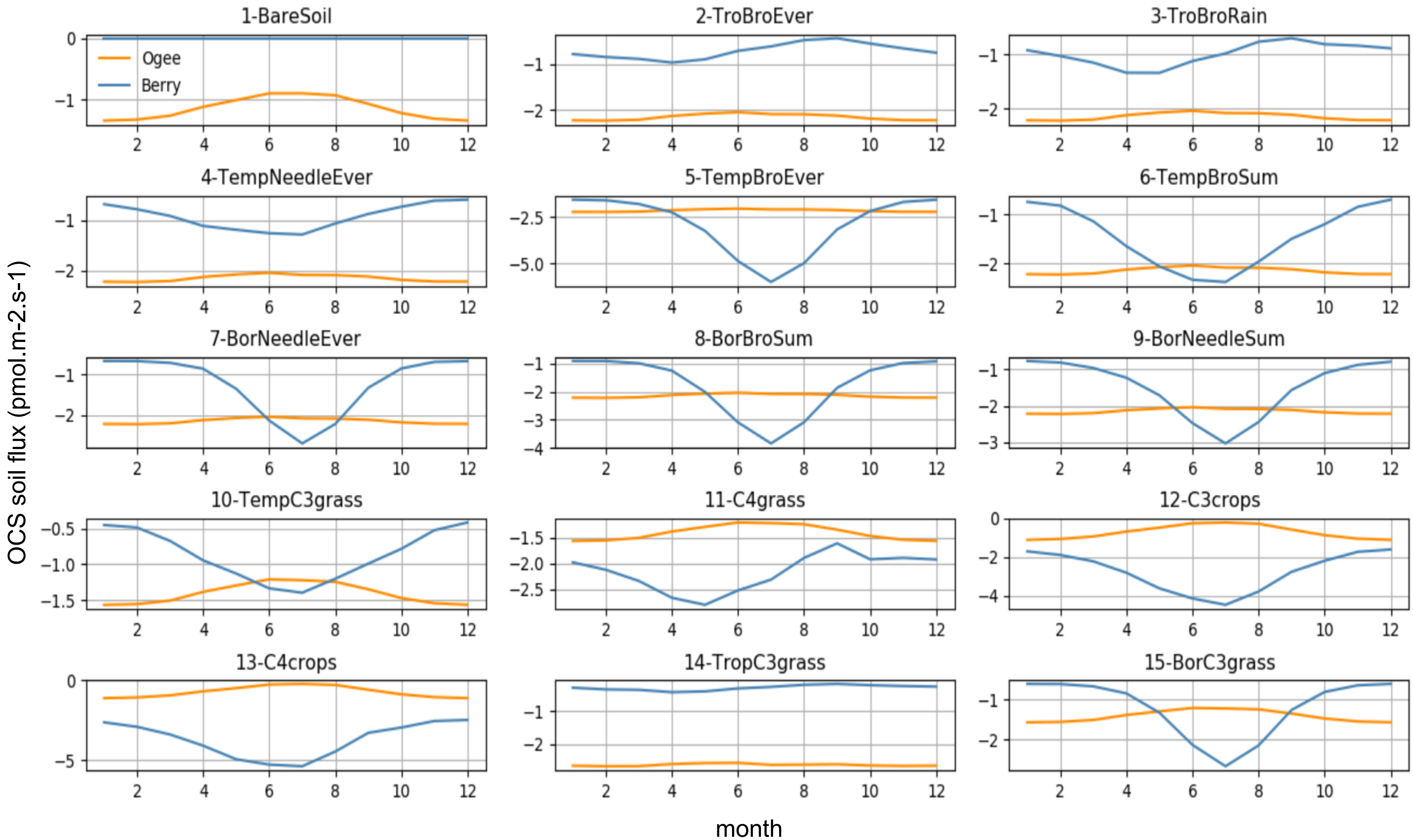
fCA = 66 000
COS soil flux = [-7;-1]
→ *No OCS net production*



fCA depends on biomes
COS soil flux = [-3;3]

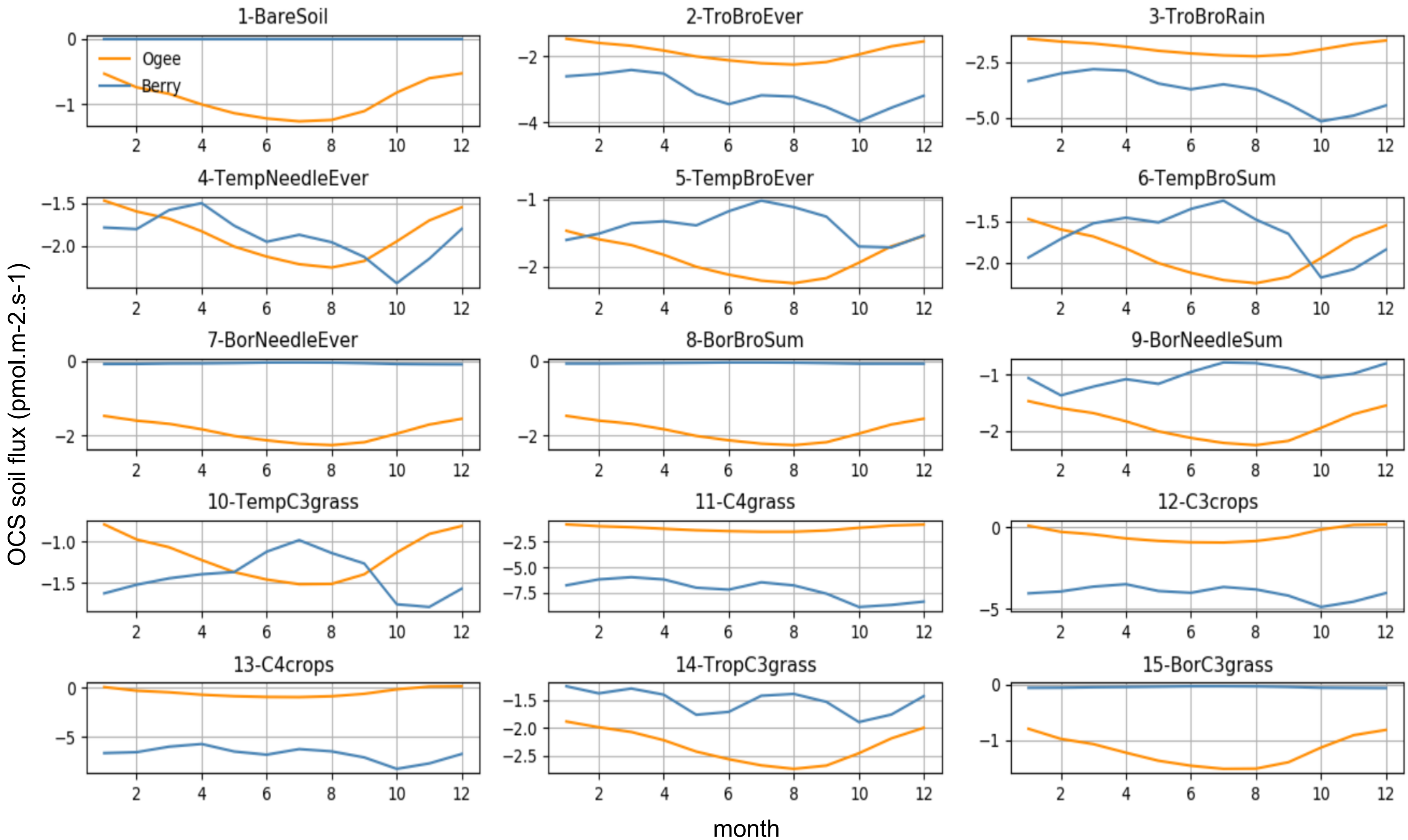
TEMPORAL DISCREPANCY BETWEEN COS SOIL MODELS

- COS soil flux for each biome in the Northern hemisphere



Temporal discrepancy between COS soil models

- COS soil flux for each biome in the Southern hemisphere



Conclusion & Perspectives

Vegetation

Be careful with the LRU approach.
A mechanistic model is preferable.

Soil

Improve the implementation thanks to collaborations J.Ogée, I. Baker, M. Whelan & E. Campbell.

Next steps

Collect more COS fluxes data.
Start optimization of mechanistic models' parameters.
Co-assimilation of COS and SIF data.

VEGETATION UPTAKE OF COS: THE LEAF RELATIVE UPTAKE (LRU) APPROACH

$$LRU_{PFT} = \frac{F_{COS}}{GPP}\frac{[CO2]}{[COS]}$$

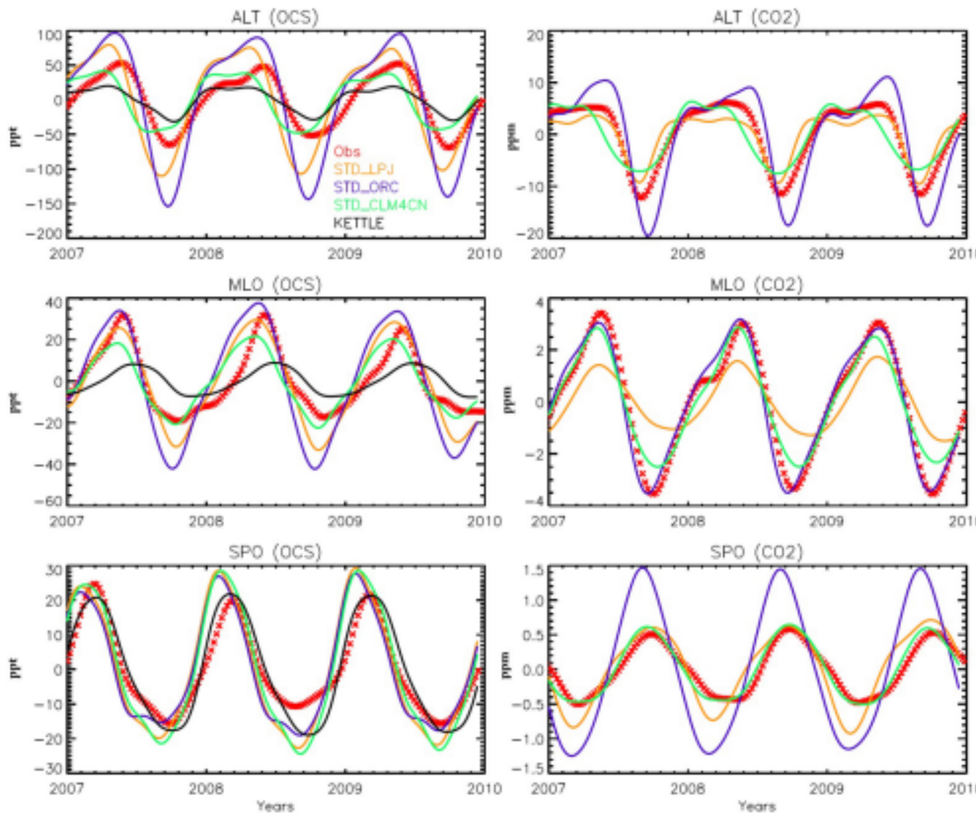


Figure 5. Smoothed seasonal cycles of OCS (left column) and CO_2 (right column) monthly mean mixing ratios, simulated at ALT, MLO and SPO, and obtained after removing the annual trends. Simulations obtained with the LMDZ model using the STD_ORC, STD_CLM4CN, STD_LPJ setups (Table 1). Data derived solely from the Kettle et al. (2002) surface fluxes are shown by the black solid line. Observations (red crosses) are from the NOAA/ESRL global monitoring network (Montzka et al., 2007).

Launois et al. (2015)

Results: night-time COS fluxes

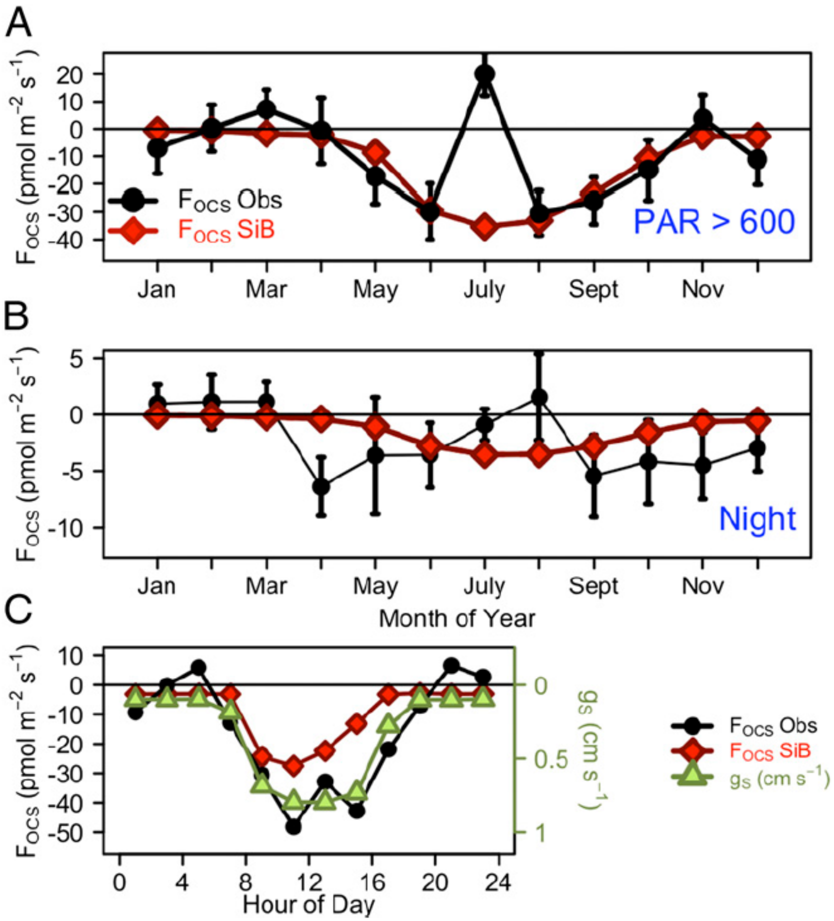
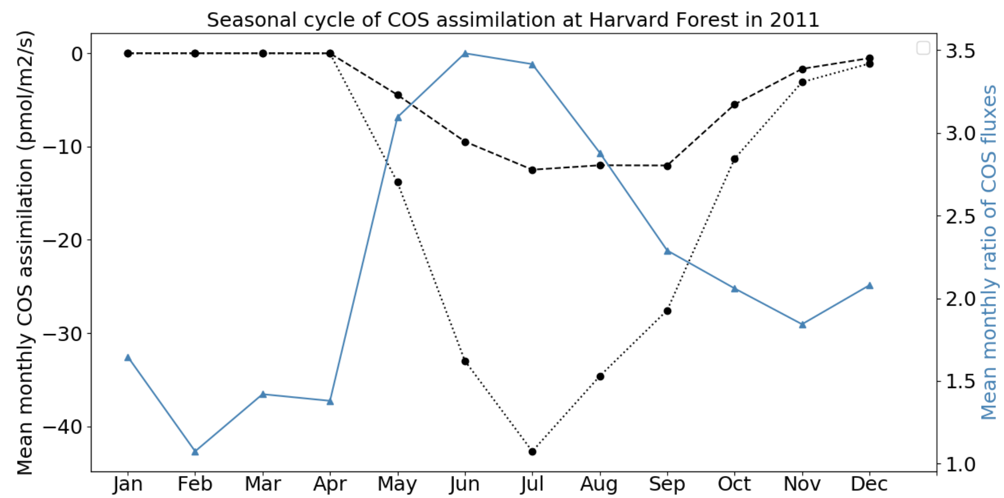


Fig. 3. Monthly mean observed OCS (F_{OCS} Obs, pmol·m^{-2}·s^{-1}; black) and Simple Biosphere (SiB3) model simulated OCS (F_{OCS} SiB, pmol·m^{-2}·s^{-1}; red) fluxes for (*A*) daytime (PAR > 600 μE·m^{-2}·s^{-1}) and (*B*) nighttime. (*C*) Mean diel cycle of observed (black) and simulated (red) OCS fluxes and stomatal conductance of OCS, g_S (cm·s^{-1}; green) for August–September 2011.

Commane et al. (2015)

ORCHIDEE seasonal cycle



day-time COS fluxes

night-time COS fluxes

ratio day-time/night-time