

# A carbon sink-driven approach to estimate gross primary production from microwave satellite observations

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## Abstract

Global estimation of Gross Primary Production (GPP) – the uptake of atmospheric carbon dioxide by plants through photosynthesis - is commonly based on optical satellite remote sensing data. This presents a source-driven

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approach since it uses the amount of absorbed light, the main driver of photosynthesis, as a proxy for GPP. Vegetation Optical Depth (VOD) estimates obtained from microwave sensors provide an alternative and independent data source to estimate GPP on a global scale, which may complement existing GPP products. Recent studies have shown that VOD is related to aboveground biomass, and that both VOD and temporal changes in VOD relate to GPP. In this study, we build upon this concept and propose a model for estimating GPP from VOD. Since the model is driven by vegetation biomass, as observed through VOD, it presents a carbon sink-driven approach to quantify GPP and, therefore, is conceptually different from common source-driven approaches. The model developed in this study uses single frequencies from active or passive microwave VOD retrievals from C-, X- and Ku-band (Advanced Scatterometer (ASCAT) and Advanced Microwave Scanning Radiometer for Earth Observation (AMSR-E)) to estimate GPP at the global scale. We assessed the ability for temporal and spatial extrapolation of the model using global GPP from FLUXCOM and in situ GPP from FLUXNET. We further performed upscaling of in situ GPP based on different VOD data sets and compared these estimates with the FLUXCOM and MODerate-resolution Imaging Spectroradiometer (MODIS) GPP products. Our results show that the model developed for individual grid cells using VOD and change in VOD as input performs well in predicting temporal patterns in GPP for all VOD data sets. For spatial extrapolation of the model, however, additional input variables are needed to represent the spa-

tial variability of the VOD-GPP relationship due to differences in vegetation type. As additional input variable, we included the grid cell median VOD (as a proxy for vegetation cover), which increased the model performance during cross validation. Mean annual GPP obtained for AMSR-E X-band data tends to overestimate mean annual GPP for FLUXCOM and MODIS but shows comparable latitudinal patterns. Overall, our findings demonstrate the potential of VOD for estimating GPP. The sink-driven approach provides additional information about GPP independent of optical data, which may contribute to our knowledge about the carbon source-sink balance in different ecosystems.

*Keywords:* microwave remote sensing, vegetation optical depth, ecosystem productivity, ASCAT, AMSR-E, AMSR2

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## 1 **1. Introduction**

2     The uptake of the greenhouse gas carbon dioxide by vegetation during  
3 photosynthesis, i.e. Gross Primary Production (GPP), is a key ecosystem  
4 process. Estimation of GPP from satellite observations commonly uses op-  
5 tical data together with empirical or semi-empirical models (Gilabert et al.,  
6 2017; Running et al., 2004) or machine learning approaches (Beer et al.,  
7 2010; Jung et al., 2011; Tramontana et al., 2016; Yang et al., 2007). Bio-  
8 physical properties obtained from optical remote sensing that are often used  
9 to estimate GPP include the fraction of Absorbed Photosynthetically Active  
10 Radiation (fAPAR), Normalized Difference Vegetation Index (NDVI), or Leaf

11 Area Index (LAI). These approaches rely on the light-use efficiency theory  
12 (Monteith, 1972) whereby GPP depends on the incoming Photosynthetically  
13 Active Radiation (PAR), the fraction of PAR that is absorbed, i.e. fAPAR,  
14 and the efficiency of converting light to assimilated carbon (Beer et al., 2010;  
15 Gilabert et al., 2017; Jung et al., 2011; Running et al., 2004; Tramontana  
16 et al., 2016; Yang et al., 2007). Another variable retrieved from optical data  
17 is Solar-Induced chlorophyll Fluorescence (SIF), which is a measure for pho-  
18 tosynthetic activity (Frankenberg et al., 2011; Guan et al., 2016). SIF has  
19 received much attention in recent years, because of its linear relationship with  
20 GPP at canopy scale (Damm et al., 2015; Frankenberg et al., 2014; Guanter  
21 et al., 2014; Zhang et al., 2016), especially at coarser temporal resolution  
22 like monthly sampling (Guanter et al., 2014). SIF has also been used for  
23 estimating GPP globally through the use of artificial neural networks (Ale-  
24 mohammad et al., 2017). Optical biophysical properties provide an estimate  
25 for the amount of carbon that is taken up by plants based on the absorption  
26 (fAPAR) or re-emission (SIF) of sunlight (source-driven). In recent years,  
27 however, it has been proposed that plant growth may be stronger limited by  
28 sink- rather than source-activity (Fatichi et al., 2014; Körner, 2015), and that  
29 considering sinks of fixed carbon can improve constrains in global vegetation  
30 models (Leuzinger et al., 2013).

31 Microwave Vegetation Optical Depth (VOD) is a measure of the atten-  
32 uation of microwave radiation caused by vegetation (Woodhouse, 2005) and  
33 thus relates to the total vegetation water content (Jackson and Schmugge,

34 1991). VOD can be retrieved from different frequencies/wavelengths in the  
35 microwave region, which can provide information on different parts of the  
36 canopy. In theory, lower frequencies like L-band are more sensitive to large  
37 plant structures like stems and large branches, while higher frequencies like  
38 X-band are more closely related to small structures like leaves and twigs  
39 (Woodhouse, 2005). Microwave satellite observations at frequencies below  
40 10 GHz are not affected by cloud cover (Woodhouse, 2005). Therefore, VOD  
41 can provide valuable information on the vegetation layer in addition to prod-  
42 ucts derived from optical remote sensing data.

43 In recent years, studies have proposed to use VOD to estimate above-  
44 ground living biomass (Liu et al., 2011, 2015; Momen et al., 2017; Rodríguez-  
45 Fernández et al., 2018; Tian et al., 2016). Biomass and/or temporal change  
46 in biomass, however, relate to Net Primary Production (NPP) (Clark et al.,  
47 2001a,b; Girardin et al., 2010; Gower et al., 2001; Lavigne and Ryan, 1997;  
48 Luysaert et al., 2007) and to Autotrophic Respiration ( $R_a$ ) (Lavigne and  
49 Ryan, 1997; Ryan, 1990), the sum of which constitutes GPP (e.g. Bonan,  
50 2015; Odum, 1959). Due to this causal relationship between biomass and  
51 GPP, a relationship is expected between VOD and GPP. Teubner et al.  
52 (2018) showed that both the original VOD time series ( $VOD$ ) and the tem-  
53 poral change in VOD ( $\Delta VOD$ ) are correlated to GPP and suggested that  
54 the combination of  $VOD$  and  $\Delta VOD$  has the potential to provide comple-  
55 mentary information to GPP estimates from optical data.

56 In this study, we build upon the explorative work of Teubner et al. (2018)

57 and develop a model to estimate GPP based on VOD using Generalized  
58 Additive Models (GAM; Hastie and Tibshirani, 1987). Complementary to  
59 source-driven approaches, we are proposing a model that is driven by vegeta-  
60 tion biomass, as expressed through VOD, which thus presents a sink-driven  
61 approach that does not depend on PAR as model input. We assessed the  
62 performance of VOD observations from different sensors and multiple fre-  
63 quencies, since it is not clear which frequencies most closely relate to GPP.  
64 As input variables to the model, we use different VOD variables, i.e.  $VOD$ ,  
65  $\Delta VOD$  and the temporal grid cell median VOD ( $mdnVOD$ ). The latter  
66 serves as a proxy for land cover and thus aids the spatial extrapolation of  
67 the model to different vegetation types without requiring further ancillary  
68 data. Due to the complex relationship between VOD and GPP, we con-  
69 ducted a separate analysis based on SIF using similar experimental setups  
70 as for VOD. This additional analysis gives insight into differences in model  
71 performance between setups that are not caused by using VOD variables as  
72 input to the model. The aim of this study is 1) to assess the model's ca-  
73 pability for temporal extrapolation, 2) to evaluate the model's performance  
74 in spatial extrapolation and determine the required model structure using  
75 model selection, and 3) to perform upscaling of in situ FLUXNET GPP and  
76 compare the upscaled VOD-based GPP estimates with global GPP estimates  
77 from FLUXCOM and the MODerate-resolution Imaging Spectroradiometer  
78 (MODIS).

## 79 **2. Data sets**

80 The analysis is based on the period from 2007 to 2015 and uses VOD  
81 data from C-, X- and Ku -band and various GPP data sets. The data sets  
82 have different temporal coverage, which is summarized for VOD and GPP  
83 data in Table 1. Global temporal median maps of the remotely sensed VOD  
84 and GPP data sets are displayed in Fig. S1. For FLUXNET data, a list of  
85 the sites and graphs illustrating the location and data coverage are given in  
86 Table S1 and Fig. S2.

87 Our analysis was carried out for different passive VOD frequencies from  
88 both the Advanced Microwave Scanning Radiometer for Earth Observation  
89 System (AMSR-E) and its successor the Advanced Microwave Scanning Ra-  
90 diometer 2 (AMSR2). The overlap period between AMSR2 and in situ  
91 FLUXNET data, however, is considerably short (2 years and 5 months) and  
92 is further reduced by the lower number of FLUXNET sites in the later period,  
93 which potentially leads to less robust results in some parts of the analysis.  
94 For this reason and because AMSR-E and AMSR2 generally yielded similar  
95 results, the study focuses on results for AMSR-E. For results using AMSR2  
96 frequencies, please see the supplement.

### 97 *2.1. VOD data sets*

#### 98 *2.1.1. ASCAT VOD*

99 The Advanced Scatterometer (ASCAT) is an active microwave sensor  
100 measuring C-band (5.25 GHz) backscatter in vertical co-polarization and flies

Table 1: Data set overview for VOD and GPP data sets. Acronyms – EVI: Enhanced Vegetation Index, fAPAR: fraction of Absorbed Photosynthetically Active Radiation, LAI: Leaf Area Index, MIR: MODIS band 7 - Middle Infrared Reflectance, NDVI: Normalized Difference Vegetation Index, NDWI: Normalized Difference Water Index, LPRM: Land Parameter Retrieval Model.

Variable name	Data set/sensor	Period used	Frequency/wavelength/data input	Sampling	Type	Method/algorithm	Reference/URL
ASCAT	ASCAT	1/2007 - 12/2015	5.25 GHz	Daily, 12.5 km	Active microwave	TU-Wien change detection	Melzer (2013); Vreugdenhil et al. (2016a,b)
AMSRE-C, AMSRE-X, AMSRE-Ku	AMSRE-E	1/2007 - 9/2011	6.9 GHz, 10.7 GHz, 18.7 GHz	Daily, 0.25°	Passive microwave	LPRMv06	van der Schalie et al. (2017)
AMSR2-C1, AMSR2-C2, AMSR2-X, AMSR2-Ku	AMSR2	7/2012 - 12/2015	6.9 GHz, 7.3 GHz, 10.7 GHz, 18.7 GHz	Daily, 0.25°	Passive microwave	LPRMv06	van der Schalie et al. (2017)
FLUXCOM GPP	FLUXCOM	1/2007 - 12/2015	MODIS EVI, LAI, MIR, NDVI, NDWI	8-daily, 10 km	Optical	Machine learning	Tramontana et al. (2016)
MODIS GPP	MOD17A2H v006	1/2007 - 12/2015	MODIS fAPAR	8-daily, 500 m	Optical	Semi-empirical model	Running et al. (2004); Running and Mu (2015); Zhao et al. (2005)
SIF	GOME2_F v26	1/2007 - 12/2015	740 nm	Monthly, 0.5°	Optical		Joiner et al. (2013); Joiner et al. (2014)
FLUXNET GPP	FLUXNET2015 Tier1	1/2007 - 12/2014		Daily	in situ	Eddy covariance	<a href="http://fluxnet.fluxdata.org/">http://fluxnet.fluxdata.org/</a>



101 onboard the meteorological operational satellite A (MetOp-A). The retrieval  
102 of daily VOD at 12.5 km sampling is based on the TU-Wien change detection  
103 model developed by Wagner et al. (1999). VOD is derived using slope and  
104 curvature of the angular backscatter dependency, which describe the volume  
105 scattering caused by vegetation (Melzer, 2013; Vreugdenhil et al., 2016a,b).  
106 The VOD retrieval uses observations from both ascending and descending  
107 mode (ascending/descending at 9:30 a.m./p.m. equatorial crossing).

### 108 *2.1.2. AMSR-E VOD*

109 AMSR-E is a passive microwave sensor measuring brightness tempera-  
110 ture at different frequencies. VOD was retrieved using the Land Parameter  
111 Retrieval Model (LPRM) v06 (van der Schalie et al., 2017). LPRM is a radia-  
112 tive transfer model, which estimates VOD and soil moisture simultaneously  
113 with the use of an analytical solution based on the Microwave Polarization  
114 Difference Index (Meesters et al., 2005; Mo et al., 1982). We analyzed VOD  
115 from C- (6.9 GHz), X- (10.7 GHz) and Ku-band (18.7 GHz) obtained for  
116 descending mode (equatorial crossing at 1:30 a.m.), since the assumption in  
117 LPRM that soil and vegetation temperature are similar is best met during  
118 nighttime. Data are available at daily, 0.25° sampling.

### 119 *2.1.3. AMSR2 VOD*

120 AMSR2 measures brightness temperature both at the same frequencies  
121 as AMSR-E as well as at additional frequencies. VOD was retrieved anal-  
122 ogously to AMSR-E using LPRM v06. In the analysis, we used VOD from

123 C- (C1: 6.9 GHz, C2: 7.3 GHz), X- (10.7 GHz) and Ku-band (18.7 GHz) in  
124 descending mode (1:30 a.m. equatorial crossing) at daily, 0.25° sampling.

## 125 *2.2. GPP data sets*

### 126 *2.2.1. FLUXCOM GPP*

127 FLUXCOM is a global GPP product that is based on upscaling site-level  
128 eddy covariance estimates of GPP by using variables from optical satellites  
129 and different machine learning algorithms including tree-based methods, re-  
130 gression splines, neural networks and kernel methods (Tramontana et al.,  
131 2016). For comparability with satellite VOD data, we used the satellite-  
132 based version of FLUXCOM GPP. The data set represents the median of 18  
133 ensemble members, which consist of 9 machine learning algorithms applied  
134 to both daytime and nighttime GPP estimates. Data are available at 8-daily,  
135 10 km sampling.

### 136 *2.2.2. MODIS GPP*

137 MODIS GPP (Running et al., 2004; Zhao et al., 2005) is based on the  
138 light-use efficiency concept introduced by Monteith (1972) in which absorbed  
139 solar energy is related to plant productivity. MODIS GPP is provided by  
140 the land product MOD17; the algorithm uses fAPAR derived from optical  
141 data for calculating the absorbed PAR (Running et al., 1999, 2000). Several  
142 versions of MOD17, differing in spatial and temporal resolution, are available.  
143 We used the MOD17A2H v006 GPP, which has 8-daily, 500 m sampling.

144 *2.2.3. GOME-F SIF*

145 SIF observations at 740 nm (GOME-F v26) are obtained from measure-  
146 ments of the Global Ozone Monitoring Experiment-2 (GOME-2) sensor flying  
147 onboard MetOp-A (Joiner et al., 2013, 2014, 2016). The retrieval algorithm  
148 of SIF proposed by Joiner et al. (2013) utilizes the filling-in of Fraunhofer  
149 lines caused by the plants chlorophyll fluorescence. Data are available at  
150 monthly, 0.5° sampling.

151 *2.2.4. FLUXNET2015 GPP*

152 FLUXNET2015<sup>1</sup> provides a compilation of in situ flux observations spread  
153 around the world. The stations measure water, heat and carbon fluxes by  
154 means of the eddy covariance method (Baldocchi, 2003). The carbon diox-  
155 ide flux, i.e. net ecosystem exchange, is further partitioned into ecosystem  
156 respiration and GPP using the daytime (Lasslop et al., 2010) or nighttime  
157 (Reichstein et al., 2005) partitioning method. For our analysis, we used GPP  
158 estimates from the publicly available Tier 1 data set that were obtained with  
159 the daytime partitioning method with a variable friction velocity threshold.

160 *2.3. Meteorological data sets*

161 *2.3.1. Precipitation*

162 We used daily, 1° precipitation estimates from the Global Precipitation  
163 Climatology Project (GPCP) 1DD version 1.2 to aid the interpretation of the

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<sup>1</sup>Fluxnet2015 data set (accessed June 9, 2016): [http://fluxnet.fluxdata.org/  
/data/fluxnet2015-dataset/](http://fluxnet.fluxdata.org/data/fluxnet2015-dataset/)

164 time series plot. Precipitation is estimated using a combination of satellite  
165 observations and gauge measurements (Huffman et al., 2001). The satel-  
166 lite data include microwave observations of frequencies above 10 GHz and  
167 infrared radiation.

### 168 *2.3.2. Temperature and snow depth*

169 Frozen conditions and snow cover lead to erroneous VOD retrievals. For  
170 this reason, we masked VOD observations using skin temperature and snow  
171 depth from ERA-Interim. ERA-Interim is a global atmospheric reanaly-  
172 sis produced by the European Centre for Medium-Range Weather Forecasts  
173 which incorporates a 4-dimensional variational analysis (Dee et al., 2011).  
174 Data are available at 0.7° horizontal sampling at the equator for the period  
175 from 1979 onwards.

### 176 *2.3.3. Aridity Index*

177 Since water availability is a main driver for plant growth, we analyzed  
178 results along a gradient of aridity in order to determine whether VOD-based  
179 GPP estimates perform differently in different climatic regions. The aridity  
180 index is typically calculated as the ratio of the long-term averages of potential  
181 evaporation and precipitation (Good et al., 2017; Greve et al., 2014). For  
182 computing this index, we used long-term averages of potential evaporation  
183 from the Global Land Evaporation Amsterdam Model (GLEAM; Miralles  
184 et al., 2011) v3.a (Martens et al., 2017) and precipitation from the Multi-  
185 Source Weighted-Ensemble Precipitation (MSWEP; Beck et al., 2017) v1.1

186 for the period 1980 to 2017. Both data sets are available at 0.25° sampling.

### 187 **3. Theoretical model for estimating GPP based on VOD**

188 For describing the relationship between VOD and GPP, we consider the  
189 following equation which relates GPP to NPP and  $R_a$  (e.g. Bonan, 2015;  
190 Odum, 1959):

$$191 \quad \text{GPP} = R_a + \text{NPP} \quad (1)$$

192  $R_a$  represents the portion of the assimilates that is used by plants for their  
193 metabolism.  $R_a$  can be further separated into growth and maintenance res-  
194 piration, which are proportional to the change in biomass ( $\frac{dB}{dt}$ ) and biomass  
195 (B), respectively (Lavigne and Ryan, 1997; Ryan, 1990):

$$196 \quad R_a = a_0 \frac{dB}{dt} + b_0 B \quad (2)$$

197  $R_a$  generally depends on temperature and is often modelled by assuming  
198 an exponential increase of  $R_a$  with temperature (Atkin and Tjoelker, 2003;  
199 Atkin et al., 2005; Smith and Dukes, 2013; Tjoelker et al., 2001; Vander-  
200 wel et al., 2015; Wythers et al., 2013). Consequently, the coefficients  $a_0$   
201 and  $b_0$  in equation (2) are functions of temperature, although this tempera-  
202 ture sensitivity is mainly attributed to the maintenance term of  $R_a$  (Ryan,  
203 1990). Modelling the relationship between  $R_a$  and temperature, however, is  
204 not straight forward. Acclimation and adaptation of plants to changes in  
205 temperature further modulate the temperature sensitivity of  $R_a$  (Atkin and

206 Tjoelker, 2003; Gifford, 2003; Smith and Dukes, 2013; Vanderwel et al., 2015),  
207 although these two processes are acting on different time scales (Smith and  
208 Dukes, 2013). Therefore, representation of  $R_a$  in models presents a complex  
209 task (Atkin and Tjoelker, 2003; Atkin et al., 2005; Gifford, 2003; Ryan, 1991;  
210 Smith and Dukes, 2013; Vanderwel et al., 2015). For simplicity of our model,  
211 we assume that the coefficients  $a_0$  and  $b_0$  are independent of temperature  
212 and discuss the potential impact of this simplification in Section 6.5.

213 NPP is the remaining portion of the assimilates, i.e. the difference be-  
214 tween GPP and  $R_a$ , and contains the following terms (Clark et al., 2001a,b;  
215 Girardin et al., 2010; Gower et al., 2001; Luysaert et al., 2007):

$$216 \quad \text{NPP} = \frac{dB}{dt} + \text{VOC} + \text{Herbivory} + \text{Root exudates} \quad (3)$$

217 VOC stands for volatile organic compounds and are organic molecules pro-  
218 duced by plants that are released into the ambient air. VOC may play an  
219 important role in ecology and atmospheric chemistry but constitute only a  
220 small fraction of NPP (Guenther, 2002; Kesselmeier et al., 2002). Herbivory  
221 describes the loss of above- and belowground plant biomass through animals  
222 that are feeding on these plants. Root exudates are plant-produced com-  
223 pounds that are released into the ground to enhance nutrient uptake or feed  
224 mycorrhiza and can also be used as a defense mechanism (Bais et al., 2006;  
225 Bertin et al., 2003; Jones et al., 2009). All these terms are not directly re-  
226 flected in VOD and are thus neglected in the current model description for

227 relating VOD to GPP. Combining equations (1)-(3) and setting  $a = 1 + a_0$   
228 and  $b = b_0$ , we arrive at the following differential equation for GPP:

$$229 \quad \text{GPP} = a \frac{dB}{dt} + b B \quad (4)$$

230  $a$  and  $b$  represent coefficients for growth and maintenance related terms,  
231 respectively, analogous to the concept developed by Ryan (1990) for  $R_a$ , i.e.  
232 equation (2), but now extended for GPP.

233 The last step in the formulation of the relationship between VOD and  
234 GPP requires a description of the relationship between VOD and biomass.  
235 This relationship, or more specifically that between VOD and aboveground  
236 biomass (AGB), is not straightforward. Liu et al. (2015) proposed an empir-  
237 ical, non-linear function for converting VOD to AGB using a passive merged  
238 VOD data set. Similar to this concept, but without explicitly stating the re-  
239 lationship between AGB and  $VOD$ , we assume that AGB can be expressed  
240 as a function of  $VOD$ :

$$241 \quad \text{AGB} = f(VOD) = \widetilde{VOD} \quad (5)$$

242 Assuming that above- and belowground terms in equation (4) are pro-  
243 portional, which allows to express  $B$  as a function of  $VOD$ , we arrive at the  
244 relationship between VOD and GPP, which can be described by the following

245 differential equation:

$$246 \quad \text{GPP} = a \frac{d\widetilde{\text{VOD}}}{dt} + b \widetilde{\text{VOD}} + c \quad (6)$$

247  $c$  is a time-invariant offset, which is added from a mathematical point  
248 of view and does not necessarily reflect the neglected terms in equation (3)  
249 but rather aids the conversion of VOD to GPP if the offset is not already  
250 included in  $f(\text{VOD})$ .

251 Equation (6) presents the theoretical concept in this study, which we aim  
252 to model for different VOD data sets through the use of GAM (Hastie and  
253 Tibshirani, 1987).

## 254 4. Methods

### 255 4.1. Generalized Additive Models

256 GAM is a regression approach which can utilize different link functions  
257 for fitting a limited set of predictor variables ( $\mathbf{x}$ ) against the expected value  
258 of the response variable ( $y$ ) (Hastie and Tibshirani, 1987). For calculating  
259 the conditional expected value ( $\mathbb{E}[y \mid \mathbf{x}]$ ), the algorithm requires specifica-  
260 tion of the data distribution for the response variable. The approach allows  
261 non-linear and non-monotonic relationships between a response variable and  
262 predictor variables, which are represented by fitting smooth spline functions  
263 ( $f$ ) for each predictor (Hastie and Tibshirani, 1987, 1990). As such, GAM  
264 does not require specification of the underlying relationship between pre-



265 dictor and response variable. Since we do not explicitly know the shape of  
266 the relationship between biomass and each VOD data set, GAM presents a  
267 suitable method in this study for estimating GPP based on VOD.

268 For the analysis, we used LinearGAM from the python package pygam  
269 (Servén et al., 2018), which uses the normal distribution together with the  
270 identity as link function. In this case, GAM with  $p$  input variables has the  
271 form (Hastie and Tibshirani, 1987):

$$272 \quad \mathbb{E}[y \mid \mathbf{x}] = \alpha + \sum_{j=1}^p f_j(x_j) \quad (7)$$

273 We used LinearGAM with 25 splines of order 3, which allows variability in  
274 the shape of the fitted spline across the data range, together with a value of  
275 200 for the smoothing parameter lambda, which provides strong smoothing  
276 to ensure generalizability.

277 We applied GAM by fitting different sets of input variables against global  
278 or in situ GPP estimates. To indicate which set of input variables was used for  
279 training GAM, we refer to the model as GPP() with a list of input variables  
280 in parenthesis. For example, GPP(VOD,  $\Delta$ VOD) denotes a GAM setup  
281 that uses VOD and  $\Delta$ VOD as input.

#### 282 4.2. *Experimental setups*

283 Our analysis comprises three experiments. The first experiment assesses  
284 the model's performance in temporal extrapolation, while the second exper-  
285 iment evaluates the model's capability in spatial extrapolation using cross

286 validation and model selection. These experiments allow to determine the  
287 model’s performance during periods or at locations it has not been trained  
288 on, which relates to the situation during the upscaling of in situ GPP assessed  
289 in the third experiment.

#### 290 *4.2.1. Testing temporal extrapolation*

291 For testing the model’s ability to reproduce the temporal dynamics of  
292 GPP, we trained  $GPP(VOD, \Delta VOD)$  at each grid cell against the global  
293 GPP from FLUXCOM. The comparison with an existing global GPP product  
294 has the advantage of minimizing the impact of scale differences, which are  
295 often observed for in situ observations versus satellite data. It can thus  
296 demonstrate if the model can be used in general for estimating GPP. For the  
297 analysis, we split the data in time using the first two years of each data set  
298 for training the model (AMSR-E, ASCAT, SIF: 1/2007 to 12/2008; AMSR2:  
299 7/2012 to 6/2014) and the remaining period for testing (AMSR-E: 1/2009  
300 to 9/2011; ASCAT, SIF: 1/2009 to 12/2015, AMSR2: 7/2014 to 12/2015).  
301 To support global results, we repeated the analysis using in situ FLUXNET  
302 observations. For this setup, AMSR2 data are omitted since the overlap  
303 period with FLUXNET extends only through 2014.

304 In addition to the analysis of  $GPP(VOD, \Delta VOD)$ , we determined the  
305 added value of using the combination of  $VOD$  and  $\Delta VOD$  compared to  
306  $VOD$  or  $\Delta VOD$  alone. The reason for treating  $VOD$  and  $\Delta VOD$  sepa-  
307 rately against our proposed theory, was to exclude the possibility that either

308 signal alone is able to match the GPP signal merely by applying a non-linear  
309 regression like GAM.

#### 310 *4.2.2. Testing spatial extrapolation using cross validation and model selection*

311 Using leave-site-out cross validation with FLUXNET GPP as target vari-  
312 able, we assessed the model’s ability for spatial extrapolation. For each site,  
313  $GPP(VOD, \Delta VOD)$  or  $GPP(SIF)$  was trained with data from all sites ex-  
314 cept the site under evaluation. The model was then applied to the data  
315 that was left out and compared against the target variable. As the data  
316 were split in space, the training and testing period each span the full overlap  
317 period with FLUXNET for each data set. Apart from the full signal, we  
318 also assessed the performance of anomalies of the resulting GPP estimates  
319 in order to evaluate the strength of the relationship in the absence of season-  
320 ality. Anomalies were calculated as differences to the mean seasonal cycle  
321 during the testing period for the VOD- or SIF-based GPP estimates (i.e.,  
322 after model application) and FLUXNET GPP.

323 We further assessed if the additional use of the temporal grid cell median  
324 of each data set ( $mdnVOD$  or  $mdnSIF$ ) can improve the spatial extrap-  
325 olation of the model, i.e.  $GPP(VOD, \Delta VOD, mdnVOD)$  or  $GPP(SIF,$   
326  $mdnSIF)$ .  $mdnVOD$  is a static component for each data set, which varies  
327 with each grid cell and thus does not contribute to the temporal dynamic of  
328 the resulting estimate.  $mdnVOD$  identifies areas of similar biomass and thus  
329 further relates to land cover, since grassland generally has a lower biomass

330 than shrubland, which in turn has a lower biomass than a dense forest.  
331 In contrast, *mdnSIF* identifies areas of similar photosynthetic activity and  
332 therefore reflects a different property than *mdnVOD*.

333 To assess whether an improvement in model performance can be at-  
334 tributed to a gain in information through the addition of the respective vari-  
335 able or is caused by an additional degree of freedom, we computed the Akaike  
336 Information Criterion (AIC; Akaike, 1974). For this analysis, we randomly  
337 split the station data into two data sets. We used one half of the stations for  
338 training and the remaining half for testing.

#### 339 *4.2.3. Upscaling*

340 In the third experiment, we estimated GPP globally based on VOD using  
341 the best performing model setup as assessed during cross validation and  
342 model selection. The upscaling was performed similarly to cross validation  
343 with the difference that the model for each setup was trained against all  
344 available in situ FLUXNET GPP. After applying the model to the global  
345 VOD data sets, we evaluated the model’s performance by comparing the  
346 VOD-based GPP estimates with global GPP estimates from FLUXCOM and  
347 MODIS. For the analysis of mean annual GPP, we additionally performed an  
348 uncertainty analysis to determine the influence of the choice of the stations  
349 on the GPP estimation. For this, we repeated the VOD-based upscaling ten  
350 times, each time reducing the number of stations by 10%. The excluded  
351 stations were randomly drawn without replacement. Therefore, each model

352 run in the uncertainty analysis is based on data from 90% of the stations.

### 353 4.3. Data preparation

354 The analysis is based on two different resolutions: for the comparison  
355 between VOD, FLUXCOM and MODIS data, the common sampling is 8-  
356 daily,  $0.25^\circ$  while for the comparison with SIF, the common sampling is  
357 monthly,  $0.5^\circ$ . We aggregated data sets with a higher resolution using the  
358 average over 8 days or the average over the grid cell. For data sets with a  
359 lower spatial resolution like snow depth and temperature data, we performed  
360 nearest neighbor resampling.

361 VOD observations were masked when temperature was below  $0^\circ\text{C}$  and  
362 snow cover was present. The masking was also applied to GPP data sets  
363 for comparability. In addition to snow and temperature masking, VOD from  
364 passive sensors was masked for radio frequency interference using the accom-  
365 panying flags, since it can also lead to erroneous retrievals of VOD (Li et al.,  
366 2004; Njoku et al., 2005).

367 We approximate the derivative of VOD at each grid cell ( $\mathbf{x}_i$ ) with the  
368 change of the smoothed *VOD* signal between two consecutive *VOD* obser-  
369 vations:

$$370 \quad \Delta VOD(\mathbf{x}_i, t_j) = VOD(\mathbf{x}_i, t_j) - VOD(\mathbf{x}_i, t_{j-1}) \quad (8)$$

371 The smoothing was computed using a Savitzky-Golay filter (Savitzky and  
372 Golay, 1964) with a window size of 11 time steps for 8-daily data and 5 time  
373 steps for monthly data. The window size for each resolution was chosen after

374 visual inspection of the smoothed time series at the location of the FLUXNET  
375 sites. Additionally, we performed a cross validation similar to the temporal  
376 extrapolation experiment for 8-daily AMSRE\_X and for GPP(*VOD*,  $\Delta VOD$ )  
377 but using different window sizes during the computation of  $\Delta VOD$  (Figs. S3).  
378 Results for Spearman correlation and *RMSE* confirmed that a window size of  
379 11 time steps is a suitable choice presenting a trade-off between a preferably  
380 high median correlation, low median *RMSE* and still relatively low window  
381 length.

382 During cross validation, we additionally assessed the performance of the  
383 GPP anomalies relative to the mean seasonal cycle. We calculated anomalies  
384 for sites with more than two years of data using the python package pytesmo  
385 (Paulik et al., 2015).

#### 386 4.4. Statistical analysis

387 Prior to the analysis, we tested if grid cell data of the global data sets fol-  
388 low normal distribution using the D’Agostino and Pearson’s test (D’Agostino,  
389 1971; D’Agostino and Pearson, 1973). We found that on average 75% of the  
390 grid cells differ from normal distribution. For this reason, we calculated the  
391 non-parametric Spearman rank correlation and used the temporal grid cell  
392 median instead of the mean in the analysis.

393 We evaluated model performance by calculating the Spearman rank cor-  
394 relation coefficient ( $r$ ) and root mean square error (*RMSE*). For the leave-  
395 site-out cross validation, we additionally analyzed the index of agreement

396 (*IoA*), which is a standardized measure for the model prediction error and  
397 is defined after Willmott (1981) as:

$$398 \quad IoA = 1 - \frac{\sum_{i=1}^n (p_i - o_i)^2}{\sum_{i=1}^n (|p_i - \bar{o}| + |o_i - \bar{o}|)^2} \quad \text{with } n = \text{number of observations} \quad (9)$$

399 where  $p$  represents the model output and  $o$  the in situ observations. The  
400 index ranges between 0 (worst agreement) and 1 (best agreement).

401 For model selection, we computed AIC using the python package RegscorePy<sup>2</sup>.  
402 AIC is a relative measure for the goodness of fit for different model setups  
403 while penalizing higher numbers of input variables (Akaike, 1974). The model  
404 setup with the lowest AIC is then considered as the optimal choice.

## 405 5. Results

### 406 5.1. Temporal extrapolation

407 The application of GAM for each grid cell is illustrated for a grid cell dom-  
408 inated by rainfed cropland in Fig. 1. In this example, GPP( $VOD$ ,  $\Delta VOD$ )  
409 is able to capture the temporal dynamics of FLUXCOM GPP (Fig. 1a). In  
410 contrast,  $VOD$  shows a positive temporal lag with respect to GPP (Fig. 1b),  
411 while  $\Delta VOD$  results in a negative lag with GPP. Making use of both  $VOD$   
412 and  $\Delta VOD$ , the model can largely compensate the observed lags for the  
413 individual signals of  $VOD$  and  $\Delta VOD$ .

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<sup>2</sup>RegscorePy v1.0: <https://pypi.org/project/RegscorePy/>

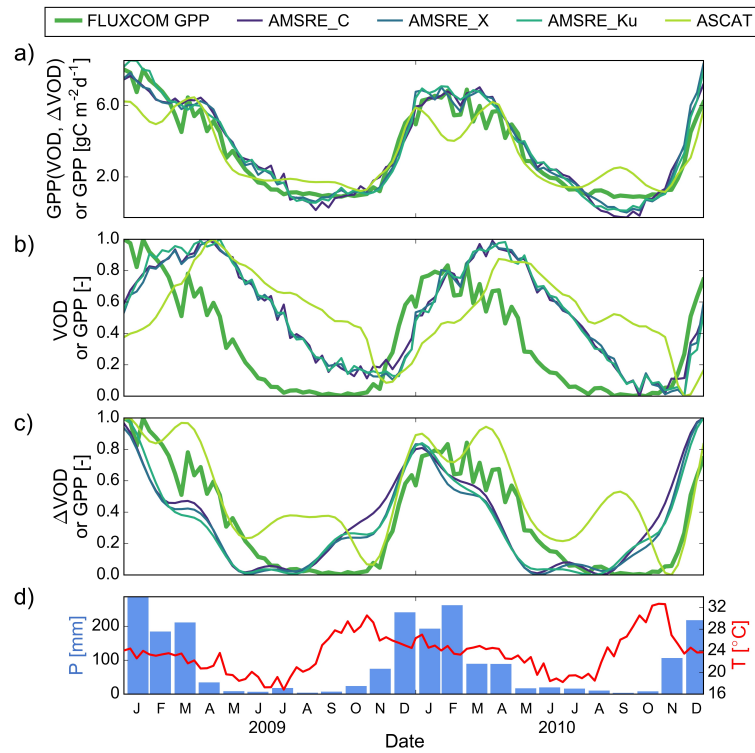


Figure 1: Time series plot for a grid cell dominated by rainfed cropland ( $35.125^{\circ}\text{E}$ ,  $15.125^{\circ}\text{S}$ ) for different VOD data sets for the period 1/2009 to 12/2010: 8-daily FLUXCOM GPP and a)  $\text{GPP}(VOD, \Delta VOD)$ , b)  $VOD$  and c)  $\Delta VOD$ .  $\text{GPP}(VOD, \Delta VOD)$  was trained at this grid cell against FLUXCOM data for the period 1/2007 to 12/2008. Data in (b) and (c) are scaled between 0 and 1 to aid visual comparison of the temporal dynamics. (d) Monthly precipitation and 8-daily surface temperature.



414 Applying the model per grid cell globally at 8-daily,  $0.25^\circ$  sampling, the  
 415 resulting GPP estimates show high temporal agreement with FLUXCOM  
 416 GPP (Fig. 2). Correlations are higher for passive VOD data sets ( $0.69 \leq$   
 417 median  $r \leq 0.72$ ) than for the active VOD data set (median  $r=0.61$ ). For  
 418 passive VOD data sets, correlations are especially high over Africa, parts of  
 419 Australia and Europe. For the active VOD, high correlations are observed  
 420 over Europe, North America and parts of South America. Consistent with  
 421 the correlation results,  $RMSE$  (Fig. S4) yields lower global median values for  
 422 passive VOD data sets ( $0.85 \leq$  median  $RMSE \leq 0.88 \text{ gCm}^{-2}\text{d}^{-1}$ ) than for  
 423 the active VOD (median  $RMSE=0.99 \text{ gCm}^{-2}\text{d}^{-1}$ ). Comparing the different  
 424 frequencies of the passive VOD data sets, Ku-band results in the lowest  
 425 median  $RMSE$  closely followed by X-band. Regions with lowest  $RMSE$  are  
 426 observed over Australia for all VOD data sets, while regions with highest  
 427  $RMSE$  are found mainly in northern latitudes.

428 The correlations increase for all data sets when performing the analysis at  
 429 monthly,  $0.5^\circ$  sampling (Table S2), yielding median  $r$  between 0.80 and 0.82  
 430 for passive VOD and 0.74 for the active VOD. When repeating the analysis  
 431 using either  $VOD$  or  $\Delta VOD$  alone as input, we found that  $GPP(VOD)$ ,  
 432  $\Delta VOD$ ) outperforms  $GPP(VOD)$  and  $GPP(\Delta VOD)$  at both resolutions  
 433 (Table S2) with an average difference in median  $r$  of about 0.1 and 0.2 for  
 434  $GPP(VOD)$  and  $GPP(\Delta VOD)$ , respectively. The different frequencies of  
 435 AMSR-E generally yield similar results. However, X-band data consistently  
 436 showed the highest correlation at both resolutions. This finding was also

437 observed for AMSR2 frequencies (Table S2). Compared with correlations  
438 obtained for SIF (median  $r=0.73$ ),  $GPP(VOD, \Delta VOD)$  at monthly,  $0.5^\circ$   
439 sampling shows comparable or slightly higher median correlations for active  
440 and passive VOD, respectively.

441 The added value of combining  $VOD$  and  $\Delta VOD$  can be further confirmed  
442 using in situ FLUXNET GPP. Correlations for  $GPP(VOD, \Delta VOD)$  are  
443 higher than for the individual signals, i.e.  $GPP(VOD)$  and  $GPP(\Delta VOD)$   
444 (Fig. S5) with an average increase in median  $r$  of about 0.1 and 0.3 for  
445  $GPP(VOD)$  and  $GPP(\Delta VOD)$ , respectively. Comparing median correla-  
446 tions of the in situ analysis with those obtained in the global comparison,  
447 the median  $r$  for SIF yields almost the same value (0.73 obtained for global  
448 GPP compared to 0.72 for in situ GPP). For VOD data sets, however, me-  
449 dian  $r$  for the in situ analysis is on average lower by 0.1 than for the global  
450 comparison.

451 These results, especially for the global comparison, demonstrate the model's  
452 capability in temporal extrapolation and support our theory of representing  
453 the relationship between VOD and GPP with a differential equation.

## 454 5.2. Spatial extrapolation

455 Using leave-site-out cross validation, we evaluated the performance in  
456 spatial extrapolation of the relationship between VOD and GPP. For the full  
457 signals (Fig. 3, S6 and S7), the performance for SIF is generally higher than  
458 for VOD data. Median values of  $IoA$  and  $r$  are comparable to or lower for

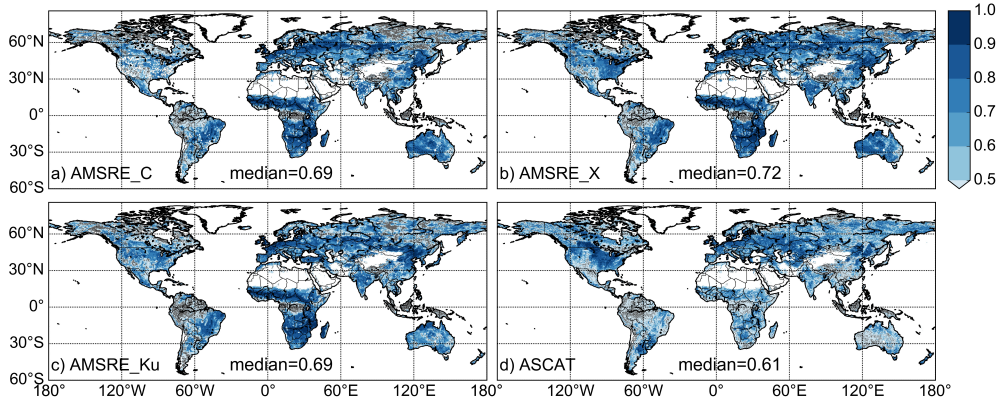


Figure 2: Spearman rank correlation ( $r$ ) between FLUXCOM GPP and GPP( $VOD$ ,  $\Delta VOD$ ) for different VOD data sets for the testing period (AMSR-E: 1/2009 to 9/2011; ASCAT: 1/2009 to 12/2015). The analysis is based on data at 8-daily and  $0.25^\circ$  sampling. GPP( $VOD$ ,  $\Delta VOD$ ) is trained at each grid cell separately against FLUXCOM using data from the period 1/2007 to 12/2008. Correlations that are not significant ( $p > 0.05$ ) are masked in grey. The median values denote the median of significant correlations for each data set.

459 VOD than for SIF, while median  $RMSE$  is higher for VOD than for SIF in  
 460 all cases. The addition of the temporal median as input to GAM does not  
 461 appear to have the same effect for VOD and SIF. While the performance  
 462 for  $VOD$  increases when adding  $mdnVOD$ ,  $SIF$  does not appear to ben-  
 463 efit from including  $mdnSIF$  since the correlations do not differ markedly  
 464 between GPP( $SIF$ ) and GPP( $SIF$ ,  $mdnSIF$ ). For VOD, however, the in-  
 465 crease in performance upon adding  $mdnVOD$  indicates that the offset, which  
 466 is already implicitly included in GAM, is not a globally constant value but  
 467 instead varies for each grid cell. The relationship between VOD and GPP  
 468 thus is additionally modified by a static component of vegetation biomass  
 469 within a grid cell as represented by  $mdnVOD$ . In contrast, the offset in the

470 relationship between SIF and GPP presents a global value and does not vary  
471 with *mdnSIF*.

472 Results for the anomalies of the VOD- or SIF-based GPP estimates  
473 (Fig. 4, S8 and S9) reveal a slightly higher performance for VOD than for SIF.  
474 Median values of *IoA* and *r* are comparable or in some cases higher for VOD  
475 than for SIF, while median *RMSE* is lower for VOD than for SIF in all cases.  
476 Including the temporal median does not affect the metrics except for *IoA* for  
477 VOD. In this case, the anomalies for  $GPP(VOD, \Delta VOD, mdnVOD)$  result  
478 in slightly higher *IoA* values than for  $GPP(VOD, \Delta VOD)$ .

479 For the different AMSR-E frequencies, the cross validation results further  
480 reveal that X-band data result in higher performance than C- and Ku-band  
481 data in most cases, which is especially true for data at 8-daily,  $0.25^\circ$  sampling.

482 The two extrapolation experiments for the full signals further show that  
483 correlations for the spatial extrapolation (Fig. 3) are generally lower than for  
484 the temporal extrapolation (Fig. S5). Even when adding *mdnVOD*, median  
485 *r* during spatial extrapolation is on average lower by about 0.1 than during  
486 temporal extrapolation at both resolutions. Similarly, SIF also experiences a  
487 reduction in correlation during spatial extrapolation compared to temporal  
488 extrapolation. The difference in median *r*, however, is about 0.05 and thus  
489 smaller than for VOD. This indicates that the reduction in performance for  
490 VOD data is not alone caused by the model representation itself but is also  
491 strongly affected by scale differences between point measurements and the  
492 spatial coverage of the grid cell data.

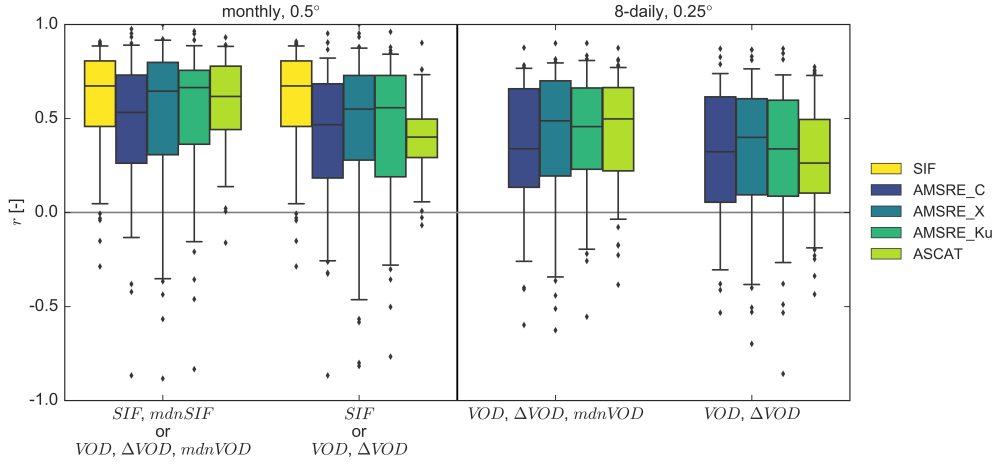


Figure 3: Leave-site-out cross validation for Spearman rank correlation ( $r$ ) at monthly,  $0.5^\circ$  and 8-daily,  $0.25^\circ$  sampling. The analysis is based on the full signals of in situ FLUXNET GPP and GPP estimates based on VOD or SIF. Labels on the x-axis indicate which input variables are used for each model. Box plot whiskers extend to the 5th and 95th data percentile. Abbreviations – *mdnSIF*: temporal grid cell median *SIF*;  $\Delta VOD$ : temporal change in *VOD* between two consecutive observations; and *mdnVOD*: temporal grid cell median *VOD*.

493 Cross validation results for the full signals for AMSR2 (Fig. S10, S11 and  
 494 S12) are generally similar to those obtained for AMSR-E. AMSR2 frequen-  
 495 cies, however, show a slight decrease in performance for  $r$  and  $IoA$  and a  
 496 slight increase in performance for  $RMSE$  compared to AMSR-E frequen-  
 497 cies (Fig. S12). Consistent with AMSR-E data, AMSR2 X-band often shows  
 498 higher performance than the remaining frequencies.

499 The previous results suggest that the combination of all three input vari-  
 500 ables, i.e.  $VOD$ ,  $\Delta VOD$  and  $mdnVOD$ , can improve model performance.  
 501 Results of AIC for the different model setups relative to AIC for  $GPP(VOD,$   
 502  $\Delta VOD, mdnVOD)$  in Fig. 5 further confirm this finding. For all VOD data  
 503 sets at both resolutions, the combination of  $VOD$  and  $\Delta VOD$  yields lower

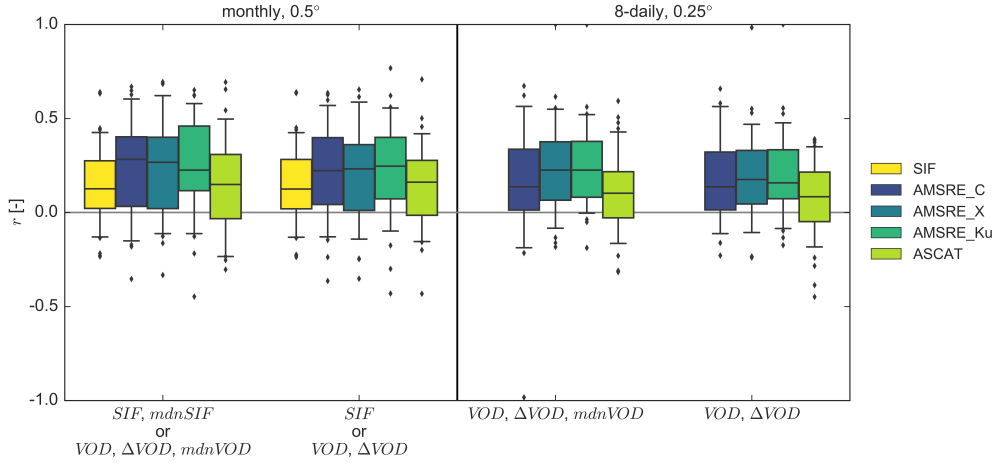


Figure 4: As Fig. 3 but for the anomalies of in situ FLUXNET GPP and GPP estimates based on VOD or SIF.

504 AIC values than for each input variable alone. When adding  $mdnVOD$ , AIC  
 505 is further reduced in the majority of cases. Exceptions from this rule are  
 506 found for AMSRE\_C and AMSRE\_X at 8-daily,  $0.25^\circ$  sampling, where the  
 507 use of all three variables increases AIC. Since this finding is not consistent  
 508 with results at monthly,  $0.5^\circ$  sampling for the same frequencies, we suspect  
 509 that this might be an artifact of the choice of stations. We thus still suggest  
 510 the use of all three variables for upscaling GPP based on VOD data. In case  
 511 of SIF, the difference in AIC between  $GPP(SIF)$  and  $GPP(SIF, mdnSIF)$   
 512 is negligible. This confirms that, unlike for VOD, the relationship between  
 513 SIF and GPP does not depend on the data set median.

### 514 5.3. Upscaling of in situ GPP

515 Based on the results for cross validation and model selection, we used  
 516  $GPP(VOD, \Delta VOD, mdnVOD)$  for the global upscaling with VOD and

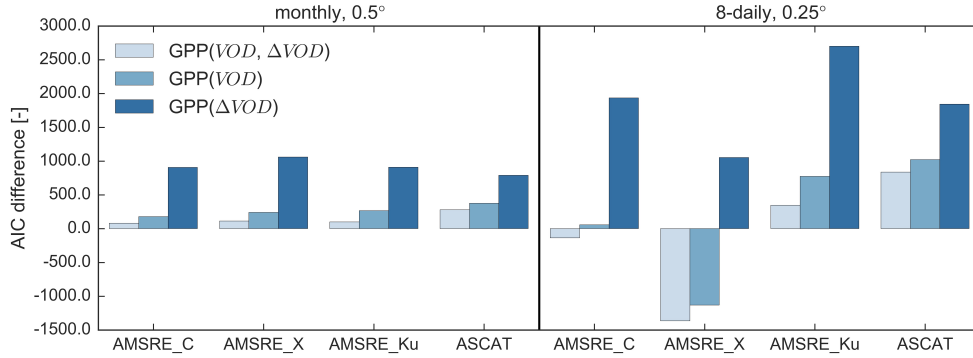


Figure 5: Difference in AIC between model setups with respect to AIC for  $GPP(VOD, \Delta VOD, mdnVOD)$  for each VOD data set. For SIF, the AIC difference between  $GPP(SIF)$  and  $GPP(SIF, mdnSIF)$  is very low (1.67) compared with VOD data sets and therefore not displayed. The analysis is based on data at monthly,  $0.5^\circ$  or 8-daily,  $0.25^\circ$  sampling. Positive values indicate model improvement when using all three variables as input compared to models with a lower number of input variables.

517  $GPP(SIF)$  for the upscaling with SIF for further analysis. We will put an  
 518 emphasis on the output from X-band due to the overall better performance  
 519 during the temporal and spatial extrapolation experiments.

### 520 5.3.1. Relationship between VOD and GPP

521 The partial dependence plots for  $GPP(VOD, \Delta VOD, mdnVOD)$ , which  
 522 are exemplified for AMSRE\_X in Fig. 6, demonstrate the contribution of the  
 523 three input variables to the model. For all VOD data sets, we observed that  
 524 the functions for  $VOD$  and  $\Delta VOD$  mainly increase, while the function for  
 525  $mdnVOD$  decreases. The increase for  $\Delta VOD$  is true for the region where  
 526 the majority of data are located and the confidence interval is small. For  
 527 AMSRE\_X, this region ranges between -0.3 and 0.4 (Fig. 6e). The inverse re-  
 528 lationship between  $VOD$  and  $mdnVOD$  and the additive linking of variables

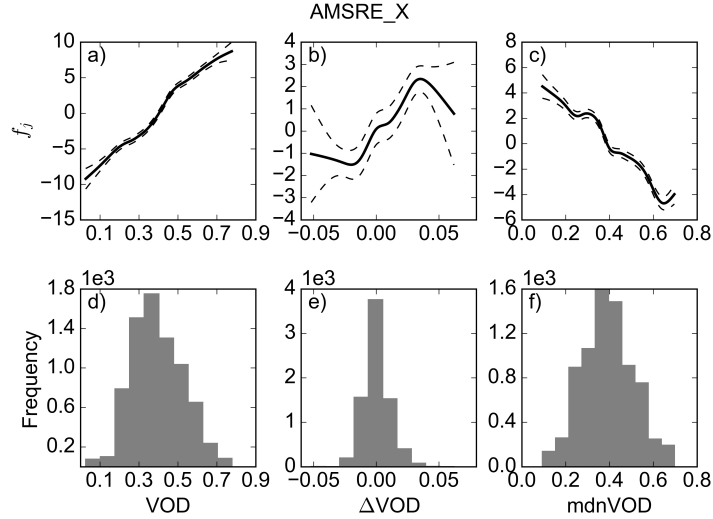


Figure 6: GAM Partial dependence plots for  $GPP(VOD, \Delta VOD, mdnVOD)$  obtained during upscaling (a-c) and histogram of input variables (d-f) for AMSRE\_X at 8-daily and  $0.25^\circ$  sampling. Dashed lines in (a-c) indicate the confidence intervals.

529 in GAM suggest that  $mdnVOD$  is subtracted from  $VOD$ .

### 530 5.3.2. Global correlation of upscaled GPP

531 Results for  $GPP(VOD, \Delta VOD, mdnVOD)$  at 8-daily,  $0.25^\circ$  sampling  
 532 show moderate temporal agreement with FLUXCOM and MODIS GPP  
 533 (Fig. 7). Median  $r$  ranges between 0.54 and 0.62 for FLUXCOM and be-  
 534 tween 0.52 and 0.60 for MODIS. The correlations also include some negative  
 535 values (Fig. S13). For significant correlations, the fraction of negative corre-  
 536 lations lies between 5 to 9% for passive VOD and about 12% for active VOD.  
 537 Highest median correlations are observed for X-band data, which is consistent  
 538 with the results from temporal and spatial extrapolation. At monthly,  $0.5^\circ$   
 539 sampling, the global median  $r$  increases, ranging between 0.67 and 0.71 for



540 FLUXCOM and between 0.66 and 0.70 for MODIS. For GPP(*SIF*), median  
541  $r$  reaches 0.71 for FLUXCOM and 0.66 for MODIS.

542 Results for AMSR2 frequencies (Fig. S15) are generally similar to those  
543 obtained for AMSR-E, although AMSR2 frequencies yield slightly lower me-  
544 dian correlations than AMSR-E frequencies.

545 Comparing correlations with FLUXCOM between the upscaling and the  
546 global temporal extrapolation (Section 5.1), median  $r$  for SIF is similar.  
547 For VOD, however, correlations for the upscaling are markedly lower than  
548 during temporal extrapolation, which is consistent with the reduction in  
549 model performance during cross validation.

### 550 5.3.3. Comparison of annual GPP

551 In addition to assessing the temporal dynamics, we compared mean an-  
552 nual GPP for GPP(*VOD*,  $\Delta$ *VOD*, *mdnVOD*) from AMSRE\_X with mean  
553 annual GPP for FLUXCOM and MODIS. The analysis is based on data  
554 points where all three data sets are available. In general, GPP(*VOD*,  $\Delta$ *VOD*,  
555 *mdnVOD*) shows the expected spatial pattern with highest values observed  
556 in tropical regions (Fig. 8a). Nevertheless, GPP(*VOD*,  $\Delta$ *VOD*, *mdnVOD*)  
557 for AMSRE\_X tends to overestimate annual GPP in many regions compared  
558 to FLUXCOM and MODIS (Fig. 8b-c). Closest agreement between AM-  
559 SRE\_X and FLUXCOM or MODIS is observed for tropical regions. Consis-  
560 tent with these results, we observed lowest differences between AMSRE\_X  
561 and FLUXCOM or MODIS at low aridity (Fig. 9), which represents very

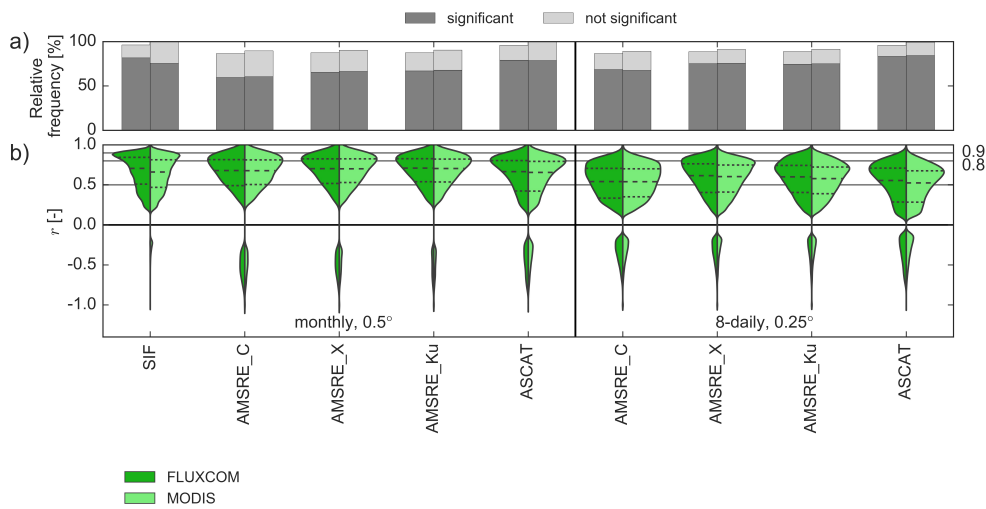


Figure 7: Spearman rank correlation ( $r$ ) between GPP data sets (FLUXCOM, MODIS) and upscaling for GPP( $VOD$ ,  $\Delta VOD$ ,  $mdnVOD$ ) or GPP( $SIF$ ). Data were trained against in situ GPP estimates (FLUXNET) at 8-daily,  $0.25^\circ$  or monthly,  $0.5^\circ$  sampling. a) Relative frequency of grid cells with significant and not significant correlations with respect to all possible land grid cells at each resolution. Areas that do not contain results relate to gaps obtained during masking for radio frequency interference or to not produced pixels in the original data products. b) Violin plot of significant correlations. Horizontal grey lines indicate correlation values of 0.5, 0.8 and 0.9. Dashed lines indicate the median (long dashes) and the 25th and 75th percentile (short dashes).

562 humid regions like the tropics. Under mesic conditions, differences between  
563 products are slightly higher than for very dry or very humid regions.

564 The observed overestimation is also apparent in the zonal mean (Fig. 8d).  
565  $GPP(VOD, \Delta VOD, mdnVOD)$  consistently overestimates annual GPP from  
566 FLUXCOM and MODIS and is closest to FLUXCOM and MODIS near the  
567 equator. Despite the overestimation,  $GPP(VOD, \Delta VOD, mdnVOD)$  shows  
568 similar latitudinal features as for FLUXCOM and MODIS. The uncertainty  
569 analysis of  $GPP(VOD, \Delta VOD, mdnVOD)$  for AMSR2\_X further demon-  
570 strates that the choice of stations for the upscaling has an effect on the GPP  
571 estimation (Fig. 8d). The range of the ten model runs is larger in the trop-  
572 ics and the southern hemisphere than in the northern hemisphere, which is  
573 caused by differences in station density in these regions. The map of the  
574 standard deviation for the ten model runs (Fig. S16) shows that differences  
575 between the model runs are most pronounced in the tropics, the Sahel, south-  
576 ern parts of Africa and large parts of Australia.

577  $GPP(VOD, \Delta VOD, mdnVOD)$  for AMSR2\_X results in a higher agree-  
578 ment with FLUXCOM and MODIS than for AMSR2\_X. In contrast to AM-  
579 SR2\_X, AMSR2 yields smaller differences in annual GPP with FLUXCOM  
580 and MODIS (Fig. S17a-c), which is in line with the smaller *RMSE* observed  
581 for AMSR2 during cross validation. Annual GPP for AMSR2, however, also  
582 exhibits areas where FLUXCOM and MODIS are underestimated, which are  
583 located mainly in the Sahel and Australia. The latitudinal distribution of  
584 annual GPP (Fig. S17d) shows that AMSR2\_X overall yields a closer agree-

585 ment between with FLUXCOM or MODIS than for AMSRE\_X. Similar as  
586 for AMSRE\_X, AMSR2\_X deviates less from FLUXCOM and MODIS in the  
587 tropics.

## 588 **6. Discussion**

### 589 *6.1. Relationship between VOD and GPP*

590 Our study presents a model for estimating GPP based on VOD, which de-  
591 scribes the relationship between VOD and GPP through a differential equa-  
592 tion. The model uses different VOD variables, i.e.  $VOD$ ,  $\Delta VOD$ , and  
593  $mdnVOD$ , as input. The approach is based on the assumption that VOD  
594 provides an estimate for aboveground living biomass (Liu et al., 2011, 2015),  
595 which has been employed by multiple studies for detecting trends in biomass  
596 (Andela et al., 2013; Liu et al., 2013b,a, 2015; Marle et al., 2016). In support  
597 of this theory, Tian et al. (2016) have demonstrated the applicability of the  
598 biomass-VOD relationship in a dryland ecosystem.

599 The relationship between biomass and VOD, however, is rather complex.  
600 Since VOD presents a measure of vegetation water content (Jackson and  
601 Schmugge, 1991), it can also be considered as the product of biomass and  
602 relative water content (Momen et al., 2017), a quantity that is closely related  
603 to the water potential of vegetation (Barnard et al., 2011; Brodribb and Hol-  
604 brook, 2003; Momen et al., 2017). For this reason, VOD has also been used as  
605 a surrogate for fuel moisture in fire modelling (Forkel et al., 2017) or for leaf  
606 water potential and isohydricity of vegetation (Konings and Gentine, 2016;

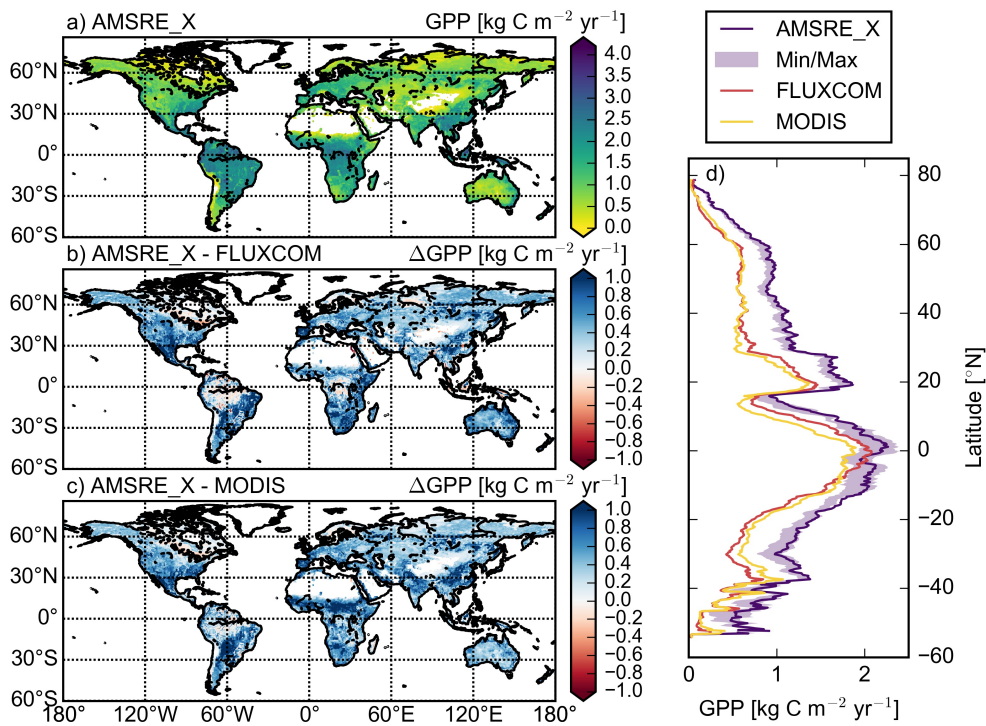


Figure 8: Mean annual GPP for the period 2007 to 2010: a) upscaling of  $GPP(VOD, \Delta VOD, mdnVOD)$  for VOD AMSRE\_X, b) difference in mean annual GPP between FLUXCOM and AMSRE\_X c) difference in mean annual GPP between MODIS and AMSRE\_X. Values in (b) and (c) are displayed between -1 and 1. d) Zonal mean of mean annual GPP. Estimates for  $GPP(VOD, \Delta VOD, mdnVOD)$  were produced using data at 8-daily, 0.25° sampling. The area denoted by Min/Max represents the minimum and maximum of the zonal means for the ten model runs obtained during the uncertainty analysis for  $GPP(VOD, \Delta VOD, mdnVOD)$  with VOD AMSRE\_X.

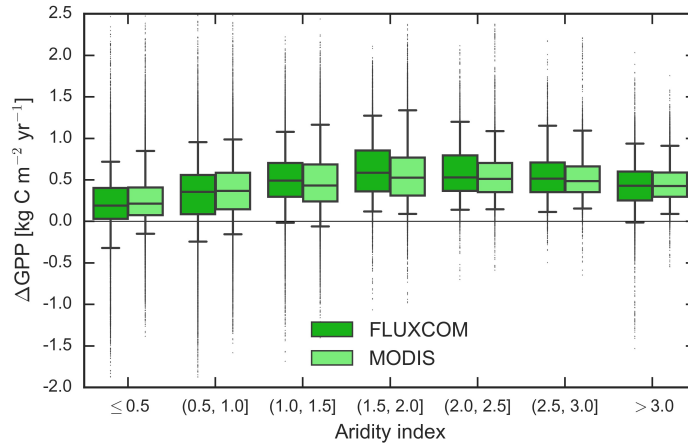


Figure 9: Differences in mean annual GPP between AMSRE\_X and FLUXCOM or MODIS stratified along the aridity index. The analysis is based on the period 2007 to 2010 and uses 8-daily,  $0.25^\circ$  data. Mean annual GPP for AMSRE\_X is computed using  $GPP(VOD, \Delta VOD, mdnVOD)$ . Box plot whiskers represent the 5th and 95th data percentile.

607 Konings et al., 2017a,b). The impact of the relative water content on the  
 608 relationship between biomass and VOD, however, is not entirely clear. Using  
 609 in situ estimates of leaf water potential, Momen et al. (2017) have shown  
 610 that variations in VOD are largely driven by changes in leaf water potential  
 611 or the interaction of leaf water potential and LAI rather than LAI alone.  
 612 Nevertheless, studies connected leaf water potential to maximum stomatal  
 613 conductivity (Klein, 2014; Running, 1976). Since stomatal conductivity con-  
 614 trols photosynthesis by regulating the  $CO_2$  uptake (e.g. Damour et al., 2010),  
 615 this can provide an additional indication for the potential use of VOD to es-  
 616 timate GPP. Considering VOD as a proxy for leaf water potential, however,  
 617 cannot explain the increase in temporal agreement when combining the orig-  
 618 inal VOD signal and its derivative as observed in our study. Therefore, we

619 propose that in our context VOD presents an estimate of the metabolically  
620 active biomass.

## 621 *6.2. Impact of VOD frequency on the relationship with GPP*

622 We observed that VOD data from X-band appear to be a suitable pre-  
623 dictor for estimating GPP. This finding may be counter-intuitive since VOD  
624 from lower frequencies (i.e. longer wavelengths), such as L-band, rather  
625 than from higher frequencies was demonstrated to correlate closely with total  
626 aboveground vegetation biomass (Rodríguez-Fernández et al., 2018). Total  
627 aboveground biomass, however, is a rather poor predictor of GPP due to the  
628 presence of large-size plant parts functioning as structural components that  
629 are less metabolically active (Litton et al., 2007). This is in accordance with  
630 observations of lower correlations between VOD and GPP for L-band than  
631 for C- or X-band VOD (Teubner et al., 2018). In contrast, the metabolically  
632 active plant parts, i.e. leaves and fine roots, present a suitable estimator for  
633 GPP (Litton et al., 2007). Since metabolically active cells contain water, the  
634 use of VOD in our model can present a suitable proxy for the aboveground  
635 metabolically active parts, which in turn can be related to GPP. In addition  
636 to this, Litton et al. (2007) demonstrated that in forests the partitioning of  
637 carbon to leaves is a constant fraction of GPP. This implies that total GPP  
638 can be obtained by estimating the portion of GPP that goes into the leaf  
639 compartment. Those two concepts together with the theoretically stronger  
640 sensitivity of higher VOD frequencies to small vegetation parts, i.e. leaves

641 and small structural components (Woodhouse, 2005), can explain why high  
642 frequency VOD rather than low frequency VOD is suited for retrieving GPP.

### 643 *6.3. Extrapolation of VOD-GPP relationship*

644 In both extrapolation experiments (temporal and spatial), we observed a  
645 lower agreement of VOD-based estimates with in situ GPP than with global  
646 GPP. In contrast, SIF only showed a slight reduction in performance dur-  
647 ing spatial extrapolation. This indicates that subpixel heterogeneity plays a  
648 more important role for the relationship between VOD and GPP than be-  
649 tween SIF and GPP. From a mathematical point of view, the relationship  
650 between VOD and GPP strongly depends on the appropriate weighting of  
651 the two dynamic terms in the model,  $VOD$  and  $\Delta VOD$ , in order to match  
652 the temporal dynamic of the reference GPP. Since variations in the weight-  
653 ing result in a temporal shifting of the VOD-based GPP estimate, weights  
654 that are not representative for the respective grid cell may decrease model  
655 performance. Therefore, scale differences potentially have a stronger impact  
656 on the upscaling of GPP with VOD than with SIF.

657 For the spatial extrapolation experiment, we further found that the off-  
658 set in the VOD-GPP relationship varies between grid cells, unlike for the  
659 SIF-GPP relationship for which the offset is a global value. The reason for  
660 this may be linked to the contribution of structural components to VOD.  
661 VOD contains information both on woody and leaf parts (Tian et al., 2017).  
662 For estimating total GPP, however, the relevant aboveground information



663 are mainly the leaves (Litton et al., 2007). Larger plant parts, which also  
664 contribute to the VOD signal, exhibit lower metabolic activity than leaves  
665 (Litton et al., 2007). Adding *mdnVOD* as input to GAM thus seems to en-  
666 sure that structural components within the grid cells are subtracted, thereby  
667 making the remainder more closely related to the leaves. When considering  
668 longer periods, the static *mdnVOD* should thus be replaced with a metric  
669 that varies over time in order to reflect changes in land cover.

670 The extrapolation experiments overall indicated that further input vari-  
671 ables may be needed to enhance the model’s extrapolation capability. In-  
672 cluding land cover information, which is commonly used in upscaling of in  
673 situ GPP (Chen et al., 2010; Jung et al., 2009; Tramontana et al., 2015,  
674 2016), may help reduce the impact of scale differences. A second variable,  
675 which may improve extrapolation, is the fraction of C3, C4 and CAM plants  
676 within a grid cell. These plants employ different strategies for carbon uptake  
677 and, hence, have a different efficiency in photosynthesis (e.g. Bonan, 2015).  
678 In turn, this may alter the VOD-GPP relationship.

#### 679 *6.4. Performance of GPP upscaling*

680 The VOD-based upscaling of GPP generally compared well with GPP  
681 from FLUXCOM and MODIS. Some areas exhibit inverse temporal dynamics  
682 with GPP. This, however, is not an issue of the model formulation but of  
683 the VOD observations itself. Microwave VOD observations can exhibit an  
684 inverse relationship to optical vegetation parameters in wet regions for passive

685 VOD and in dry regions for active VOD (Jones et al., 2011; Liu et al., 2011;  
686 Vreugdenhil et al., 2016b). Without explicitly accounting for this behavior,  
687 these patterns of negative correlations are propagated through to the VOD-  
688 based GPP estimates.

689       Considering annual GPP, we observed a closer agreement with GPP from  
690 FLUXCOM and MODIS for X-band VOD from AMSR2 than from AMSR-E.  
691 On the one hand, this finding may be linked to differences between the sensors  
692 themselves. Du et al. (2017) reported that small differences between the  
693 performance for AMSR-E and AMSR2 exist. In line with this, we observed  
694 lower RMSE for AMSR2 than for AMSR-E during cross validation. On  
695 the other hand, the differences between AMSR-E and AMSR2 could also  
696 be caused by the different analysis periods. Considering that the temporal  
697 coverage of FLUXNET stations varies for AMSR-E and for AMSR2, this  
698 likely has the same effect as seen for the uncertainty analysis, because stations  
699 used for upscaling AMSR-E were not necessarily present in the period for  
700 AMSR2, and vice versa. The reason for these differences still requires further  
701 investigation.

702       Apart from methodological differences between the VOD-based GPP es-  
703 timation and GPP from FLUXCOM or MODIS, further variations may arise  
704 from differences in the setup. FLUXCOM and MODIS GPP products both  
705 have a higher spatial resolution than VOD data, which potentially reduces the  
706 impact of scale differences. The FLUXNET data set used for the upscaling in  
707 FLUXCOM also differs in the data period and incorporates a larger number

708 of sites (Tramontana et al., 2016). As shown for the uncertainty analysis,  
709 the choice of FLUXNET stations has an impact on the VOD-based upscal-  
710 ing and, thus, likely contributes to observed differences between VOD-based  
711 GPP and FLUXCOM GPP. In addition, FLUXCOM and MODIS incorpo-  
712 rate ancillary information on land cover (Running et al., 1999; Tramontana  
713 et al., 2016), which was already discussed in Section 6.3 as possibility for  
714 model improvement.

#### 715 *6.5. Impact of model simplifications*

716 The framework neglects the temperature dependency of  $R_a$ , which is of-  
717 ten represented as an exponential increase of  $R_a$  with temperature (Wythers  
718 et al., 2013; Vanderwel et al., 2015; Tjoelker et al., 2001; Smith and Dukes,  
719 2013; Atkin et al., 2005; Atkin and Tjoelker, 2003). Not accounting for this  
720 effect thus may explain the observed overestimation of the VOD-based GPP  
721 estimates. The comparison of estimates from AMSR-E and AMSR2, how-  
722 ever, showed a closer agreement with FLUXCOM and MODIS for AMSR2  
723 than for AMSR-E even without including temperature in the model. This  
724 indicates that, in addition to the temperature dependency of  $R_a$ , other effects  
725 play an important role, which need to be considered for a more robust esti-  
726 mation of GPP based on VOD. These parameters likely include the choice of  
727 training data as demonstrated by the variability in mean annual GPP during  
728 the uncertainty analysis.

729 Another simplification is that our model assumes similar temporal dy-

730 namics of above- and belowground biomass, which allows expressing biomass  
731 as function of VOD. The ratio of above- and belowground growth, however,  
732 may vary between years in response to environmental stresses like droughts,  
733 as shown by Doughty et al. (2015) for forest plots in the Amazon basin.  
734 Depending on the strength of this effect, mismatches in above- and below-  
735 ground dynamics can potentially lead to differences between the VOD-based  
736 upscaling of GPP and GPP retrieved from optical data.

737 In general, differences and temporal shifts between GPP derived from  
738 microwave and optical data can point towards additional terms of carbon  
739 loss or storage that were not considered in the simplified model formulation.  
740 A study conducted by Würth et al. (2005) demonstrated for a semi-deciduous  
741 tropical forest how seasonal variations in the concentration of non-structural  
742 carbohydrates can support temporal shifts between carbon assimilation and  
743 vegetation growth. Therefore, differences between source- and sink-driven  
744 GPP can potentially give further insight into large-scale patterns of carbon  
745 partitioning or allocation.

## 746 **7. Conclusion**

747 We have proposed a model for estimating GPP globally based on single  
748 frequency microwave satellite VOD. The approach uses VOD as proxy for  
749 aboveground living biomass and describes the relationship between VOD and  
750 GPP through a differential equation, which connects VOD and its derivative.  
751 Using temporal changes in consecutive VOD observations ( $\Delta VOD$ ) as ap-

752 proximation for the derivative, we implemented the model using Generalized  
753 Additive Models. The proposed model is driven by VOD-based observations  
754 of vegetation biomass, and thus presents a sink-driven approach. Our results  
755 show that the model performs well in temporal extrapolation but requires  
756 further input variables like the grid cell median VOD for spatial extrapo-  
757 lation of the VOD-GPP relationship. We have attributed this behavior to  
758 varying proportions of structural components captured by the VOD signal,  
759 which contribute less to the GPP estimation and may be reduced by includ-  
760 ing median VOD. Our approach tends to overestimate GPP with respect  
761 to FLUXCOM and MODIS GPP, which is probably caused by the lack of  
762 temperature dependency of autotrophic respiration in the current model for-  
763 mulation. Overall, our results demonstrate the global applicability of the  
764 model and highlight the potential use of microwave VOD for providing GPP  
765 estimates that are complementary to source-driven approaches based on op-  
766 tical remote sensing data.

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Figure1  
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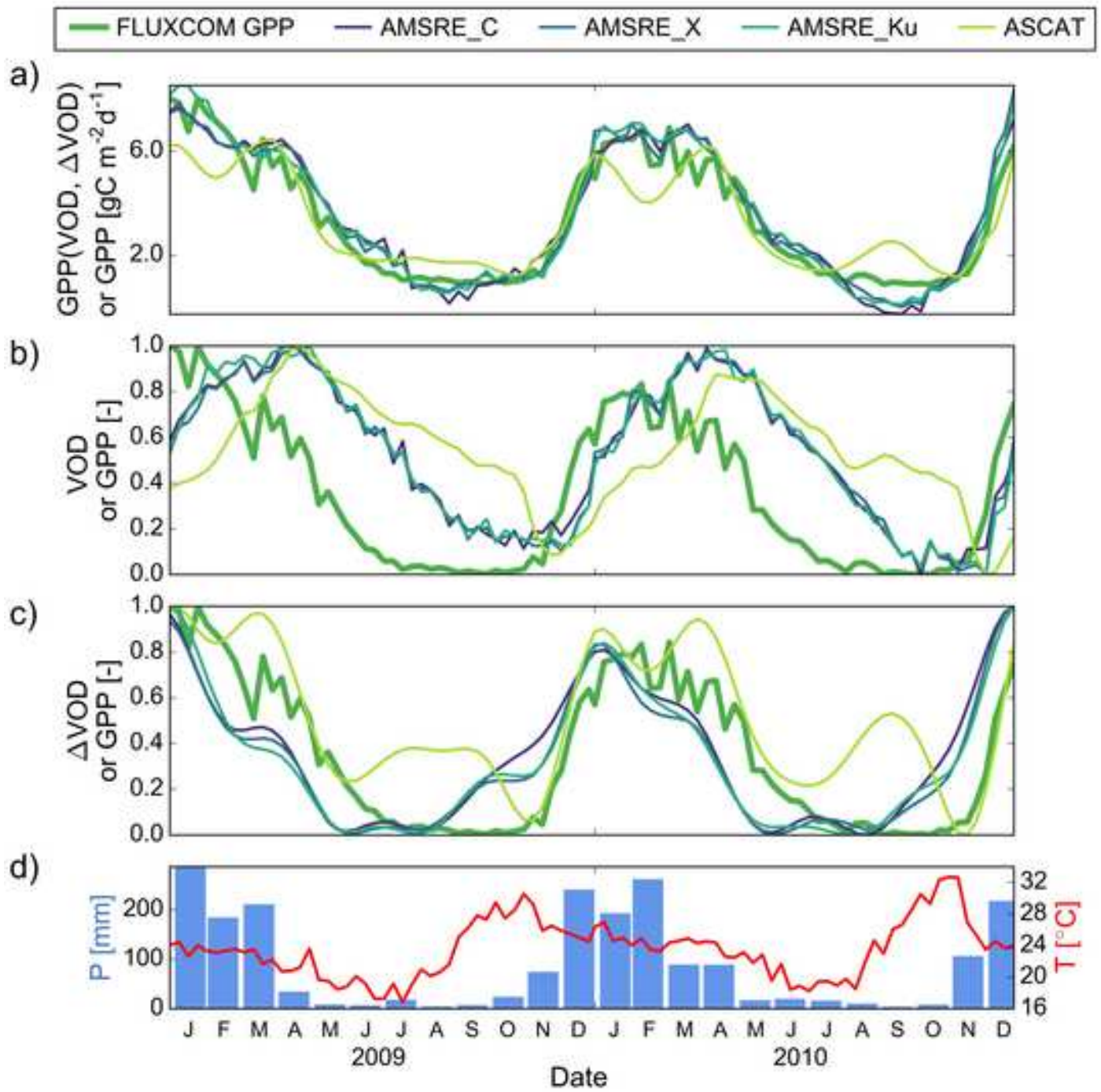


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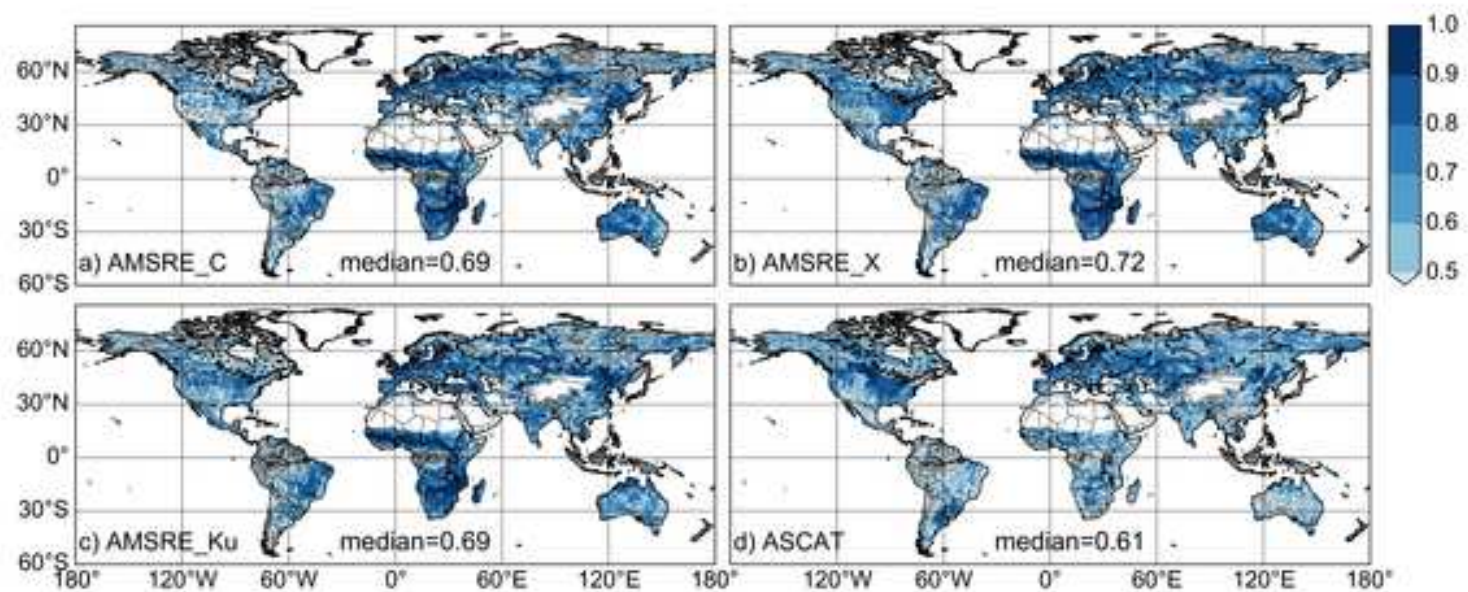


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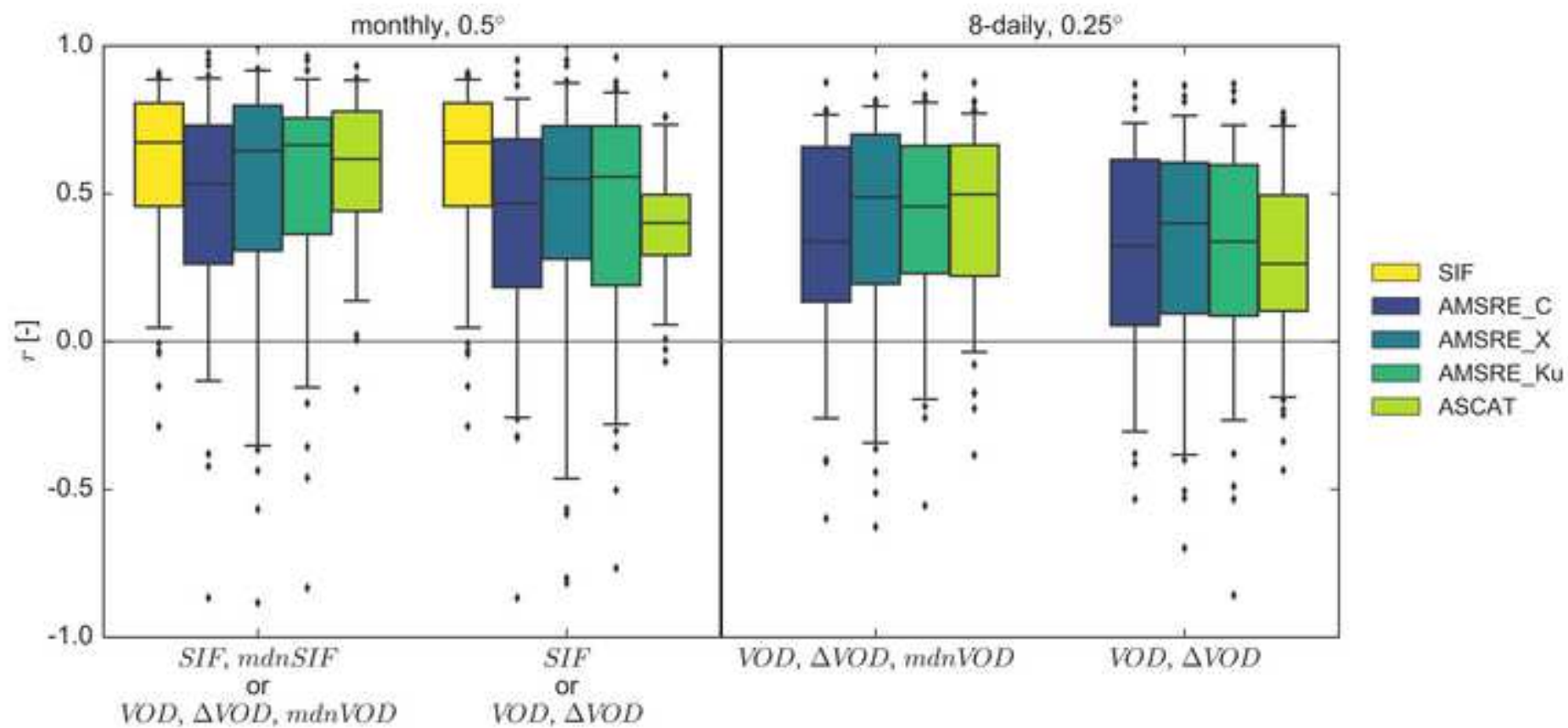


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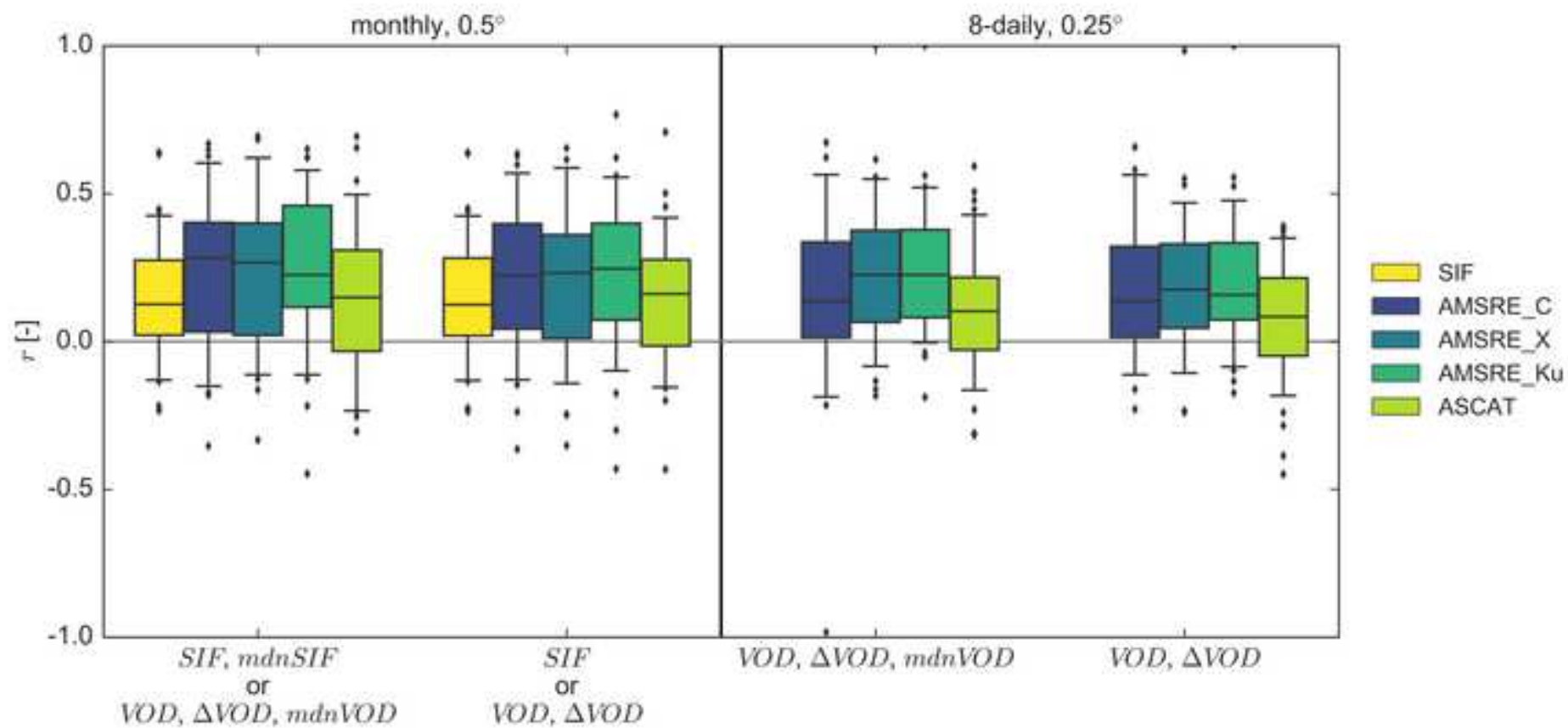


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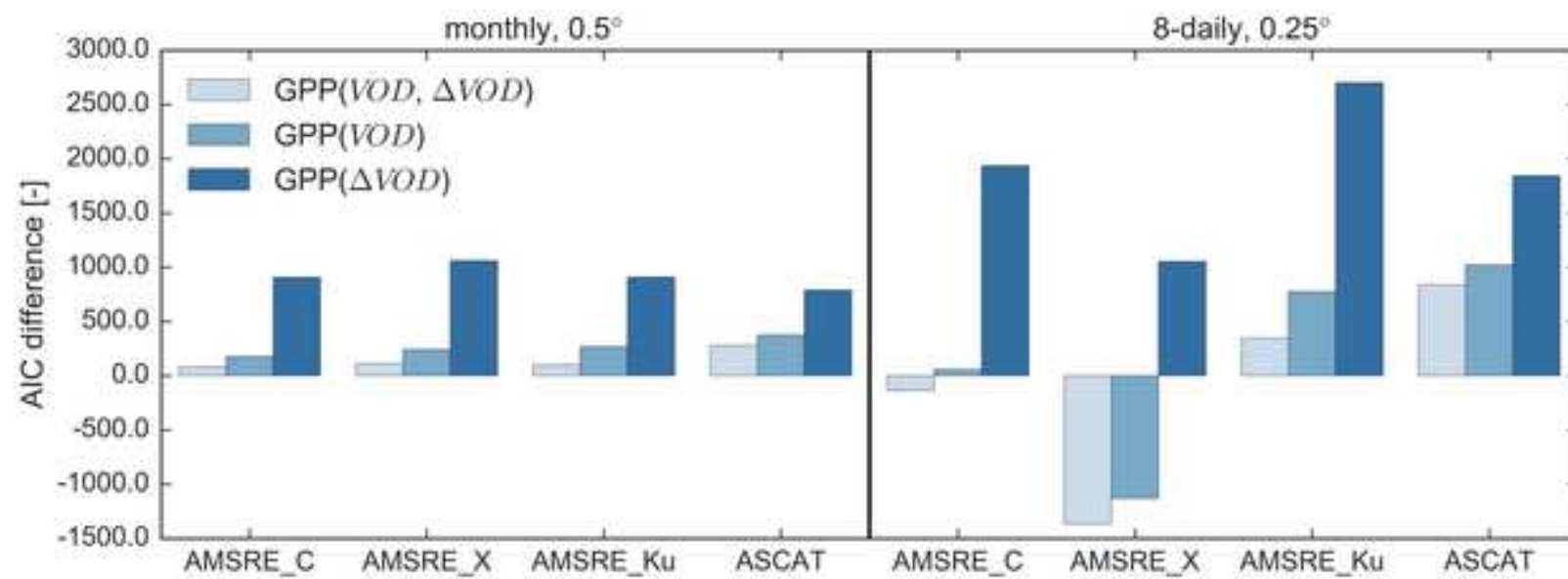


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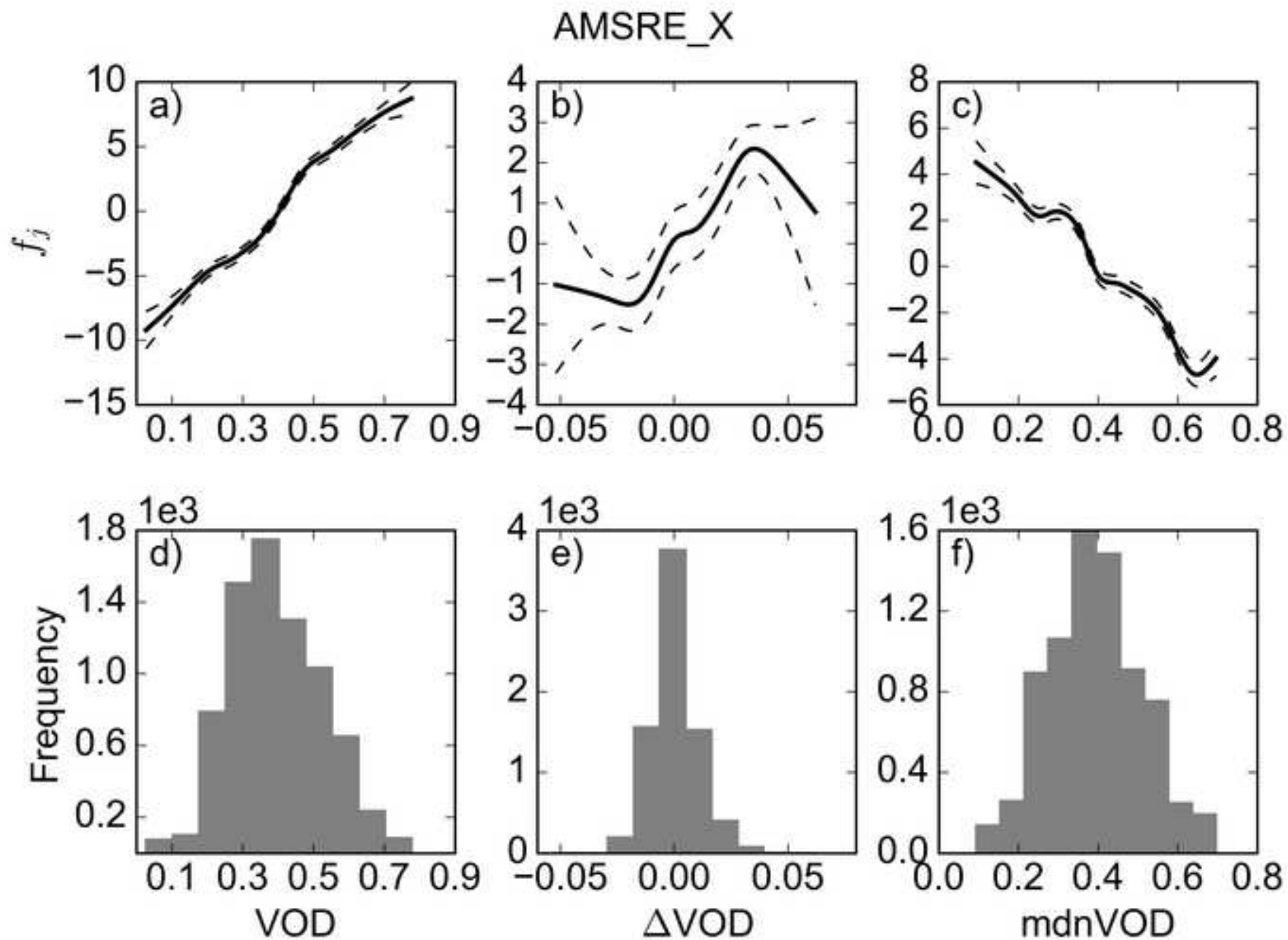


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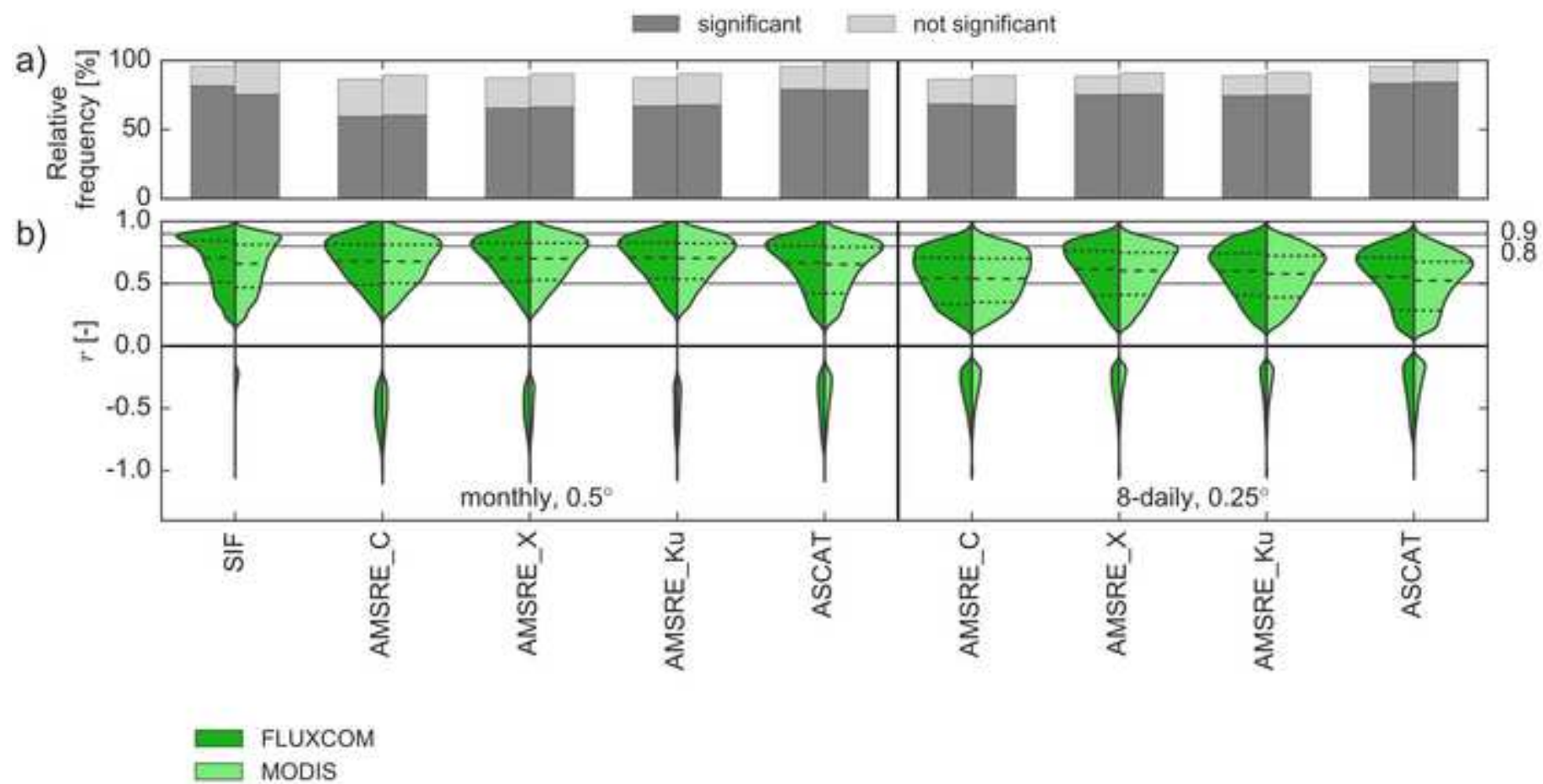




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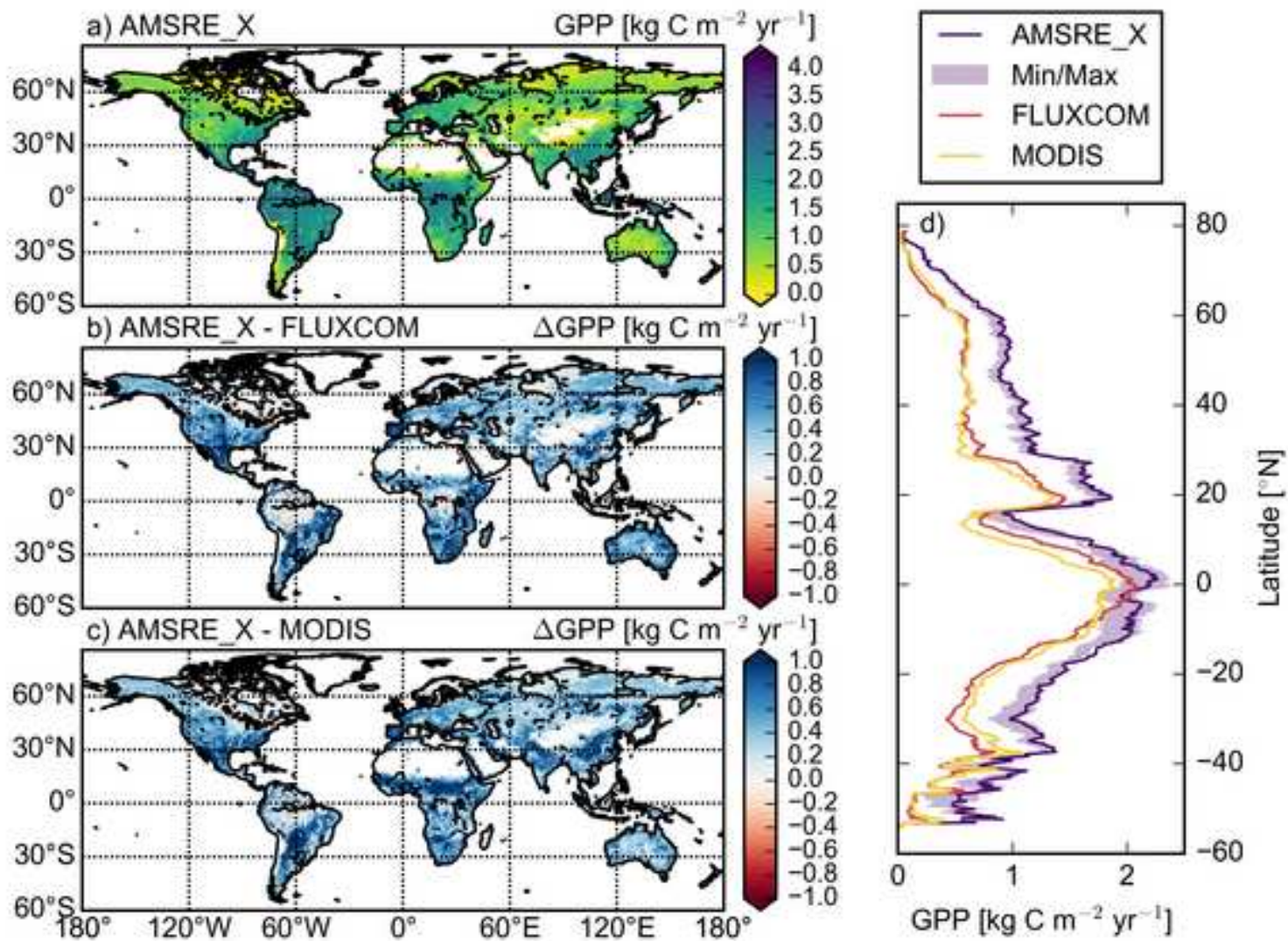


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