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10 **Title:** A novel approach to partitioning evapotranspiration into evaporation and transpiration  
11 in flooded ecosystems  
12  
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14  
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33

34 **Abstract:** Reliable partitioning of micrometeorologically measured evapotranspiration (ET)  
35 into evaporation (E) and transpiration (T) would greatly enhance our understanding of the  
36 water cycle and its response to climate change related shifts in local-to-regional climate  
37 conditions and rising global levels of vapor pressure deficit (VPD). While some methods on  
38 ET partitioning have been developed, their underlying assumptions make them difficult to  
39 apply more generally, especially in sites with large contributions of E. Here, we report a  
40 novel ET partitioning method using Artificial Neural Networks (ANN) in combination with a  
41 range of environmental input variables to predict daytime E from nighttime ET  
42 measurements. The study uses eddy covariance data from four restored wetlands in the  
43 Sacramento-San Joaquin Delta, California, USA, as well as leaf-level T data for validation.  
44 The four wetlands vary in their vegetation make-up and structure, representing a range of ET  
45 conditions. The ANNs were built with increasing complexity by adding the input variable  
46 that resulted in the next highest average value of model testing  $R^2$  across all sites. The order  
47 of variable inclusion (and importance) was: VPD > gap-filled sensible heat flux ( $H_{gf}$ ) > air  
48 temperature ( $T_{air}$ ) > friction velocity ( $u_*$ ) > other variables. The model using VPD,  $H_{gf}$ ,  $T_{air}$ ,  
49 and  $u_*$  showed the best performance during validation with independent data and had a mean  
50 testing  $R^2$  value of 0.853 (averaged across all sites, range from 0.728 to 0.910). In  
51 comparison to other methods, our ANN method generated T/ET partitioning results which  
52 were more consistent with  $CO_2$  exchange data especially for more heterogeneous sites with  
53 large E contributions. Our method improves the understanding of T/ET partitioning. While it  
54 may be particularly suited to flooded ecosystems, it can also improve T/ET partitioning in  
55 other systems, increasing our knowledge of the global water cycle and ecosystem  
56 functioning.

57

58 **Key-words:** artificial neural networks; eddy covariance; machine learning; latent energy;  
59 terrestrial water cycle; wetlands; vapor pressure deficit.

60 **1 Introduction**

61

62 Evapotranspiration (ET) is the combined water loss from terrestrial ecosystems via  
63 transpiration (T), i.e., water lost by plants during the process of carbon assimilation, and  
64 evaporation (E), i.e., water lost via direct evaporation of soil and surface water (including  
65 evaporation of intercepted precipitation; NB: There is some discussion in the community  
66 around the correct use of the terms evapotranspiration vs evaporation (Miralles et al, 2020);  
67 We have opted to follow the common use of the term evapotranspiration throughout this  
68 manuscript to describe the total biosphere-atmosphere water flux, including transpiration as  
69 well as direct evaporation from soil and surface waters). Through these processes, ET adds on  
70 the order of 65 to 75 thousand km<sup>3</sup> of water to the atmosphere every year (Oki & Kanae,  
71 2006; Trenberth, Fasullo, & Kiehl, 2009; Jung et al., 2018; Dorigo et al., 2021) and  
72 constitutes an important component of the terrestrial water cycle. Despite its importance to  
73 the global water cycle, ET is, however, currently poorly constrained in global land surface  
74 models (LSM), and although there is general consensus that ET will increase under climate  
75 change, the processes and trends are unclear, which creates large uncertainties in climate  
76 predictions (Brutsaert & Parlange, 1998; Zeng et al., 2018; Pascolini-Campbell et al., 2021).  
77 This partly occurs because E and T have different drivers and mechanisms.

78 Vapor pressure deficit (VPD) is recognized as one of the most important drivers to  
79 control water cycling by means of interacting with T and plant stomata (Novick et al., 2016;  
80 Yuan et al., 2019; Grossiord et al., 2020; López, Way, & Sadok, 2021). VPD levels are  
81 projected to limit ET in most biomes, with climate change increasing the importance of  
82 evaporative demands worldwide (Novick et al., 2016). Thus, the continuous rise in the global  
83 levels of atmospheric VPD is of major concern as it can have drastic effects on plant  
84 communities, mainly increasing T (Grossiord et al., 2020) and reducing plant productivity  
85 (Yuan et al., 2019; López, Way, & Sadok, 2021), impacting on water cycling. Previous work  
86 in several flooded ecosystems, however, identified air and water temperatures as strong  
87 drivers of nighttime ET, considered to be mainly E at these sites, with VPD playing a less  
88 important role (Eichelmann et al., 2018). Increasing global temperatures could, therefore,  
89 have significant implications for evaporative water loss from these systems. Consequently,  
90 improving our understanding of the relative contribution of E and T to ET will allow us to  
91 analyze the physiological responses of plant communities to climate change, as well as  
92 improve our ability to predict how the water cycle will evolve with climate change within and  
93 across ecosystems (Stoy et al., 2019).

94 Assessments of E and T fluxes at an ecosystem scale (i.e., 100 m to km) have been  
95 attempted using a variety of methods (Stoy et al., 2019). While some methods attempt to

96 determine E and T components by direct measurements (e.g., measurement of soil  
97 evaporation, sap-flux measurements for transpiration, and isotopic tracer approaches), these  
98 are often time and labor intensive and present significant challenges upscaling results to  
99 ecosystem level (Wilson et al., 2001). Micrometeorological methods, such as eddy  
100 covariance (EC), are well-established methods that assess biosphere-atmosphere fluxes of  
101 trace gases at the ecosystem scale (Baldocchi et al., 1988). With EC (see Fluxnet.org, 2021)  
102 continuous measurements of ecosystem trace gas fluxes such as water vapor can be made on  
103 time scales from individual half hours to years (Baldocchi, 2003). However, it can generally  
104 only provide direct measurements of the net biosphere-atmosphere flux above the plant  
105 canopy. In the case of water vapor fluxes, this includes the net flux of E and T combined. The  
106 ability to partition micrometeorologically measured ET fluxes into E and T components  
107 would greatly improve our understanding of the pathways by which ecosystems use water,  
108 including how E and T components change on different timescales and with changing  
109 climatic conditions, as well as the impact of site-specific characteristics like vegetation cover  
110 heterogeneity (Eichelmann et al., 2018).

111 While there are several well tested and established methods to partition net  
112 ecosystem CO<sub>2</sub> fluxes into its components of gross primary production and ecosystem  
113 respiration (Baldocchi, 2003; Reichstein et al., 2005; Desai et al., 2008), less work has been  
114 done on partitioning ET fluxes (Stoy et al., 2019). Stoy et al. (2019) provide a review of the  
115 most common methods for determining E and T fluxes at ecosystem level. Most methods  
116 proposed for partitioning micrometeorologically measured ET fluxes use the intrinsic  
117 relationship between CO<sub>2</sub> uptake and transpirational water loss, linked through stomatal  
118 exchange at the plant level, to estimate ecosystem T (e.g., Scanlon and Sahu, 2008; Zhou et  
119 al., 2016; Scott and Biederman, 2017; Nelson et al., 2018; Li et al., 2019). Scott and  
120 Biederman (2017) proposed a method to partition long-term ET measurements into E and T.  
121 Their method provides multi-year averages of partitioning on a weekly to yearly timescale.  
122 However, it requires datasets of multiple year lengths with high interannual consistency in  
123 seasonal ecosystem ET behavior. Furthermore, it is unclear if this method provides reliable  
124 results in systems that have a large contribution of E or large interannual variation in  
125 ecosystem water exchange behavior.

126 Similarly, the partitioning method proposed by Scanlon and Sahu (2008), Scanlon  
127 and Kustas (2010), and Skaggs et al. (2018), uses the correlation between the high frequency  
128 fluctuation of water vapor and CO<sub>2</sub> concentrations to determine the stomatal and non-  
129 stomatal mediated components of the net water and CO<sub>2</sub> fluxes. However, this method relies

130 on the knowledge of water use efficiency (WUE), which is the ratio of carbon uptake through  
131 photosynthesis to water loss through T, at the plant or leaf-level. Since information on WUE  
132 is not always readily available at the temporal scale required for this method, and because  
133 WUE can change over time with successional age and environmental factors like stomatal  
134 response to increasing atmospheric CO<sub>2</sub> concentration (van der Sleen et al., 2015), it restricts  
135 the wider use of this method. Another method based on the relationship between CO<sub>2</sub> uptake  
136 and T proposed by Zhou et al. (2016) to partition ET data from EC measurements works with  
137 the underlying assumption that there will be periods for which E is zero and T/ET approaches  
138 one. Similarly, the method proposed by Nelson et al. (2018) assumes that the ecosystem will  
139 be dominated by T for some time periods. While such methods are an advancement on T/ET  
140 partitioning, there is space for other new approaches particularly if they do not need  
141 specialized data or costly equipment to increase the wider use and applicability of such  
142 techniques.

143 Ecosystems with large contributions of E, where total ET is not always dominated  
144 by T and which have complex interrelationships between ecosystem productivity, E, and T,  
145 might violate some or all of the underlying assumptions necessary for partitioning methods  
146 based on the relationship between CO<sub>2</sub> uptake and water loss to work (Stoy et al., 2019). This  
147 is the case for wetlands, where the contribution of E-T is altered significantly by structural  
148 factors such as areas of open water, as well as environmental factors, for instance, diurnal  
149 fluctuations in air or water temperature and water table (Drexler et al., 2004; Goulden et al.,  
150 2007; Eichelmann et al., 2018). In addition, the before-mentioned methods only work when  
151 the ecosystem CO<sub>2</sub> flux is known in conjunction with ET. Although this is often the case for  
152 EC measurements, there are other micrometeorological methods that provide measurements  
153 of ET without measuring CO<sub>2</sub> fluxes. Consequently, a partitioning method that does not rely  
154 on knowledge of CO<sub>2</sub> flux and assumptions of carbon-water flux correlations would greatly  
155 enhance our ability to partition T/ET in a diversity of settings.

156 Methods applied to partition CO<sub>2</sub> fluxes usually use relationships of environmental  
157 drivers with the individual flux components determined from time periods where only one  
158 flux component is present and extrapolate these to the other periods (Reichstein et al., 2005;  
159 Desai et al., 2008). Many methods (e.g., Barr et al., 2004; Reichstein et al., 2005) use  
160 relationships between temperature and ecosystem respiration based on nighttime fluxes, when  
161 CO<sub>2</sub> uptake is zero, and extrapolate these to calculate daytime ecosystem respiration. The  
162 gross CO<sub>2</sub> uptake component is then determined as the difference between the net flux and  
163 the estimated daytime ecosystem respiration. While this method works well for carbon flux

partitioning, where the primary driver of ecosystem respiration is considered to be temperature, it can face limitations in the case of water fluxes where nighttime fluxes are often very small and the drivers of E and T are complex. However, it has been shown that nighttime T from plants is usually very small in many ecosystems (Caird et al., 2006; Dawson et al., 2007). Thus, for non-water limited systems with large contributions of E, such as wetlands, we can approximate nighttime water fluxes as exclusively E.

A newer approach used to partition net ecosystem carbon fluxes into the individual components of gross primary production and ecosystem respiration uses Artificial Neural Networks (ANN) (Papale & Valentini, 2003; Desai et al., 2008; Tramontana et al., 2020). ANNs and other machine learning approaches have also been successfully applied in the context of interpolating ecosystem biosphere-atmosphere exchange, including evapotranspiration fluxes, both spatially and temporally (Jung et al. 2010; Jung et al., 2011; Zhao et al., 2019; Kim et al., 2020; Tramontana et al., 2020; Irvin et al., 2021). Although the use of ANNs could also be directed at T/ET partitioning, the application of this technique has not been done yet and needs further exploration. Since machine learning methods can resolve complex, nonlinear relationships between environmental drivers and flux variables (Papale & Valentini, 2003; Tramontana et al., 2020), ANNs are a promising approach to partition T/ET in ecosystems where existing ET partitioning methods face limitations, such as wetlands and river deltas.

There has been a growing interest in restoring freshwater wetlands in regions where they historically existed, such as the Sacramento-San Joaquin River Delta, California, USA (hereafter, the Delta). While restoring freshwater wetlands can have many benefits, including those related to wildlife habitat, climate, and carbon sequestration, it can also lead to increased water loss through ET depending on the vegetation cover characteristics (Eichelmann et al., 2018). Moreover, given that changes in local and regional ET can affect cloud formation and precipitation distribution (Gerken et al., 2018), this may have a knock-on effect on the water cycle and on the climate feedback of wetlands (Hemes et al., 2018). In locations that experience spatial and temporal water shortages, such as California, increasing our knowledge of the local water cycle and understanding how ET is affected by external drivers is extremely important.

Here, we show that we can partition ET measurements above flooded wetlands in the Delta by predicting daytime E from nighttime ET measurements using ANNs in combination with environmental driver variables such as VPD, temperature, atmospheric turbulence, canopy greenness index, and others. The meso-network of diverse wetland EC

198 sites used in this study is ideal to test this new ET partitioning method as it provides a  
199 continuum of T/ET conditions across complex canopy architectures. We present the most  
200 promising models and discuss the application of ANN to partition T/ET measurements.  
201 While there is an emphasis on wetlands, we show evidence that our method may be applied  
202 to other ecosystems as well, increasing the knowledge of the water cycle and shedding light  
203 on plant-water productivity relationships at an ecosystem level.

204

## 205 **2 Methods**

206

### 207 **2.1 Site Description**

208

209 The Delta plays an essential role in the water supply of the state of California, USA.  
210 It supplies the majority of freshwater to large metropolises in Southern California and  
211 provides water for irrigation of crops in the Central Valley (Deverel & Rojstaczer, 1996).  
212 Historically, the peat soils were flooded with large areas of freshwater marsh, but the  
213 majority of the Delta land area is now actively drained and cultivated for agriculture. More  
214 recently, there has been growing interest in restoring freshwater wetlands to prevent further  
215 soil subsidence. In one of the approaches used, the restored wetlands in the Delta are flooded  
216 with a water table that is above ground level at all times (Hemes et al., 2019). The four  
217 restored wetlands in the Delta selected for this study represent a range of conditions with  
218 some sites dominated by open water areas and others covered in dense vegetation throughout  
219 (Eichelmann et al., 2018), representing varying amounts of T/ET ratios expected at the  
220 different sites.

221 We conducted EC measurements at four wetland sites in the Sacramento-San  
222 Joaquin river delta in Northern California: West Pond ( $38^{\circ} 6.44'N$ ,  $121^{\circ} 38.81'W$ , Ameriflux  
223 ID: US-TW1; Valach et al., 2021b), East End ( $38^{\circ} 6.17'N$ ,  $121^{\circ} 38.48'W$ , Ameriflux ID: US-  
224 TW4; Eichelmann et al., 2021), Mayberry Farms ( $38^{\circ} 2.99'N$ ,  $121^{\circ} 45.90'W$ , Ameriflux ID:  
225 US-MYB; Hatala-Matthes et al., 2021), and Sherman Island ( $38^{\circ} 2.21'N$   $121^{\circ} 45.28'W$ ,  
226 Ameriflux ID: US-Sne; Shortt et. al., 2021). All sites are part of the Ameriflux network and  
227 the EC data from these sites are available for download through the Ameriflux data sharing  
228 platform (<https://ameriflux.lbl.gov/>). The sites have been described in detail in other  
229 publications (Detto et al., 2010; Hatala et al., 2012; Knox et al., 2015; Eichelmann et al.,  
230 2018; Hemes et al., 2018, 2019) and their main characteristics will only be briefly  
231 summarized here. Overall the dataset used in this study covers 24 site-years of data with

232 individual sites spanning between 4 and 7 years of data coverage. All four wetlands are  
233 artificially constructed wetlands managed by the Department of Water Resources to reverse  
234 soil subsidence in the area. The water table is actively managed to be above ground level  
235 throughout the flooded portions of the wetlands at all sites.

236 The West Pond wetland is the oldest of the four wetlands, originally constructed in  
237 1998. It is the most homogeneous of the study sites, with a fairly even, but slightly sloping,  
238 ground surface and dense vegetation covering the whole wetland (97% vegetation cover  
239 within EC footprint in 2018, Valach et al., 2021a). The water table varies slightly throughout  
240 the wetland due to the sloping ground level but is generally between 20 and 40 cm above  
241 ground level. The Mayberry Farms wetland was constructed in 2010 and has a very  
242 heterogeneous footprint. With a heterogeneous bathymetry this wetland features small islands  
243 of vegetation and deeper channels and pools of open water (64% vegetation cover within EC  
244 footprint in 2018, Valach et al., 2021a). The water depth varies from 2 m above ground level  
245 to 2 cm above ground level in the flooded portions, with some dry areas. The East End  
246 wetland was constructed in 2013 and also features some areas of open water channels and  
247 pools. The vegetation at East End has filled in more evenly since its establishment and it has  
248 a greater vegetation cover than Mayberry Farms (96% vegetation cover within EC footprint  
249 in 2018, Valach et al., 2021a). The Sherman Island wetland is the newest wetland constructed  
250 in 2016. Similarly to Mayberry Farms, it features a very heterogeneous bathymetry and the  
251 footprint is dominated by large portions of open water. Vegetation has only taken hold in  
252 very few and small patches within the footprint of the EC measurements (45% vegetation  
253 cover within EC footprint in 2018, Valach et al., 2021a). While the individual make-up and  
254 proportions vary slightly between sites, the dominant vegetation species at all sites are tules  
255 (*Schoenoplectus acutus*) and cattails (*Typha* spp.) (O'Connell et al., 2015).

256

## 257 **2.2 Eddy Covariance Data**

258

259 We measured continuous fluxes of  $H_2O$ ,  $CO_2$  and sensible heat using the EC method  
260 at all sites (Baldocchi et al., 1988). A detailed description of the instrument set-up and  
261 calculation procedures can be found in previously published papers (Detto et al., 2010; Hatala  
262 et al., 2012; Knox et al., 2015; Eichelmann et al., 2018; Hemes et al., 2018, 2019) and will  
263 only be summarized here. At each site, the EC instrumentation consisted of a sonic  
264 anemometer (WindMaster 1590 or WindMaster Pro 1352, Gill Instruments Ltd, Lymington,  
265 Hampshire, England) and an open path trace gas analyzer for  $H_2O$  and  $CO_2$  concentrations

266 (LI-7500 or LI-7500A, LI-COR Inc., Lincoln, NE, USA). The instruments were mounted at a  
267 fixed height at least 1 m above the maximum height of the canopy.

268 High frequency (20 Hz) measurements of sonic temperature, three-dimensional wind  
269 speed, and trace gas concentrations were recorded on USB drives in the field through the  
270 analyzer interface (LI-7550, LI-COR Inc., Lincoln, NE, USA). The data were collected  
271 approximately every two weeks, with routine maintenance and servicing of the instruments  
272 taking place at the same time. The LI-7500 trace gas analyzers were calibrated approximately  
273 every three to six months in the laboratory. The performance of the EC set-up was also cross  
274 checked periodically at individual sites by the Ameriflux mobile EC reference system  
275 (Schmidt et al., 2012).

276 All data processing and filtering was performed offline. Thirty-minute average  
277 fluxes were calculated using custom software written in-house (MATLAB, MathWorks Inc.,  
278 R2015b, version 8.6.0) after basic de-spiking of high frequency data and filtering for  
279 instrument malfunctioning (Detto et al., 2010; Hatala et al., 2012; Knox et al., 2015;  
280 Eichelmann et al., 2018). A rotation into the mean wind was performed for each 30-minute  
281 averaging interval and the Webb-Pearman-Leuning correction for air density fluctuations for  
282 open path sensors was applied to the calculated fluxes (Webb et al., 1980). Fluxes were  
283 filtered for low friction velocity ( $u_*$ ), as well as based on stability and turbulence conditions  
284 (Foken & Wichura, 1996). Low friction velocity thresholds are based on the point where  
285 nighttime CO<sub>2</sub> fluxes become independent of  $u_*$  and are defined individually at each site. The  
286 thresholds can vary seasonally and usually range from 0.12 m s<sup>-1</sup> to 0.2 m s<sup>-1</sup>. Because of the  
287 narrow shape of the wetland, the West Pond wetland fluxes were also filtered by wind  
288 direction to ensure flux footprints originated from the ecosystem of interest.

289 Energy budget closure is often used as a quality indicator for EC data (Wilson et al.,  
290 2002). At the flooded wetland sites covered in this study the energy budget closure of daily  
291 totals was between 73% and 81%, which is slightly lower than typically found in dry  
292 ecosystems. H<sub>2</sub>O fluxes from the West Pond, Mayberry Farms, and East End wetland sites  
293 used in this study have been published and discussed in detail by Eichelmann et al. (2018),  
294 including a discussion of data quality, energy budget closure, and the difficulties estimating  
295 energy storage components in the flooded wetlands. Because of the importance of storage  
296 terms in the context of these sites, energy fluxes measured by the EC method have not been  
297 adjusted for incomplete energy budget closure (Eichelmann et al., 2018). In this study,  
298 positive fluxes indicate a gain to the atmosphere and negative fluxes indicate a loss from the

299 atmosphere. All analyzes and data processing described in this study were performed using  
300 MATLAB (MathWorks Inc., R2018a, version 9.4.0).

301

### 302 **2.3 Auxiliary Data**

303

304 Meteorological and environmental data were also measured continuously in addition  
305 to EC data at all sites. The following auxiliary measurements were available at all wetland  
306 sites: Air temperature ( $T_{air}$ ); water temperature at 3 to 6 different water depths ( $T_{water}$ , depths  
307 vary between site due to differences in water tables); soil temperature at 6 different depths  
308 ( $T_{soil}$ ); relative humidity (RH); atmospheric pressure; incoming and outgoing shortwave  
309 radiation; incoming and outgoing longwave radiation; net radiation; incoming and outgoing  
310 photosynthetically active radiation; water table depth; water conductivity; and vegetation  
311 greenness index from camera data. Moreover, the West Pond and East End wetland sites were  
312 equipped with a rain gauge to measure precipitation and the East End wetland site was  
313 equipped to measure ground heat flux (G).

314 Data were recorded as half hour averages (or totals in the case of precipitation) with  
315 individual sampling frequency varying between 1 and 15 minutes depending on the sensor.  
316 Specifically of interest for this study are measurements of vapor pressure deficit (VPD),  
317 water table depth (WT), air temperature ( $T_{air}$ ), vegetation greenness index (green chromatic  
318 coordinate; GCC), and net radiation (Rnet). VPD was calculated from relative humidity  
319 measurements in combination with air temperature data, both measured with aspirated and  
320 wind-shielded humidity and temperature probes (HMP-60, Vaisala Inc., Helsinki, Finland).  
321 Net radiation was measured using either a net radiometer (NR-LITE Radiometer, Hukseflux,  
322 Delft, the Netherlands; at Mayberry Farms) or a four-component net radiometer (NR01 Net  
323 Radiometer, Hukseflux, Delft, the Netherlands; at West Pond, East End, and Sherman  
324 Island).

325

### 326 **2.4 Artificial Neural Network Partitioning Routine**

327

328 Artificial Neural Networks have been applied for gap-filling and partitioning EC  
329 fluxes in the past (Papale & Valentini, 2003; Oikawa et al., 2017; Tramontana et al., 2020).  
330 Specifically, for  $\text{CO}_2$  fluxes, ANNs have shown to perform well when used to gap-fill  
331 missing data (Moffat et al., 2007) and partitioning net  $\text{CO}_2$  fluxes into the component fluxes  
332 of gross primary production (GPP) and ecosystem respiration ( $R_{eco}$ ) (Desai et al., 2008;

333 Oikawa et al., 2017; Tramontana et al., 2020). Following a similar approach to partitioning  
334 CO<sub>2</sub> data, we assumed that nighttime ET data is dominated by E at these flooded sites:

335

336  $ET = T + E$  (1)

337  $T_{night} \cong 0$  (2)

338  $ET_{night} = E$  (3)

339

340 In this study, daytime and nighttime are distinguished by the local solar zenith angle  
341 (ze) with nighttime being defined as ze >= 90°. We conducted several leaf-level chamber  
342 measurements using a LI-6400 Portable Photosynthesis System (LI-COR Inc., Lincoln, NE,  
343 USA) throughout the growing season of 2017 to confirm that nighttime and dark T flux is  
344 indeed negligible at these sites. The available nighttime E data is used in combination with  
345 environmental input variables to train the ANN routine to predict daytime E. Daytime T was  
346 then calculated as the difference between total ET and E:

347

348  $T_{day} = ET_{measured} - E_{predicted}$  (4)

349

350 Before ET partitioning was performed all flux data were gap-filled using ANN  
351 routines described in previous studies (Knox et al., 2015, 2016; Oikawa et al., 2017,  
352 Eichelmann et al., 2018).

353

#### 354 2.4.1 Artificial Neural Network Routine Set-up

355

356 To partition ET data using ANNs in this study, we followed a similar set-up and  
357 architecture as described for gap-filling and partitioning CO<sub>2</sub> data in previous studies  
358 (Balocchi & Sturtevant, 2015; Knox et al., 2015, 2016; Oikawa et al., 2017). We applied  
359 feedforward networks specialized for function fitting using symmetric sigmoid transfer  
360 functions in all layers except the final layer which uses a linear transfer function. The  
361 networks are trained using the Levenberg-Marquardt optimization algorithm. For each site,  
362 the entire available (multi-year) explanatory dataset was split into 20 data clusters using the  
363 k-means clustering algorithm. The data used for training, testing, and validation of the ANNs  
364 was proportionally sampled from these clusters with one third of the available data used for  
365 training, testing, and validation each. This procedure avoids a sampling bias towards periods  
366 when more data are available, such as a specific time of the year or time of the day.

367 Proportional data sampling from the k-means clusters into training, testing, and validation  
368 data was repeated 20 times. For each of the 20 re-sampled training, testing, and validation  
369 datasets several ANN architectures were tested starting with one hidden layer and the same  
370 number of nodes as the number of explanatory input variables ( $n_{inputvar}$ ). Each architecture  
371 was initialized 10 times with random starting weights and the initialization with the lowest  
372 mean sampling error was used. The complexity of the ANN architecture was increased first  
373 by increasing the number of nodes to 1.5 times  $n_{inputvar}$  and then by increasing the number of  
374 hidden layers until a further increase in complexity results in less than 5% reduction of the  
375 mean standard error. For our datasets, this commonly resulted in the use of an architecture  
376 with two hidden layers, the first one with  $n_{inputvar}$  nodes, the second one with  $0.5*n_{inputvar}$   
377 nodes, although for some sites and input variable combinations architectures with only one  
378 hidden layer produced better results. The ‘validation’ step within the ANN procedure  
379 described above is performed on nighttime data only and is therefore distinctly different from  
380 the validation with flooding and leaf level data described below. Throughout the remainder of  
381 the manuscript when we use the term ‘validation’ we refer to the independent flooding and  
382 leaf level data validation. The ANN internal validation routine based on nighttime data is  
383 referred to as ‘testing’. An overview of the ANN training, testing, and validation process is  
384 presented in the flowchart in Fig. S1.

385

#### 386 **2.4.2 Selection of Explanatory Variables**

387

388 A number of different explanatory environmental input variables were tested  
389 individually and in combination. Based on the general understanding of the drivers of E  
390 fluxes in terrestrial and aquatic ecosystems we tested the following input parameters:  
391 Meteorological and environmental variables: VPD, Rnet, GCC, WT,  $T_{air}$ ; Flux variables:  
392 friction velocity ( $u_*$ ), gap-filled sensible heat flux ( $H_{gf}$ ), gap-filled  $CO_2$  flux ( $wc_{gf}$ ), and  
393 ecosystem respiration ( $er_{Reichstein}$ ) partitioned using the temperature dependency method  
394 proposed by Reichstein et al. (2005). In addition, we used a running decimal timestamp  
395 (`datetime`) as input variable in all our ANN runs. VPD,  $u_*$ , and  $T_{air}$  describe the atmospheric  
396 demand driving E. Rnet and  $H_{gf}$  are connected to ET (or latent energy) through the energy  
397 balance equation. GCC,  $wc_{gf}$ , and  $er_{Reichstein}$  are directly or indirectly related to plant  
398 physiological responses that can impact ET components. Finally, WT is related to the water  
399 budget of the ecosystem. Given the strong correlation of water temperature ( $T_{water}$ ) with  
400 nighttime ET documented at these sites in a previous study (Eichelmann et al., 2018) we

401 would also expect  $T_{water}$  to perform well as an environmental input variable. Unfortunately,  
402 we were unable to include  $T_{water}$  as an input variable in this study since we did not have  
403 consistent  $T_{water}$  measurements across time for any of the four sites.

404 We ran the ANN routine for each of these parameters individually and recorded the  
405  $R^2$  value, slope, and RSME of the linear regression of the nighttime EC data initially set aside  
406 for testing within the ANN routine versus the predictions. This  $R^2$  value is called ‘testing  $R^2$ ’  
407 throughout this manuscript and is based only on nighttime data. Starting with the input  
408 parameter with the highest testing  $R^2$ , we ran the ANN routine with increasing numbers of  
409 input variables, each time adding on the variable with the next highest testing  $R^2$  value. We  
410 continued this process until a further increase in input variables resulted in less than 1%  
411 increase in the testing  $R^2$  value. We averaged the testing  $R^2$  values across the four sites and  
412 used this value to estimate increases in the performance of the ANNs. While this average  
413 testing  $R^2$  does not have any statistical relevance, it gave us a good indicator on how well the  
414 models performed across all sites studied.

415

## 416 **2.5 Validation of Results**

417

418 One of the main issues facing validation of ET partitioning methods is often the lack  
419 of independent E or T data to validate against (Stoy et al., 2019). Taking independent  
420 measurements of ecosystem E or T is challenging and one of the main reasons why  
421 partitioning approaches for EC measurements of ET are much sought after. Since we do not  
422 have independent measurements of ecosystem level E or T available at our sites, we reverted  
423 to validating our partitioning data by a conditional sampling approach, selecting EC  
424 measurement data from certain time periods when E and T can be known or closely  
425 approximated to compare with the ANN predicted E or T. One of these time periods is the  
426 initial time right after flooding of the wetland (referred to as flooding data), when vegetation  
427 had not yet established within the footprint of our instruments. During this time, it can be  
428 assumed that the entire  $H_2O$  flux coming off the surface is from E, with negligible T.

429 Since we trained our ANN routines only on nighttime data, we were able to use the  
430 daytime data during the initial flooding period as an independent validation dataset for E.  
431 Apart from the initial flooding period, T can also be assumed to be small to negligible during  
432 the senescent winter months. However, since the plants are not harvested or otherwise  
433 removed and the climate in this region is fairly mild, some do stay green throughout the  
434 winter and may continue to be photosynthetically active. Additionally, vegetation on dry

435 areas such as levees usually starts to green up during the winter months in this region. Both of  
436 these would be contributing to a small T flux from the ecosystem. Moreover, ET fluxes  
437 during the winter period are generally lower and subject to larger errors due to more  
438 challenging turbulence conditions during this time. Such conditions result in large relative  
439 error in flux measurements during this period limiting the insights gained from the validation  
440 during the senescent winter period. Nonetheless, we included validation of E predicted from  
441 our ANN method against E measured during winter times to further test the performance of  
442 our method. Testing our ANN method against daytime data is particularly important as some  
443 of the drivers of E can exhibit strong diurnal patterns (e.g. H<sub>gf</sub>) and interdependencies  
444 between energy fluxes and environmental conditions (e.g. evaporation, transpiration, and  
445 canopy VPD) can change between day and night. While ANNs have been shown to provide  
446 good performance in predicting non-linear responses of biological data and extrapolating  
447 outside of the training variable space (Papale & Valentini, 2003), by using nighttime data  
448 only for training the ANNs we may not correctly capture the daytime response of E to the  
449 driver variables or changes in interdependent relationships. This would be highlighted  
450 through poor performance in the winter and flooding data validations. We compared the  
451 variable space covered by our nighttime training dataset with the variable space covered by  
452 the daytime prediction dataset and the flooding validation dataset (Fig. S2). While the  
453 daytime distributions show proportionally more values in the high end of the distributions, for  
454 most variables there is a reasonably good representation of higher values within the training  
455 and validation datasets. In addition, the proportional sampling from environmental clusters  
456 for our training dataset ensures all environmental conditions are represented equally during  
457 training.

458 In addition to the validation during periods when T was zero, we also conducted a  
459 number of leaf-level T measurements in the summer of 2017 at the East End wetland using a  
460 LI-6400 portable photosynthesis system (LI-COR Inc., Lincoln, NE, USA) with a clear  
461 conifer chamber (part number 6400-05) encasing sections of the leafs or culms. Six  
462 individual leaf-level measurement points (three for each of the dominant plant species) taken  
463 during the same half hour period were pooled to allow comparison with the half hourly EC  
464 data. These measurements provided us with an estimate of T per unit of sunlit leaf area and  
465 may potentially be converted to the ecosystem scale if the ecosystem leaf area index and the  
466 leaf angle distribution are known. Efforts have been made to estimate the leaf area index in a  
467 number of the wetlands in the study region, however, due to the high heterogeneity and litter  
468 accumulation in these systems there is a high level of uncertainty associated with the

469 measured leaf area indexes (Dronova & Taddeo, 2016). Additionally, the leaf angle  
470 distribution is unknown in these systems and can only be approximated, which is an intrinsic  
471 limitation of this technique.

472 Taking all these uncertainties into account, ecosystem T scaled up from leaf-level  
473 measurements is associated with very large error intervals and cannot serve as a reasonable  
474 constraint on the absolute values of our ANN partitioned T fluxes. However, since the scaling  
475 factors to convert leaf-level values to ecosystem level are constant multipliers, we should still  
476 be seeing a linear relationship between the leaf-level flux and the partitioned ecosystem level  
477 T if our partitioning algorithm predicts the correct T behavior across a range of  
478 environmental conditions. While we may not be able to compare the absolute T values, we  
479 can compare the response cycle of ANN predicted T with the field measurements to validate  
480 that we are predicting the right behavior.

481

## 482 **2.6 Comparison with Other T/ET Partitioning Approaches**

483

484 Direct comparisons with the Scott and Biederman's (2017) method were carried out  
485 in order to evaluate the performance of our own models against their approach. For these  
486 comparisons, we used the model (F11, see Results below) that achieved the best  $R^2$  value  
487 against the validation with leaf-level/flooding data. The Scott and Biederman (2017) method  
488 uses data from multi-year monthly ET and gross ecosystem productivity ( $GEP = -GPP$ ;  
489 determined from EC data using ANN based partitioning). At each site, regressions are  
490 calculated between all available monthly ET and GEP values measured for a specific month  
491 (e.g., July) across years (see Fig. 4 for illustration). Regressions are extrapolated to zero GEP  
492 to estimate the long-term average E for the specific month of interest. While Scott and  
493 Biederman (2017) forced all monthly regressions between ET and GEP to the same slope, we  
494 used different slopes for each regression. This was done to ensure the best fit since our  
495 datasets did not show the same uniform behavior across months. The Scott and Biederman  
496 (2017) method only provides average monthly E and T values across the entire dataset, not  
497 for individual years. Indirect comparisons with other methodologies mentioned above are  
498 also discussed.

499

## 500 **3 Results**

501

### 502 **3.1 Artificial Neural Network Architecture Performances**

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503

504 Alongside the basic timestamp (datetime), VPD and  $T_{air}$  were the meteorological  
505 variables that best explained our data when only looking at the nighttime testing data, with  
506 average testing  $R^2$  values across all sites of 0.648 (model F26) and 0.565 (model F22),  
507 respectively (Table 1 and Supplementary Table 1). The flux related variables that showed the  
508 highest average testing  $R^2$  values and added most information to the models were  $H_{gf}$   
509 (testing  $R^2$  of 0.620, model F28) and  $u_*$  (testing  $R^2$  of 0.531, model F27). To increase the  
510 ANNs complexity we, therefore, followed the variables order of  $VPD > H_{gf} > T_{air} > u_*$ ,  
511 adding each of them into the models sequentially. VPD was the variable that contributed the  
512 most to increase the testing  $R^2$  values of the ANNs, with an average increase of 24% across  
513 all sites and a maximum of 36% for West Pond, when models F21 and F26 were compared  
514 (Table 1). The incorporation of  $H_{gf}$  was responsible for an average increase of 10% in  
515 testing  $R^2$ , when comparing the ANNs F26 and F33 (Table 1).  $T_{air}$  only increased the ANNs  
516 testing  $R^2$  by 1% (i.e., when comparing models F33 and F34), however, when we added  $u_*$ ,  
517 the average testing  $R^2$  value increased across all sites by 9%, when comparing models F34  
518 and F11 (Table 1). Thus, building the ANN F11 using datetime, VPD,  $H_{gf}$ ,  $T_{air}$ , and  $u_*$ , the  
519 average testing  $R^2$  value across all sites reached 0.853, with a minimum of 0.728 (West Pond)  
520 and a maximum of 0.910 (Sherman Island; Supplementary Table 1).

521 Of all the 36 ANNs tested, the highest average testing  $R^2$  (0.891) was reached when  
522 all the explanatory variables (i.e., datetime,  $H_{gf}$ ,  $u_*$ ,  $wc_{gf}$ ,  $er_{Reichstein}$ , VPD,  $T_{air}$ , GCC,  
523  $R_{net}$  and WT) were put into the model F36 (Table 1 and Supplementary Table 1).  
524 Consequently, on average, all the other variables analyzed (i.e.,  $wc_{gf}$ ,  $er_{Reichstein}$ , GCC,  
525  $R_{net}$  and WT) accounted for less than 4% of the testing  $R^2$  value across all the four sites  
526 (when comparing models F36 and F11; Table 1). The top five ANNs (F36 > F14 > F20 > F35  
527 > F11) that performed better than 0.85 all have datetime, VPD,  $H_{gf}$ ,  $T_{air}$ , and  $u_*$  as their  
528 explanatory variables and all the 11 ANNs that scored an average testing  $R^2$  higher than 0.80  
529 have both VPD and  $u_*$  in their models (Table 1 and Supplementary Table 1). Fifteen ANNs  
530 showed an average testing  $R^2$  higher than 0.70 and the lowest average testing  $R^2$  among these  
531 (0.730) was presented by the ANN F2, constructed using only datetime,  $T_{air}$ , and  $u_*$   
532 (Supplementary Table 1). Unsurprisingly, the lowest average testing  $R^2$  (0.410) of all the 36  
533 ANNs analyzed was given by the ANN built using datetime alone (F21). The slope and  
534 RSME values (Table 1 and Supplementary Table 2) of the different ANNs followed quite  
535 closely the pattern described for the increase in testing  $R^2$  values.

536

537 **3.2 Validation of Artificial Neural Networks**

538

539 **3.2.1 Flooding Validation**

540

541 To evaluate the performance of our ANN partitioning method, we compared the  
542 model predicted E with EC measurement data from conditionally sampled post-flooding  
543 periods, during which we assume T to be negligible (Table 2). The ANN F11 showed the  
544 highest validation  $R^2$  values for East End (0.81), Mayberry Farms (0.69), and Sherman Island  
545 (0.82). These values surpassed those from the model F36 (most complex), which reached  
546 0.51, 0.56, and 0.53, for East End, Mayberry Farms, and Sherman Island, respectively. The  
547 slope values overall follow very similar patterns to the  $R^2$  values. With regards to the RSME  
548 values, models F21 and F15 have lower RSME values than model F11 for most of the sites.  
549 However, the extremely low  $R^2$  and slope values for model F21 and F15 highlight that these  
550 relationships are poorly constrained and, therefore, model performance evaluation should not  
551 be based on RSME alone (Table 2). Nevertheless, the slope and RSME values should be used  
552 as secondary selection criteria to ensure predictions are not offset by a constant factor, which  
553 would not be visible by evaluating  $R^2$  values alone. Figure 1 shows the validation comparison  
554 between F11 and F36 for the three sites.

555

556 **3.3.2 Winter Time Validation**

557

558 Judging by the observed  $R^2$  values, the validation using daytime data from senescent  
559 periods during the winter time (December to February, Table 3) performed quite poorly in  
560 comparison to the validation performed with data during the initial flooding periods (Table  
561 2). Nevertheless, the winter period validation overall did confirm the same trends and  
562 observations as the flooding validation. At Mayberry Farms and Sherman Island ANN F11  
563 again had the highest  $R^2$  values (0.56 and 0.70, respectively). However, at East End and West  
564 Pond the model F36, which included all input variables, performed best with  $R^2$  values of  
565 0.45 and 0.36, respectively. Figure 2 shows the validation comparison between F11 and F36  
566 for the four sites using winter data.

567

568 **3.3.2 Validation on Diurnal Measurements of Leaf-Level Data for East End**

569

570 To evaluate the performance of our method further, we compared the model  
571 predicted T with independent leaf-level data collected during a field campaign in summer  
572 2017 at the East End wetland. The leaf-level data showed high variability across individual  
573 measurements (Fig. 3). F11 again showed a high  $R^2$  (0.986, Table 4). Other models (F15,  
574 F33) also performed quite well in the leaf-level validation, in contrast to their performance  
575 for the validation during flooding or senescent periods. The most complex ANN (F36) had a  
576 lower  $R^2$  value (0.92) for the leaf-level validation. In general, adding too many variables did  
577 not lead to enhancement of validation values, but it is to be noted that all models showed a  
578 high level of agreement with the leaf-level data (Table 4). Figure 3 shows both F11 and F36  
579 validations against leaf-level data.

580  
581

### 582 **3.3 Artificial Neural Networks Performance Across the Wetland Sites**

583

584 To look for model consistency across diverse canopy architecture and successional  
585 stages, we compared ANN testing  $R^2$  values between the four sites. Among the four sites,  
586 East End and Sherman Island were the only sites that had ANNs with testing  $R^2$  values larger  
587 than 0.90 for the EC testing data set aside during the ANN routine (Supplementary Table 1).  
588 At Sherman Island, East End, and Mayberry Farms 22, 20, and 19 ANN models reached  
589 testing  $R^2$  values above 0.70, respectively, whereas at West Pond only 11 models reached  
590 testing  $R^2$  values above 0.7 (Supplementary Table 1). In comparison with the other three  
591 studied sites, West Pond showed testing  $R^2$  values in the order of 9-18% smaller when  
592 analyzing the top five ANNs with average testing  $R^2$  larger than 0.85 (Supplementary Table  
593 1). Considering all 36 ANNs, differences in testing  $R^2$  between the same ANN for different  
594 sites reached a maximum of 46%, when comparing model F6 at West Pond with Sherman  
595 Island (Supplementary Table 1).

596

### 597 **3.4 Comparisons with Other Partitioning Approaches**

598

599 To compare our ANN method with existing T/ET partitioning methods, we applied  
600 the Scott and Biederman (2017) long-term flux data partitioning method at all four sites. As  
601 expected, the Scott and Biederman (2017) method worked better for datasets with  $> 6$  years  
602 (Fig. 4; Mayberry Farms, West Pond, and East End). Sherman Island, the shortest dataset

603 with four years of data collection, performed poorly, showing negative correlations of ET vs  
604 GEP for the months of June to September (Fig. 4 d). Average monthly T fluxes from the  
605 Scott and Biederman (2017) method for Mayberry Farms and Sherman Island (Fig. 5a and d)  
606 both showed increases in T at the end of the growing season (i.e., October) out of line with  
607 the observed GEP patterns. Conversely, West Pond and East End (Fig. 5b and c) showed a T  
608 pattern parallel to GEP with the growing season.

609 While the T values from our ANN approach showed a similar behavior as GEP  
610 during the growing season, as would be expected, the T values from the Scott and Biederman  
611 (2017) method did deviate somewhat from the GEP pattern for all sites (Fig. 5). The best  
612 ANN (F11) also produced more reasonable T numbers for Sherman Island compared to the  
613 Scott and Bierderman (2017) method. In addition, the E values retrieved in our analysis for  
614 all sites were also more stable and did not fluctuate as much across months compared to the E  
615 values from the Scott and Biederman (2017) method (Fig. 5). While the Scott and Biederman  
616 (2017) method is not intended to produce reliable results for T/ET partitioning during winter  
617 months when GEP is small, it did show very good agreement of produced E and T values  
618 when compared to our ANN based values from October to February for all sites.

619

### 620 **3.5 Resulting Evaporation and Transpiration Estimates**

621

622 Figure 6 shows the annual (2013-2019) ANN based T/ET partitioning  
623 intercomparison for all sites using ANN F11. Only years with a full year of data are used.  
624 While ET stayed fairly consistent between 850-1250 mm for all sites and years (Fig. 6a),  
625 GEP showed more fluctuations between the different sites, as well as interannually within  
626 each site (Fig. 6b). Looking at the predicted partitioning of E and T (Fig. 6c, d), Sherman  
627 Island showed the highest values of E (approximately 1100 mm) for the three years of  
628 measurements available at this site, while West Pond had the lowest E values across all years  
629 and sites (200 to 300 mm). Although values at East End were always higher compared to  
630 Mayberry Farms for all years with measurements from both sites, decreasing pattern can be  
631 observed for E at both sites, ranging from high values of 831 mm at Mayberry Farms in 2013  
632 and 1119 mm at East End in 2014 down to low values of 449 mm at Mayberry and 630 mm  
633 at East End in 2019. Transpiration showed opposite trends compared to E, with West Pond  
634 having the highest values (between 700-800 mm in most years), followed by Mayberry Farms  
635 with T values between 300-500 mm. The T pattern predicted at Mayberry Farms follows a  
636 similar pattern as the GEP measurements, most notably is the significant reduction in GEP in

637 2016 which was caused by saltwater intrusion at the site (Eichelmann et al., 2018,  
638 Chamberlain et al., 2020). This was mirrored in a reduction of T values in 2016, however, E  
639 was not affected. Sherman Island and East End showed T values below 300 mm for all years,  
640 considerably lower than the other two sites. In the first full year of measurements (2014), T at  
641 East End was even predicted as negative (-24 mm), similar to the negative T predictions  
642 observed at East End during the winter validation (Fig. 2). However, this value falls within  
643 the uncertainty range of 91 mm for annual ET measurements at this site in 2014 (Eichelmann  
644 et al., 2018). East End and Sherman Island both had a very high open water surface area,  
645 especially in the first years after flooding, so it would be expected that E is more dominant.  
646 Sherman Island specifically had extremely sparse vegetation cover throughout the EC  
647 measurement footprint for the first two years of measurements, also evident in the very low  
648 values of GEP. For both of these sites, East End and Sherman Island, we can see that  
649 gradually E declines and T increases as the vegetation fills in from year to year.  
650 Consequently, when comparing the T/ET values across sites (Fig. 6e), West Pond had the  
651 highest value of T/ET (70%-75% on T), followed by Mayberry Farms (30%-50%), East End  
652 (0-30%), and Sherman Island (<15%). This highlights that only West Pond can be described  
653 as a T dominated site with T/ET values in the range between 0.5 and 0.8 reported for other  
654 terrestrial ecosystems (Schlesinger & Jasechko, 2014). The other three sites are clearly E  
655 dominated and have T/ET values considerably lower than those expected for terrestrial  
656 ecosystems.

657

## 658 **4 Discussion**

659

### 660 **4.1 Artificial Neural Network Architecture Performances**

661

662 The ANN F36, which was built using all studied variables, presented the highest  
663 average testing  $R^2$  value (0.891) for the nighttime-based testing dataset among all 36 ANNs  
664 analyzed. Nevertheless, there was not much improvement in testing  $R^2$  in the models (i.e.,  
665 maximum of 3-4% on average) after the ANN F11. This indicates that not all variables are  
666 necessary to provide good results in the partitioning of ET into E and T, and that less  
667 complex models can result in good predictions. For instance, using only datetime + H\_gf +  
668 VPD (F33) or datetime +  $u_*$  +  $T_{air}$  (F2) the average testing  $R^2$  value across all sites was  $> 0.70$ , indicating a good correlation. In addition, when using datetime + VPD alone the

670 average testing  $R^2$  value for three sites (i.e., East End, Mayberry Farms and Sherman Island)  
671 was  $> 0.70$ .

672 In our study, the order of variable inclusion to increase model complexity was:  
673 `datetime > VPD > H_gf > T_air > u_*`. VPD was the variable that contributed the most in the  
674 improvement of the ANNs, with an average of 24% increase in testing  $R^2$  values across all  
675 sites. VPD is routinely measured at most EC sites (e.g., Fluxnet.org, 2021) and its effect on  
676 ecosystem water cycling by limiting surface conductance and reducing transpiration under  
677 high VPD is well documented (Buckley, 2005, Novick et al., 2016). The fact that the top 14  
678 ANNs (i.e., with the highest testing  $R^2$  value) were constructed using VPD as one of the input  
679 parameters highlights the importance of VPD as a predictor of ecosystem water exchange. In  
680 addition, all the 11 ANNs that scored an average testing  $R^2 > 0.80$  have  $u_*$  in their models,  
681 indicating that information on atmospheric turbulence is important to incorporate in ET  
682 partitioning prediction if available. It may not be surprising that at these flooded sites E is  
683 mainly explained by atmospheric conditions such as VPD,  $T_{air}$ , and turbulence ( $u_*$ )  
684 underlining their importance in the ANN partitioning routine. At sites with different surface  
685 and vegetation characteristics, such as dryland sites, it would be important to investigate the  
686 importance of other variables such as soil moisture, soil temperature, or leaf wetness. It  
687 would be expected that these, together with other energy balance components such as  
688 radiation, would play a larger role in explaining E at water limited sites.

689

## 690 **4.2 Artificial Neural Network Validation Against Post-Flooding Periods and Leaf-Level 691 Data**

692

693 The validation of our models against data collected right after flooding (for East  
694 End, Mayberry Farms, and Sherman Island) and with leaf-level data (for East End only)  
695 indicated that models with less input variables (F11) performed better in comparison to the  
696 model that incorporated all 10 studied variables (F36). It might be that overfitting occurred  
697 when incorporating input variables that deal directly and/or indirectly with the same  
698 property/factor (i.e., carbon assimilation). In this case, F36 includes `er_Reichstein`, `wc_gf` and  
699 `GCC` which are all related to carbon uptake by vegetation. Thus, even with a smaller average  
700 testing  $R^2$  value, models with fewer input variables (e.g., F11) still performed better than F36  
701 during validation with ground-truth leaf-level and flooding data. Specifically, the ANN F11,  
702 which showed the best performance for all three of the sites with flooding data validation  
703 (East End, Mayberry Farms, and Sherman Island) included `datetime + H_gf + VPD + T_air +`

704 u\*. The validation based on data collected right after flooding also emphasized the importance  
705 of validating the ANN partitioning routine against data collected during daytime periods.  
706 Some of the tested input variables showed strong differences in daytime and nighttime  
707 behavior (e.g., Rnet). Using these variables as inputs can lead to incorrect daytime  
708 predictions for the nighttime-based ANN routine as seen in the poor performance of F15 for  
709 the flooding validation at East End and Mayberry Farms, despite a high testing  $R^2$  of 0.75  
710 (Supplementary Table 1).

711 The flooding validation also highlights site-specific differences in the input variables  
712 that provided good predictions. While the best performance was achieved with the same  
713 model (F11) across all three validation sites, the behavior of the other tested models varied  
714 across sites. We recommend that the selection of input parameters for ANN partitioning of  
715 ET should be based on the unique site characteristics rather than a standardized set of  
716 variables since vegetation heterogeneity and other site level characteristics can influence  
717 ecosystem ET levels (Eichelmann et al., 2018).

718 This is also evident in the validation using data from the winter/senescent period,  
719 where F11 performed best at Mayberry Farms and Sherman Island, whereas F36 performed  
720 best at East End and West Pond. The overall performance of our ANNs in predicting E  
721 during the winter/senescent periods was also considerably lower in comparison to the  
722 flooding and leaf-level data validation. This is partially due to the smaller fluxes observed  
723 overall during this period, leading to larger relative errors. In addition, the assumption that all  
724 measured ET during the winter months represents solely E is likely incorrect. Especially at  
725 the sites with high vegetation cover (Mayberry and West Pond) it is likely that a small  
726 amount of T occurs during this time which would be included in the measured ET signal,  
727 leading to an apparent under-prediction of E for the ANN. For East End and Sherman Island,  
728 however, we can see that the ANNs are actually over-predicting E (Fig. 2), leading to  
729 consistent, albeit relatively small, negative T prediction in the winter months, specifically at  
730 East End (Fig. 4). It is unclear what is causing the discrepancy between measured and  
731 modeled E at East End and Sherman Island during the winter months. However, the fact that  
732 inclusion of variables linked to vegetation growth (GCC, wc\_gf, er\_Reichstein) reduced the  
733 over-prediction at both sites (e.g., F36 or F15) could indicate that E dynamics linked to  
734 phenology and vegetation cover are not adequately reproduced in models without these input  
735 variables at East End and Sherman Island.

736 Unfortunately, a limitation in our study is that we were not able to validate our  
737 results across all sites/sampling times due to a lack of leaf-level data collected from all sites,

738 which is very time and labor intensive. In addition, no data were available from the initial  
739 flooding period at the West Pond wetland. Nonetheless, we are aware that validation of T/ET  
740 partitioning is quite scarce in the literature and that the data validated against our ANNs  
741 prove that good results can be achieved using the protocol tested here.

742

#### 743 **4.3 Artificial Neural Network Performance Across the Wetland Sites**

744

745 Concerning the performance of all the 36 ANNs across the four wetlands analyzed  
746 in this study, West Pond showed smaller testing  $R^2$  values in comparison to the three other  
747 sites. Between-site differences reached up to 46% for the same model. The main reason for  
748 this divergence was likely the differing amounts of open water surfaces and density of the  
749 vegetation between these sites. West Pond, with little to no open water, is likely to see less E  
750 compared to the other wetlands (Eichelmann et al., 2018). In addition, West Pond also has the  
751 lowest water temperature and a very dense vegetation canopy decoupling the water surface  
752 from the atmosphere and leading to further reductions in E, especially at night (Drexler et al.,  
753 2004; Goulden et al., 2007; Eichelmann et al., 2018). Because our method predicts E based  
754 on nighttime data and calculates T based on the difference between total ET and E, if E  
755 values are small the relative accuracy of the prediction will decrease, which is reflected in the  
756 testing  $R^2$  values. However, because the E values are small, the absolute error of the predicted  
757 E and T would be proportionately small, hence the total T and E values can still be reliable.  
758 Unfortunately, we did not have a set of ground-truth validation data available for the West  
759 Pond site to investigate the true performance of the ANN ET partitioning. However, our  
760 comparison with the Scott and Biederman (2017) partitioned data and expected relationships  
761 based on the observed carbon fluxes and vegetation dynamics give us high confidence in the  
762 performance of the ANN partitioning routine at the West Pond wetland site. This shows that  
763 the ANN partitioning method can also be successfully applied in situations where nighttime E  
764 fluxes are small, indicating that it could be applicable to a large variety of ecosystems. In this  
765 context it is important to note that some studies have found non-negligible nighttime  
766 transpiration values for certain ecosystems (Caird et al., 2006; Novick et al., 2009; Resco de  
767 Dios et al., 2019). To be able to apply the ANN methodology from our study to other sites or  
768 ecosystems it is essential to confirm that nighttime transpiration is indeed negligible at the  
769 respective site. Additionally, careful consideration needs to be given to the changing  
770 interactive effects between energy fluxes and environmental conditions from nighttime to

771 daytime. Any application of this methodology will require validation against independent  
772 daytime data to ensure these effects are correctly captured in the ANN models.

773

#### 774 **4.4 Comparisons with Other Partitioning Approaches and Wider Implications**

775

776 In comparison to other established methods in the literature our own approach using  
777 ANNs to determine the T/ET partitioning achieved very good results with fewer limitations,  
778 which makes it easier to apply in other contexts/ecosystems. For instance, Scott and  
779 Biederman's (2017) method only works when there are enough years of data. The shortest  
780 dataset Scott and Biederman (2017) analyzed spanned eight years, which is a considerably  
781 long time period and reduces its applicability to shorter studies. Also, in the absence of  
782 climate consistency among sampling sites or if the research takes place in areas where fluxes  
783 are not limited by water availability (e.g., wetlands), their model fails to partition T/ET  
784 correctly, limiting it to relatively dry ecosystems. This was evident from direct comparisons  
785 with our own method, particularly for Sherman Island which has the shortest dataset (i.e.,  
786 four years) and the highest area of open water, with the largest relative contribution of E (Fig.  
787 4, 5).

788 Considering the partitioning methods proposed by Scanlon and Sahu (2008),  
789 Scanlon and Kustas (2010), and Skaggs et al. (2018), *a priori* knowledge on WUE and carbon  
790 uptake is required to apply their method. Consequently, the paucity of previous  
791 data/information or lack of equipment impede the application of this method to a broader  
792 audience. We tried to run the Scanlon and Kustas (2010) and Skaggs et al. (2018) partitioning  
793 methods for our wetland sites but were not able to retrieve reliable and meaningful  
794 partitioning results for any of the sites discussed in this study. We did not test the method  
795 proposed by Zhou et al. (2016) in this study, since we believe that some of the underlying  
796 assumptions are easily violated at the wetland sites investigated here. Most importantly, the  
797 Zhou et al. (2016) method is based on the assumption that some periods within the time series  
798 represent conditions without E and the water flux is entirely based on T (i.e., T = ET). This is  
799 most certainly not the case at flooded sites where we can reasonably expect that there will  
800 always be E, albeit in varying amounts. Additionally, the potential underlying WUE is  
801 assumed to be constant, which could be violated when multiple vegetation types or species  
802 are present, as is the case with our sites. Finally, virtually all the other methods discussed  
803 here lacked validation against ground-truth data in the original studies. We included several  
804 verification types for the ANN method in this paper, which gives us confidence that our

805 approach using ANNs produces reliable and meaningful estimates for E and T in wetland  
806 ecosystems. The fact that our method does not rely on presumed relationships between water  
807 and carbon fluxes and was shown to work across a range of ecosystem properties from T to E  
808 dominated systems, provides an advantage against other methods that are limited to certain  
809 ecosystems or need specialized input data/equipment.

810 In terms of wider implications, our results can help to connect T/ET partitioning  
811 with other global atmospheric processes. An example is the constant increase in global VPD,  
812 which is cause of much concern regarding natural and agricultural systems. Most studies to  
813 date have focused on the effect of increasing VPD levels on plant physiology and reduced  
814 plant growth or productivity with concomitantly increased T (Yuan et al., 2019; Grossiord et  
815 al., 2020; López, Way, & Sadok, 2021). However, VPD was the variable that contributed the  
816 most to explain E across the 36 ANNs analyzed in our study, highlighting its importance not  
817 only for plant regulated water cycling (T), but also for driving E. Two independent studies  
818 indicated that VPD levels are increasing in our study region (i.e., southwest USA, California).  
819 Seager et al. (2015) have found a consistent rise in atmospheric VPD since 1960s and Ficklin  
820 and Novick (2017) also projected higher VPD levels with amplified effects during summer  
821 months, potentially driving more pronounced water loss through E regardless of the plant  
822 physiological response. While other factors might be more important at controlling plant  
823 productivity in some ecosystems (e.g., soil moisture in semi-arid areas; see Liu et al., 2020),  
824 atmospheric vapor demand is projected to become more important with climate change in all  
825 ecosystems (Novick et al., 2016). Consequently, the estimates of T/ET partitioning given by  
826 our new approach will be important as they allow us to explain the effects of rising global  
827 VPD levels on E and T separately.

828

## 829 **5 Summary**

830

831 A novel T/ET partitioning method using Artificial Neural Networks (ANN) to  
832 predict daytime E from nighttime ET measurements in a combination with a range of  
833 environmental variables was presented and compared to previous methods from the literature.  
834 In comparison to other approaches, the ANN method achieved better results, particularly with  
835 shorter-term data (i.e., <5 years) and was successfully applied to flooded ecosystems. The  
836 order of variable inclusion (and importance) for the ANN construction was: vapor pressure  
837 deficit (VPD) > gap-filled sensible heat flux ( $H_{gf}$ ) > air temperature ( $T_{air}$ ) > friction velocity  
838 ( $u_*$ ) > other variables. The best performing ANN, model F11, used datetime, VPD,  $H_{gf}$ ,  $T_{air}$ ,

839 and  $u_*$  inputs with an average testing  $R^2$  value across all sites of 0.85. This model also  
840 performed the best when validated against ground-truth leaf-level data and periods where  
841 sites were completely flooded with no T from vegetation. Our method sheds light on T/ET  
842 partitioning methods and applications. While here it has only been tested for flooded  
843 ecosystems, we present strong indicators that it could also perform well in other ecosystems,  
844 contributing to the understanding of the global water cycle and its response to atmospheric  
845 processes such as rising global VPD levels.

846

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862

## 863 **7 Data Availability Statement**

864 All data used in this study are publicly available through the Ameriflux network  
865 under the AmeriFlux CC-BY-4.0 License and the EC data from the sites are available for  
866 download through the Ameriflux data sharing platform (<https://ameriflux.lbl.gov/>). Specific  
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871 ID: US-Sne; <https://doi.org/10.17190/AMF/1418684>

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1146

1147 **Table 1:** Average testing R<sup>2</sup>, slope, and RSME values for 12 ANN architecture models used  
 1148 to partition evapotranspiration measurements, demonstrating an increase in complexity from  
 1149 models F21 (most basic) to F36 (most complex).

Model	Model Structure	Average testing R <sup>2</sup>	Average Slope	Average RSME
Name				
F21	datetime	0.410	0.393	0.380
F26	datetime + VPD	0.648	0.626	0.378
F17	datetime + VPD + T <sub>air</sub>	0.672	0.636	0.369
F31	datetime + VPD + T <sub>air</sub> + GCC	0.686	0.657	0.364
F32	datetime + VPD + T <sub>air</sub> + GCC + Rnet	0.689	0.665	0.364
F15	datetime + VPD + T <sub>air</sub> + GCC + Rnet + WT	0.694	0.663	0.360
F33	datetime + H <sub>gf</sub> + VPD	0.753	0.726	0.340
F34	datetime + H <sub>gf</sub> + VPD + T <sub>air</sub>	0.762	0.734	0.336
F11	datetime + H <sub>gf</sub> + VPD + T <sub>air</sub> + u <sub>*</sub>	0.853	0.831	0.264
F35	datetime + H <sub>gf</sub> + VPD + T <sub>air</sub> + u <sub>*</sub> + er Reichstein	0.863	0.851	0.258
F14	datetime + H <sub>gf</sub> + u <sub>*</sub> + VPD + T <sub>air</sub> + GCC + Rnet + WT	0.877	0.868	0.252
F36	er_Reichstein + VPD + T <sub>air</sub> + GCC +	0.891	0.880	0.237

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1151

1152 **Table 2:** Validation R<sup>2</sup>, slope, and RSME values of seven ANNs used to partition  
 1153 evapotranspiration measurements and validated with data collected right after flooding for

1154 East End, Mayberry Farms, and Sherman Island wetland sites. Models are ordered by the  
 1155 increase in complexity, from model F21 (most basic) to F36 (most complex). Refer to Tables  
 1156 1 and 3 for each model's input variables. Validation  $R^2$  values higher than 0.7 are highlighted  
 1157 in bold.

Model	East End			Mayberry Farms			Sherman Island		
	Name	$R^2$	Slope	RSME	$R^2$	Slope	RSME	$R^2$	Slope
F21	0.29	0.28	0.75	0.06	0.09	0.47	0.34	0.25	0.49
F26	0.48	0.52	0.90	0.26	0.37	0.82	0.61	0.50	0.56
F17	0.50	0.46	0.77	0.31	0.41	0.82	0.63	0.56	0.60
F15	0.24	0.15	0.44	0.16	0.13	0.39	0.37	0.28	0.50
F33	0.61	0.66	0.90	0.48	0.81	1.13	0.62	0.71	0.76
F11	<b>0.81</b>	0.86	0.70	0.69	0.95	0.85	<b>0.82</b>	1.00	0.65
F36	0.51	0.45	0.75	0.56	0.48	0.57	0.53	0.43	0.56

1158

1159

1160 **Table 3:** Validation  $R^2$ , slope, and RSME values of seven ANNs used to partition  
 1161 evapotranspiration measurements and validated with winter time data (December to  
 1162 February) for each of the four wetlands studied (East End, Mayberry Farms, Sherman Island,  
 1163 and West Pond). Models are listed according to the increase in complexity, from model F21  
 1164 (most basic) to F36 (most complex). Refer to Tables 1 and 4 for each model's input variables.  
 1165 Validation  $R^2$  values higher than 0.7 are highlighted in bold.

Model	East End			Mayberry Farms			Sherman Island			West Pond		
	Name	$R^2$	Slope	RSME	$R^2$	Slope	RSME	$R^2$	Slope	RSME	$R^2$	Slope
F21	0.06	0.02	0.05	0.06	0.06	0.21	0.15	0.11	0.23	0.08	0.30	0.09
F26	0.17	0.25	0.41	0.26	0.38	0.58	0.45	0.48	0.45	0.03	0.08	0.46
F17	0.21	0.24	0.36	0.35	0.47	0.56	0.47	0.49	0.48	0.05	0.06	0.28
F15	0.33	0.41	0.44	0.14	0.12	0.26	0.43	0.29	0.31	0.17	0.11	0.25
F33	0.21	0.71	1.03	0.22	0.48	0.77	0.19	0.42	0.79	0.01	0.01	0.12
F11	0.33	1.15	1.23	0.56	0.71	0.55	<b>0.70</b>	1.27	0.76	0.11	0.11	0.29
F36	0.45	0.95	0.79	0.43	0.59	0.60	0.69	0.87	0.54	0.36	0.17	0.21

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1167

1168 **Table 4:**  $R^2$  and slope values for linear regression of ecosystem level transpiration data  
 1169 predicted by seven ANNs versus leaf-level transpiration data collected in 2017 for East End.  
 1170 Models are ordered by the increase in complexity from model F21 (most basic) to F36 (most  
 1171 complex). Note that leaf-level transpiration is measured on a per leaf area basis, whereas  
 1172 ANN predicted transpiration is measured on a per ground area basis (see section 2.5 for  
 1173 details). The slope parameter, therefore, does not show an under-estimation of the ANN  
 1174 predicted transpiration values in this case.

Model Name	Model Structure	$R^2$ value	Slope value
F21	datetime	0.979	0.95
F26	datetime + VPD	0.984	0.79
F17	datetime + VPD + TA	0.984	0.75
F15	datetime + VPD + TA + GCC + Rnet + WT	0.987	0.81
F33	datetime + H_gf + VPD	0.99	0.93
F11	datetime + H_gf + VPD + TA + $u_*$	0.986	0.76
	datetime + H_gf + $u_*$ + wc_gf + er_Reichstein +		
F36	VPD + TA + GCC + Rnet + WT	0.922	0.70

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## 1177 **Figure Legends**

1178

1179 **Figure 1:** Comparison between the eddy covariance measured daytime evaporation flux  
 1180 ( $H_2O_{measured}$ ) and daytime evaporation predicted by ANNs ( $H_2O_{modeled}$ ) using model F11 (top  
 1181 panels, a-c) and F36 (bottom panels, d-f) based on data collected right after flooding for  
 1182 Mayberry Farms (a, d), East End (b, e), and Sherman Island (c, f). Note: the black lines are  
 1183 1:1 relationships for reference, red lines show linear regressions with standard deviation, and  
 1184 blue dots represent the data.

1185

1186 **Figure 2:** Comparison between the eddy covariance measured daytime evaporation flux  
 1187 ( $H_2O_{measured}$ ) and daytime evaporation predicted by ANNs ( $H_2O_{modeled}$ ) using model F11 (top  
 1188 panels, a-d) and F36 (bottom panels, e-h) based on data collected during senescent periods in  
 1189 winter (December to February) at Mayberry Farms (a, e), East End (b, f), Sherman Island (c,  
 1190 g), and West Pond (d, h). Note: the black lines are 1:1 relationships for reference, red lines  
 1191 show linear regressions with standard deviation, and blue dots represent the data.

1192

1193 **Figure 3:** Ecosystem level transpiration data ( $H_2O_{modeled}$ ) predicted by ANNs F11 (a) and F36  
1194 (b) validated against leaf-level (LL) transpiration data ( $H_2O_{measured}$ ) collected during the field  
1195 campaigns in 2017 for the two dominant species in the wetland: Tule (yellow triangles) and  
1196 Cattail (blue squares). The overall linear regression line (solid red line) and standard  
1197 deviation (dashed red line) is based on average leaf-level transpiration across both species  
1198 (red asterisks). Error bars represent the standard deviation from the mean for each  
1199 measurement interval and species for the leaf-level data. Leaf-level data were pooled for 30-  
1200 min intervals to match the eddy covariance averaging period (i.e. each symbol (square,  
1201 triangle or asterisks) represents measurements taken during one 30-min interval). The solid  
1202 black lines show 1:1 relationships for reference. Note that leaf-level transpiration is measured  
1203 on a per leaf area basis, whereas ANN predicted transpiration is measured on a per ground  
1204 area basis (see section 2.5 for details). The slope, therefore, does not show an under-  
1205 estimation of the ANN predicted transpiration values in this case.

1206

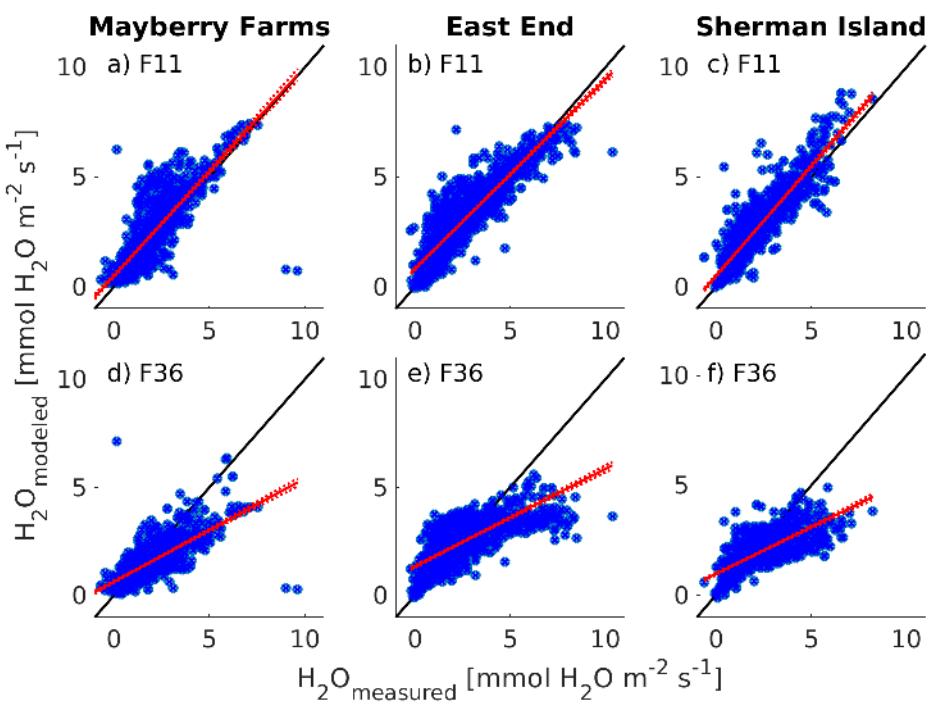
1207 **Figure 4:** Monthly regressions of evapotranspiration (ET) vs Gross Ecosystem Productivity  
1208 (GEP) data for four wetland sites Mayberry Farms (a), East End (b), West Pond (c), and  
1209 Sherman Island (d) for T/ET partitioning using the Scott and Biederman (2017) method for  
1210 long-term flux data. Each regression line represents data for the same month across multiple  
1211 years. The method is considered unreliable for winter months when GEP is small (November  
1212 through March, shown in dashed lines and cross symbols). Negative regression lines for most  
1213 months at Sherman Island (d) indicate that the methodology does not work at this site,  
1214 potentially due to the shorter time period of this dataset (4 years) or because of the large  
1215 contribution of evaporation at this site (see main text for detailed discussion).

1216

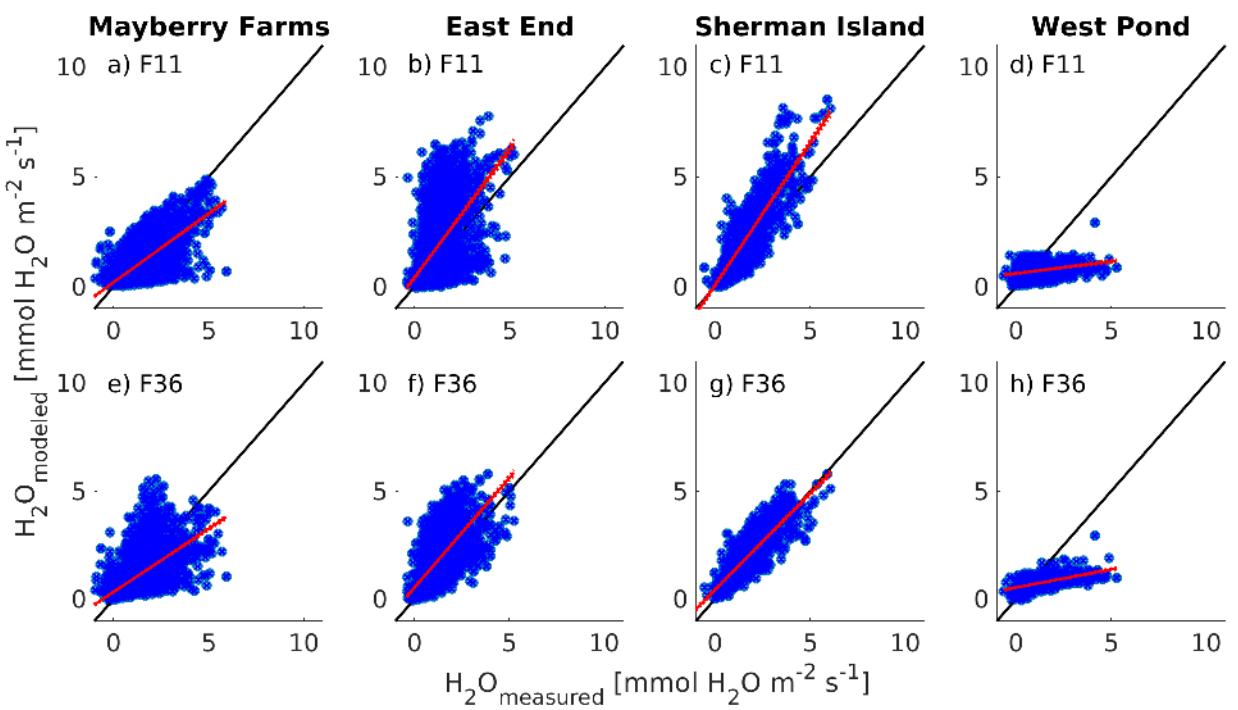
1217 **Figure 5:** Average monthly evaporation (E) (top panels, a-d) and transpiration (T) (bottom  
1218 panels, e-h) fluxes across four wetland sites: Mayberry Farms (a, e), East End (b, f), West  
1219 Pond (c, g), and Sherman Island (d, h) comparing the ANN T/ET partitioning method  
1220 described in this paper (red lines and square symbols) and the Scott and Biederman (2017)  
1221 method (blue lines and triangle symbols) on long-term flux data. Error bars are based on the  
1222 standard error of the fit intercept and slope for the Scott and Biederman (2017) method and  
1223 on the interquartile range of the 20 individual ANN runs for the ANN method. Comparisons  
1224 were done using ANN F11 for all sites. Gross Ecosystem Productivity (GEP, yellow lines and  
1225 asterisks) for each site is shown for comparison in the bottom panels with a separate y-axis on  
1226 the right.

1227

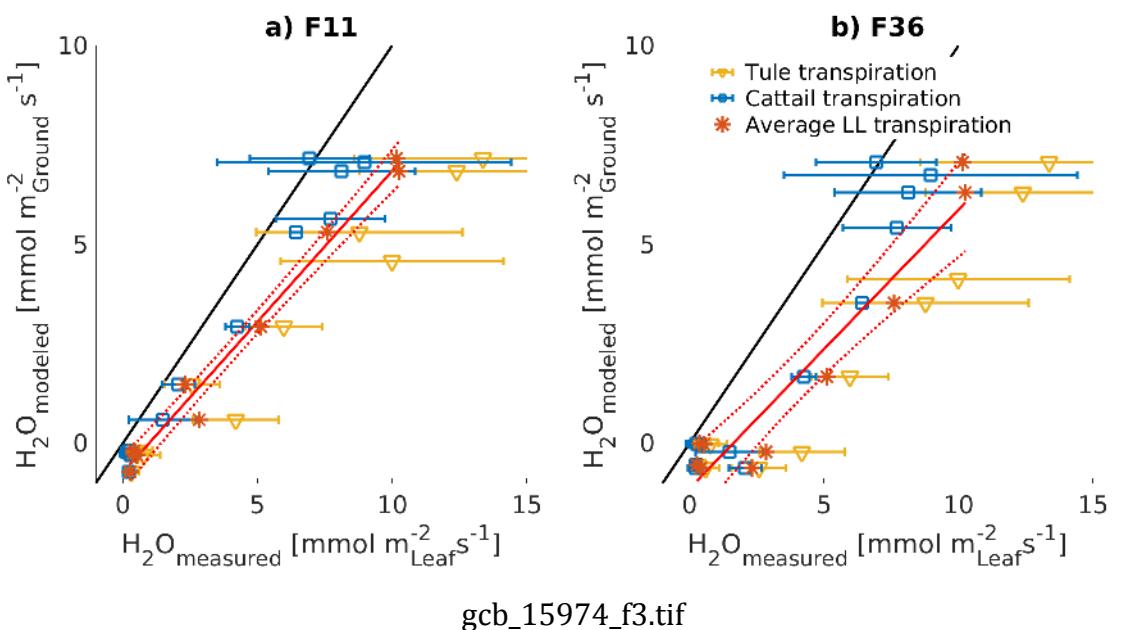
1228 **Figure 6:** Annual intercomparison of (a) total evapotranspiration (ET), (b) gross ecosystem  
1229 productivity (GEP), (c) evaporation (E), (d) transpiration (T), and (e) transpiration over  
1230 evapotranspiration ratio (T/ET) between four wetland sites (Mayberry Farms, 2013-2019,  
1231 blue triangles; West Pond, 2013-2019, red squares; East End, 2014-2019, yellow asterisks;  
1232 and Sherman Island, 2016-2019, purple circles). E and T values are based on the ANN  
1233 partitioning routine (F11) described in this study.

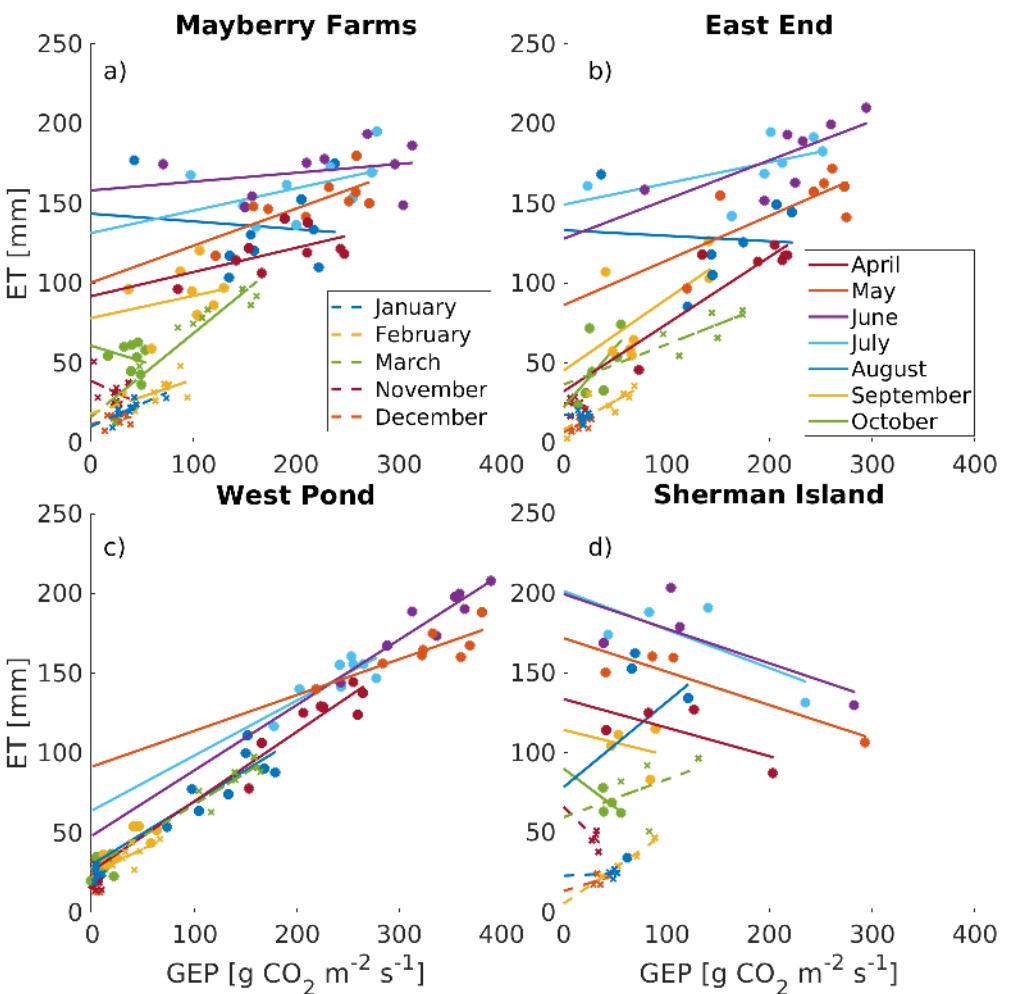


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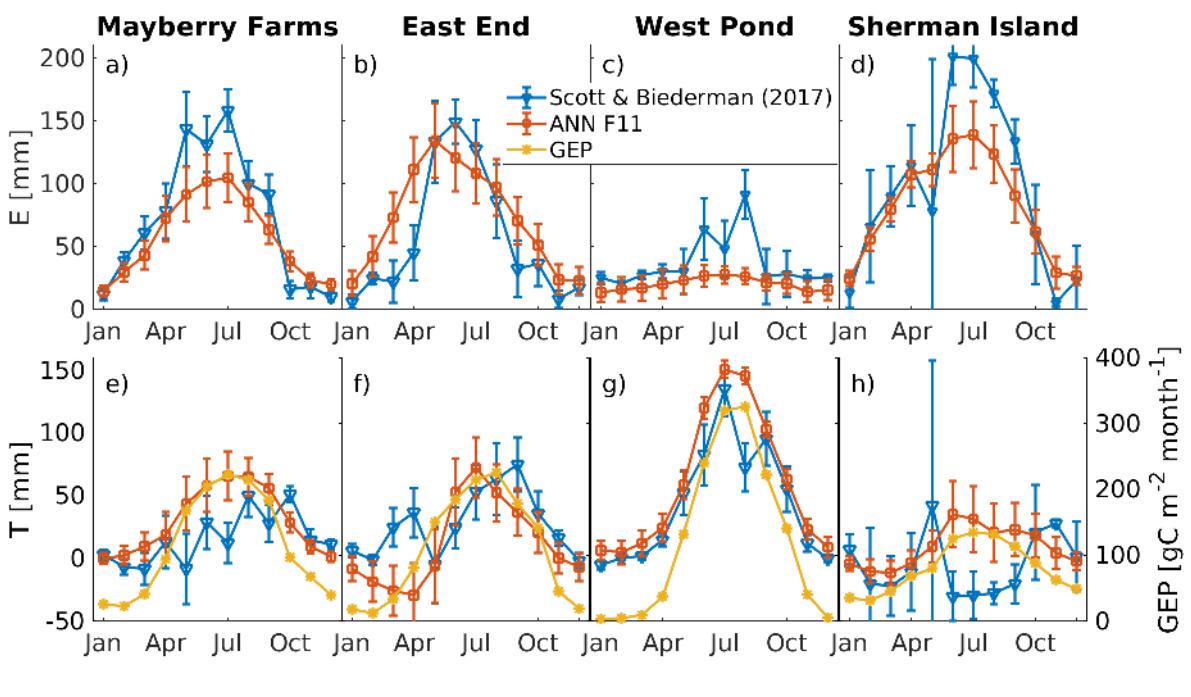


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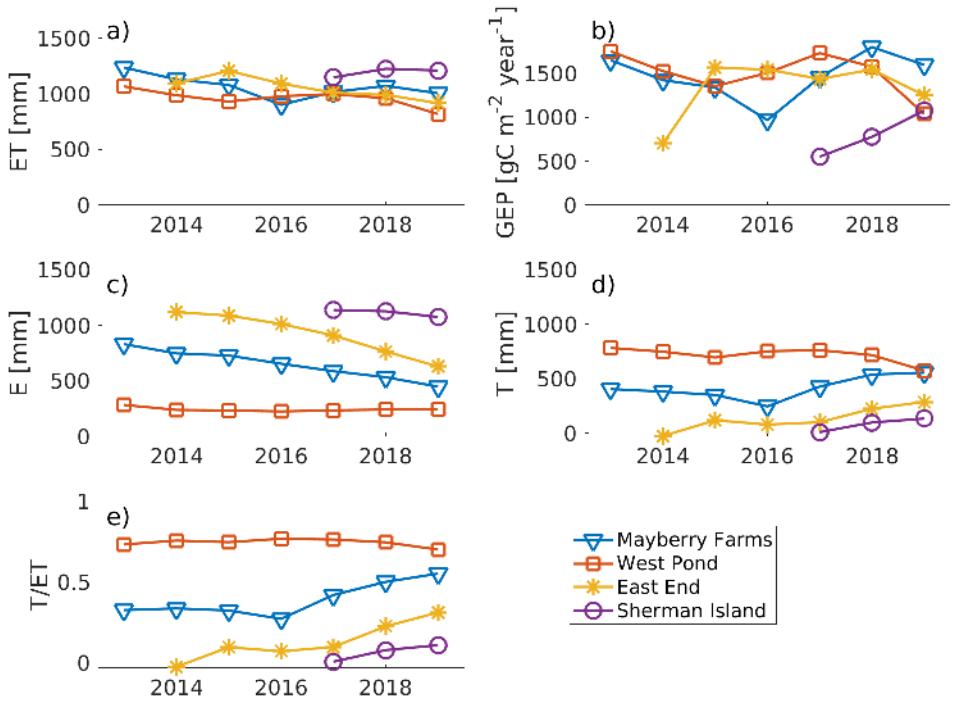




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