Evaluation of water flux predictive models developed using eddy covariance observations and machine learning: a meta-analysis

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Submitted to *Hydrology and Earth System Sciences*

Abstract.

With the rapid accumulation of water flux observations from global eddy-covariance flux sites, many studies have used data-driven approaches to model water fluxes with various predictors and machine learning algorithms used. However, ~~systematic evaluation of such models~~ it is ~~still limited. We therefore performed a meta-analysis of 32 such studies, derived 139 model records, and evaluated the impact of~~unclear how various model features ~~on model~~affect prediction accuracy ~~throughout the modeling flow~~. To fill this gap, we evaluated this issue based on records of 139 developed models collected from 32 such studies. SVM (average R-squared = 0.82) and RF (average R-squared = 0.81) outperformed over evaluated algorithms with sufficient sample size in both cross-study and intra-study (with the same data) comparisons. The average accuracy of the model applied to arid regions is higher than in other climate types. The average accuracy of the model was slightly lower for forest sites (average R-squared = 0.76) than for croplands and grasslands (average R-squared = 0.8 and 0.79), but higher than for shrubland sites (average R-squared = 0.67). Using Rn/Rs, precipitation, Ta, and FAPAR improved the model accuracy. The combined use of Ta and Rn/Rs is very effective especially in forests, while in grasslands the combination of Ws and Rn/Rs is also effective. Random cross-validation showed higher model accuracy than spatial cross-validation and temporal cross-validation, but spatial cross-validation is more important in spatial extrapolation. The findings of this study are promising to guide future research on such machine learning-based modeling.

1 Introduction

Evapotranspiration (ET) is one of the most important components of the water cycle in terrestrial ecosystems. It also represents the key variable in linking ecosystem functioning, carbon and climate ~~feedbacks~~feedback, agricultural management, and water resources (Fisher et al., 2017). The quantification of ET for ~~regional~~regions, continents, or the globe can improve our understanding of the water, heat, and carbon interactions, which is important for global change research (Xu et al., 2018). Information on ET has been used in many fields, including, but not limited to, droughts and heatwaves (Miralles et al., 2014), regional water balance closures (Chen et al., 2014; Sahoo et al., 2011), agricultural management (Allen et al., 2011), water resources management (Anderson et al., 2012), biodiversity patterns (Gaston, 2000). In addition, accurate large-scale and long-time series ET prediction at high spatial and temporal resolution has been of great interest (Fisher et al., 2017).

Currently, there are three main approaches for simulation and spatial and temporal prediction of ET: (i) physical models based on remote sensing such as surface energy balance models (Minacapilli et al., 2009; Wagle et al., 2017), Penman-Monteith equation (Mu et al., 2011; Zhang et al., 2010), Priestley-Taylor equation (Miralles et al., 2011); (ii) process-based land surface models, biogeochemical models and hydrological models (Barman et al., 2014; Pan et al., 2015; Sándor et al., 2016; Chen et al., 2019); and (iii) the observation-based machine learning modeling approach with in situ eddy covariance (EC) observations of water flux (Jung et al., 2011; Li et al., 2018; Van Wijk and Bouten, 1999; Xie et al., 2021; Xu et al., 2018; Yang et al., 2006; Zhang et al., 2021). For remote sensing-based physical models and process-based land surface models, some physical processes have not been well characterized due to the lack of understanding of the detailed mechanisms influencing ET

55 under different environmental conditions. For example, the inaccurate representation and estimation of stomatal

56 conductance (Li et al., 2019) and the linearization (McColl, 2020) of the Clausius-Clapeyron relation in the

57 Penman-Monteith equation may introduce both empirical and conceptual errors into estimates of ET. Limited by

58 complicated assumptions and model parametrizations, these process-based models face challenges in the

59 accuracy of their ET estimations over heterogeneous landscapes (Pan et al., 2020; Zhang et al., 2021).

60 Therefore, many researchers have used data-driven approaches for the simulation and prediction of ET with the

61 accumulation of a large volume of measured observational data of water fluxes in the past decades. Various

62 machine learning models have been developed to simulate water fluxes at the flux site scale. Besides, various

63 predictor variables (e.g., meteorological factors, vegetation conditions, and moisture supply conditions) have

64 been incorporated into such models for upscaling (Fang et al., 2020; Jung et al., 2009) of water flux to a larger

65 scale or understanding the driving mechanisms with the variable importance analysis performed in such models.

66

67 However, to date, the systematic assessment of the uncertainty in the processes of water flux prediction models

68 constructed using the machine learning approach is limited. Although considerable effort has been invested in

69 improving the accuracy of such prediction models, our understanding of the expected accuracy of such models

70 under different conditions is still limited. It is still not easy for us to give the general guidelines for selecting

71 appropriate predictor variables and models. Questions such as 'Which predictor variables are the best in water

72 flux simulations?' and 'How to improve the prediction accuracy of water flux effectively?' etc. still confuse the

73 researchers in the field. Therefore, we should synthesize the findings from published studies to determine which

74 predictor variables, machine learning models, and other features can significantly improve the prediction

75 accuracy of water flux. Also, we are interested in understanding under which specific conditions they are more

76 effective.

77

78 A variety of features control the accuracy of such models, including the predictor variables used, the inherent

79 heterogeneity within the dataset, the plant functional type (PFT) and characteristics of the flux sites, ~~the method~~

80 ~~of~~ model construction ~~and~~/ validation skills, and the ~~algorithm chosen~~algorithms used:

81 a) Predictor variables used: Compared to process-based models, the data used may have a more significant

82   impact on the final model performance in data-driven models. Various biophysical covariates and other

83   environmental factors have been used for the simulation and prediction of water fluxes. The most

84   commonly used factors include mainly precipitation (Prec), air temperature (Ta), wind speed (Ws), net/sun

85   radiation (Rn/Rs), soil temperature (Ts), soil texture, vapor-pressure deficit (VPD), the fraction of absorbed

86   photosynthetically active radiation (FAPAR), vegetation index (e.g., Normalized Difference Vegetation

87   Index (NDVI), Enhanced Vegetation Index (EVI)), Leaf area index (LAI), and carbon fluxes (e.g., Gross

88   Primary Productivity (GPP)). These used predictor variables and their complex interactions drive the

89   fluctuations and variability of water fluxes. They affect the accuracy of water flux simulations in two ways:

90   their actual impact on water fluxes at the process-based level and their spatio-temporal resolution and

91   inherent accuracy. The relationship between water fluxes and these variables at the process-based driving

92   mechanism level is very different under different PFTs, different climate types, and different

93   hydrometeorological conditions. For example, in irrigated croplands in arid regions, water fluxes may be

94   highly correlated with irrigation practices, and thus soil moisture may be a very important predictor

95 variable, and its importance may be significantly higher than in other PFTs. And in models that incorporate
96 data from multiple PFTs, some variables that play important roles in multiple PFTs may have higher
97 importance. In terms of data spatial and temporal resolution, the data for these predictor variables may have
98 different scales. In terms of spatial resolution, meteorological observations such as precipitation and air
99 temperature are at the flux site scale, while factors extracted from satellite remote sensing and reanalysis
100 climate datasets cover a much larger spatial scale (i.e. the grid-scale). This leads to considerable differences
101 in the degree of spatial match between different variables and the site scale EC observations (approximately
102 100 m x 100 m). It is therefore difficult for some variables to be fairly compared in the subsequent
103 importance analysis of driving factors. In terms of temporal resolution, the importance of predictor
104 variables with different temporal resolutions may be variable for models with different time scales (e.g.,
105 half-hourly, daily, and monthly models). For example, the daily or 8-day NDVI data based on MODIS
106 satellite imagery may better capture the temporal dynamics of water fluxes concerning vegetation growth
107 than the 16-daily NDVI data derived from Landsat images. Besides, data on non-temporal dynamic
108 variables such as soil texture cannot explain temporal variability in water fluxes in the data-driven
109 simulations, although soil texture may be important in the interpretation of the actual driving mechanisms
110 of ET (which may need to be quantified in detail in ET simulations by process-based models). In addition,
111 some inherent accuracy issues (e.g., remote sensing-based NDVI may not be effective at high values) of the
112 predictors may propagate into the consequent machine learning models, thus affecting the modeling and our
113 understanding of its importance. Therefore, it is necessary to consider the spatial and temporal resolution of
114 the data and their inherent accuracy for the predictors used in different studies in the systematic evaluation
115 of data-driven water flux simulations.
116 b) The heterogeneity of the dataset and model validation: the volume and inherent spatiotemporal
117 heterogeneity of the training dataset (with more variability and extremes incorporated) may affect model
118 accuracy. Typically, training data with larger regions, multiple sites, multiple PFTs, and longer year spans
119 may have a higher degree of imbalance (Kaur et al., 2019; Van Hulse et al., 2007; Virkkala et al., 2021;
120 Zeng et al., 2020). And in machine learning, in general, modeling with unbalanced data (with significant
121 differences in the distribution between the training and validation sets) may result in lower model accuracy.
122 Currently, the most common ways of model validation include spatial, temporal, and random cross-
123 validation. Spatial validation is mainly to evaluate the ability of the model to be applied in different regions
124 or flux sites with different PFT types, and one of the common methods is 'leave one site out' (Fang et al.,
125 2020; Papale et al., 2015; Zhang et al., 2021). If the data of the site left out for validation differs
126 significantly from the distribution of the training data set, the expected accuracy of the model applied at that
127 site may be low because the trained model may not capture the specific and local relationships between the
128 water flux and the various predictor variables at that site. For temporal validation, to assess the ability of the
129 models to adapt to the interannual variability, typically some years of data are used for training and the
130 remaining years for model validation (Lu and Zhuang, 2010). If a year with extreme climate is used for
131 validation, the accuracy may be low because the training dataset may not contain such extreme climate
132 conditions. In the case of PFTs that are significantly affected by human activities, such as cropland, the
133 possible different crops grown and different land use practices (e.g., irrigation) across years can also lead to
134 low accuracy in temporal validation.

135   c) Various machine learning algorithms: Some machine learning algorithms may have specific advantages
136   when applied to model the relationships between water fluxes and covariates. For example, neural networks
137   may have an advantage in nonlinear fitting, while random forests can avoid serious overfitting problems.
138   However, which algorithm is better overall in different situations (i.e. applied to different data sets)? Which
139   algorithm is generally more accurate than the others when using the same data set? A comprehensive
140   evaluation is important.

141

142   Therefore, to systematically and comprehensively assess the impact of various features in such modeling, we
143   perform a meta-analysis of published water flux simulation studies that combine the flux site water flux
144   observations, various predictors, and machine learning. The accuracy of model records collected from the
145   literature was linked with various model features to assess the impacts of predictor data types, algorithms, and
146   other features on model accuracy. The findings of this study may be promising to improve our understanding of
147   the impact of various features of the models to guide future research on such machine learning-based modeling.

148   **2 Methodology**

149   **2.1 Protocol for selecting the sample of articles**

150   We applied a general query (on December 1st, 2021) on title, abstract, and keywords to include articles with the
151   "OR" operator applied among expressions (Table 1) in the Scopus database. Preferred Reporting Items for
152   Systematic Reviews and Meta-Analyses (PRISMA) (Moher et al., 2009) are followed when filtering the papers.
153   We first excluded articles that obviously did not fit the topic of this study based on the abstract, and then
154   performed the article screening with the full-text reading.

155

156   The inclusion of articles follows the following criteria:
157   a)   Articles were filtered for those with water fluxes (or latent heat) simulated.
158   b)   The water flux or latent heat observations used in the prediction models should be from the eddy-
159   covariance flux measurements.
160   c)   Articles focusing only on gap-filling (Hui et al., 2004) techniques (i.e., the objective was not simulation
161   and extrapolation of water fluxes using machine learning) were excluded.
162   d)   Only articles that used multivariate regression (with the number of covariates greater than or equal to 3)
163   were included.
164   e)   The determination coefficient (R-squared) of the validation step should be reported as the metric of model
165   performance (Shi et al., 2021; Tramontana et al., 2016; Zeng et al., 2020) in the articles.
166   f)   The articles should be published in English-language journals.

167

168   Although RMSE is also often used for model accuracy assessment, its dependence on the magnitude of water
169   flux values makes it difficult to use for fair comparisons between studies. For example, due to the difference in
170   the range of ET values, models developed from flux stations in dry grasslands will typically have lower RMSE
171   than models developed by flux stations based on forests in humid regions. Therefore, RMSE may not be a good
172   metric for cross-study comparisons in this meta-analysis.

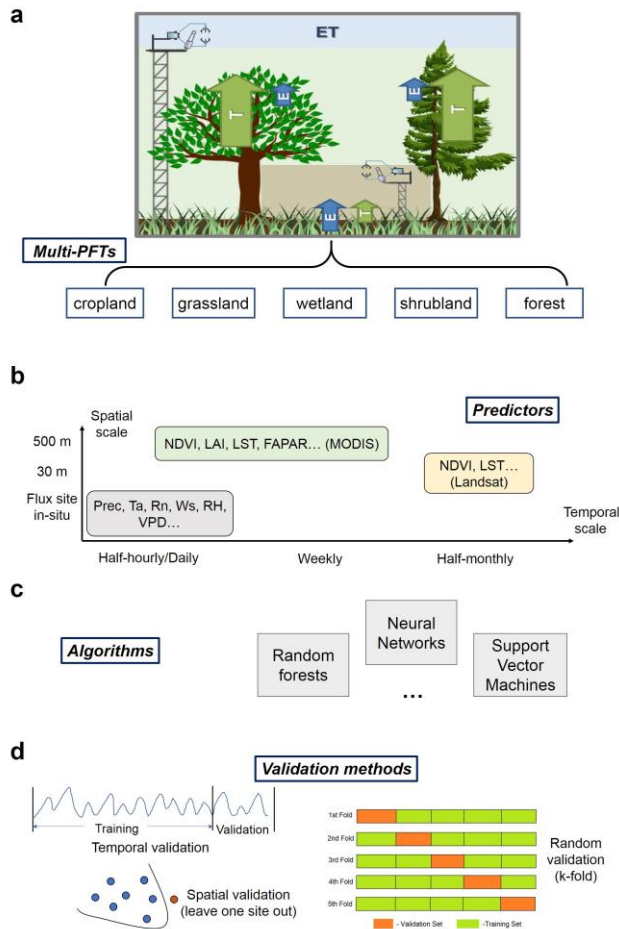
173

174   Table 1. Article search: '[A1 OR A2 OR A3...] AND [B1 OR B2 OR B3...] AND [C1 OR C2 OR C3 OR C4...]'

ID	A	B	C
1	Water flux	Eddy covariance	Machine learning
2	Evapotranspiration	Flux tower	Support Vector
3	Latent heat	Flux site	Neural Network
4			Random Forest

175

2.2 Features of the prediction processes evaluated

The various features (Table 2) involved in the water flux modeling framework (Fig. 1) include the PFTs of the sites, the predictors used, the machine learning algorithms, the validation methods, and other features. Each model for which R-squared is reported is treated as a data record. If multiple algorithms were applied to the same dataset, then multiple records were extracted. Models using different data or features are also recorded as multiple records.

182

183 Figure 1. Features of the machine learning-based water flux prediction process. (a) the eddy-covariance-based

184 water flux observations of various plant function types (PFTs), modified from Paul-Limoges et al., 2020. ET,

185 evapotranspiration. E, evaporation. T, transpiration. (b) Predictors and their spatial and temporal resolution. (c)

186 The machine learning algorithms used for the modeling, such as neural networks, random forests, etc. (d) The

187 model validation methods used including the spatial, temporal, and random cross-validations.

188

189 Table 2. ~~Description of~~Model feature-related information ~~extracted~~collected from the papers included ~~papers~~in

190 this meta-analysis.

Field	Definition & Categories adopted	Harmonization
Climate	Climate zones of the study location derived from the Köppen climate classification (Peel et al., 2007)	

Plant functional type (PFT)	PFT of the flux sites: 1-forest, 2-grassland, 3-cropland, 4-wetland, 5-shrubland, 6-savannah, and multi-PFTs	The categorization is based on the descriptions in the article. For example, cropland for various crops is classified as 'cropland', and both woody savannah and savannah are classified as 'savannah'.
Location	More precise location (with the latitude and longitude of the center of the studied sites): latitude, longitude	
Algorithms	Random Forests (RF), Multiple Linear Regressions (MLR), Artificial Neural Networks (ANN), Support Vector Machines (SVM), Cubist, model tree ensembles (MTE), K-nearest neighbors (KNN), long short-term memory (LSTM), gradient boosting regression tree (GBRT), extra tree regressor (ETR), Gaussian process regression (GPR), Bayesian model averaging (BMA), extreme learning machine (ELM), and deep belief network (DBN)	Various model algorithms with parameter optimization or other improvements are categorized as their algorithm family. For example, various improved models of RF algorithms are classified as RF, rather than as another algorithm family.
Sites number	Number of the flux sites used in the prediction model development	
Spatial scale	Area representatively covered by the flux sites: local (less than 100 x 100 km), regional, global (continent-scale and global scale)	The spatial scale is roughly categorized based on the area covered by the site. The model is classified as 'global' only when the spatial extent reaches the continental scale.
Temporal scale	The temporal scale of the model: half-hourly, hourly, daily, 4-daily, 8-daily, monthly, seasonally (i.e., 0.02, 0.04, 1, 4, 8, 30, 90 days)	Models with a temporal scale greater than one month and less than one year are classified as seasonal scale models.
Year span	The span of years of the flux ~~data used~~observations	Year span is calculated as the span from the earliest to the latest year of available flux data.
Site year	~~Describe the~~The volume of total flux data ~~with~~aggregated by the number of sites and years ~~aggregated.~~	
Cross-validation	~~Describe the chosen method of cross-~~Strategies in model validation: ~~Spatial~~spatial (e.g., 'leave one site out'), temporal (e.g., 'leave one year out'), random (e.g., 'k-fold')	
Training/validation	~~Describe the~~The ratio of the data volume in the training and validation sets~~.~~	In spatial validation, this ratio is represented by the ratio of the number of sites used for training to the number of sites used for validation. In temporal validation, this is represented by the ratio of the span of time periods used for training to the span of time periods used for validation.
Satellite images	~~Describe the~~The source of satellite images used to derive ~~NDVI, EVI,~~remote sensing-based predictors (e.g., leaf area index (LAI~~,~~ ~~LST,~~)), etc: Landsat, MODIS, AVHRR	

Biophysical predictors	~~LAI,~~ NDVI/EVI, the fraction of absorbed photosynthetically active radiation/photosynthetically active radiation (FAPAR/PAR), ~~leaf area index (~~LAI~~),~~. Carbon fluxes (CF) including NEE/GPP, etc.	The predictor variables of different measurement methods are categorized according to their definitions. For example, both using the NDVI calculated based on satellite remote sensing bands and in situ measurements were classified as the use of 'NDVI'.
Meteorological variables	~~precipitation~~Precipitation (Prec), net radiation/solar radiation (Rn/Rs), air temperature (Ta), vapour-pressure deficit (VPD), relative humidity (RH) , etc.	The way meteorological data are measured is not differentiated. For example, both using Ta from reanalysis data and Ta measured at flux sites were classified as the use of Ta.
Ancillary data	~~Describe the~~The ancillary predictor variables used in the modeling: soil texture, terrain (DEM), soil moisture/land surface water index (SM/LSWI), etc~~.~~	Both the use of in situ measured soil moisture and the use of remote sensing-based LSWI was classified as using surface moisture-related indicators SM/LSWI.
Accuracy ~~measure~~metric	Accuracy ~~measure~~metric used ~~to assess the model performance~~: R-squared (in the validation phase)	

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3 Results

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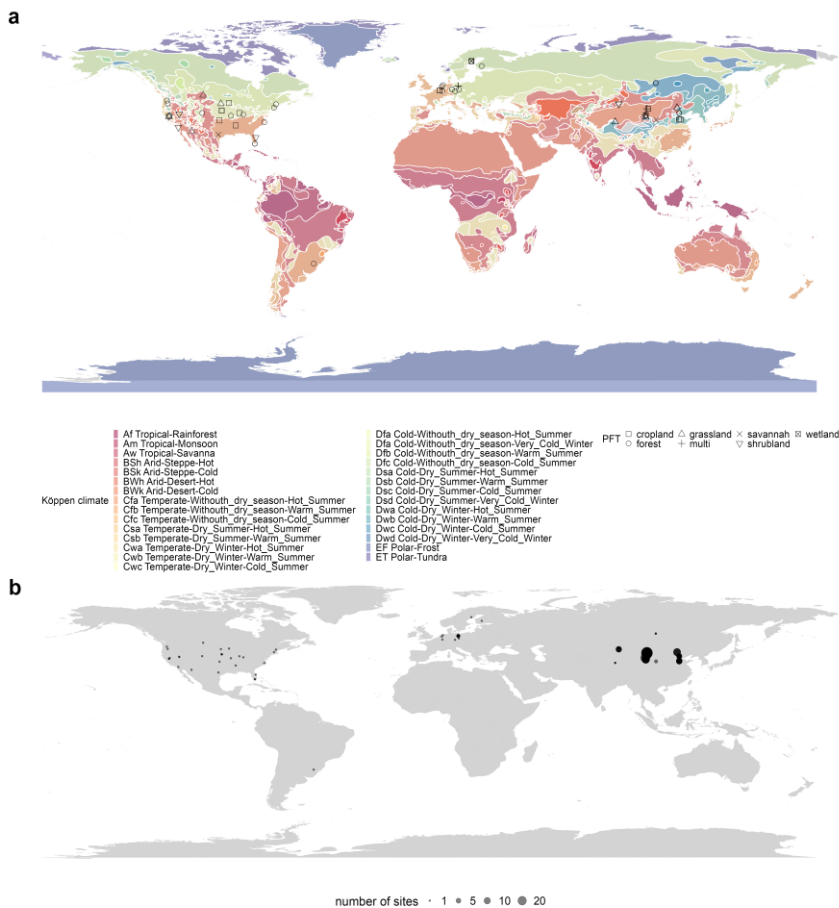
3.1 Articles included in the meta-analysis

A total of 32 articles (Table S1) containing a total of 139 model records were included. The geographical scope of these articles was mainly Europe, North America, and China (Fig. 2).

196

197 Figure 2. Location of the included studies in the meta-analysis. (a) PFTs and the climate zones (from Köppen

198 climate classification) of these studies and (b) the number of flux sites included in each study. Global and

199 continental-scale studies (e.g., models developed based on FLUXNET of the global scale) are not shown on the

200 map due to the difficulty of identifying specific locations.

3.2 The formal Meta-analysis

201

3.2.1 Algorithms

202

203 SVM and RF outperformed (Fig. 3a) across studies (better than other algorithms with sufficient sample size in

204 Fig. 3a such as ANN). These three machine learning algorithms (i.e., ANN, SVM, RF) were significantly more

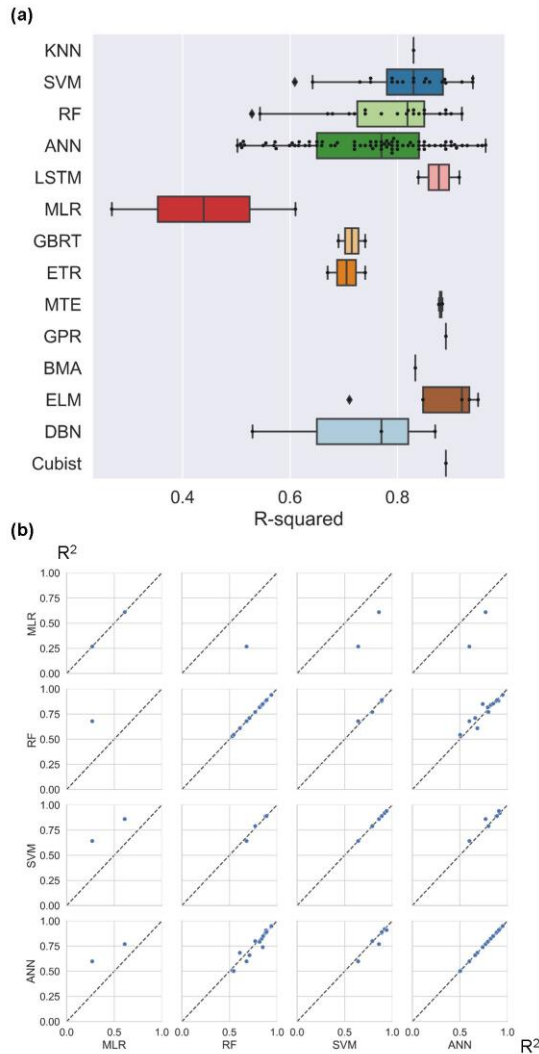
205 accurate than the traditional MLR. Other algorithms such as MTE, ELM, Cubist, etc. also correspond to high

206 accuracy, but with limited evidence sample size (Fig. 3a). In the internal comparison (different algorithms

207 applied to the same data set) in single studies, we also find that SVM and RF were slightly more accurate than

208 ANN (Fig. 3b), and all these three (i.e., ANN, SVM, RF) are considerably more accurate than MLR. Overall,

209 SVM and RF have shown higher accuracy in water flux simulations in both inter and intra-study comparisons

210 with sufficient sample size as evidence.

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212 Figure 3. Model accuracy (R-squared) using various algorithms across studies (a) and internal comparisons of

213 selected pairs of algorithms within studies (b). Algorithms: Random Forests (RF), Multiple Linear Regressions

214 (MLR), Artificial Neural Networks (ANN), Support Vector Machines (SVM), Bayesian model averaging

215 (BMA), Cubist, model tree ensembles (MTE), gradient boosting regression tree (GBRT), extra tree regressor

216 (ETR), K-nearest neighbors (KNN), long short-term memory (LSTM), Gaussian process regression (GPR),

217 extreme learning machine (ELM), and deep belief network (DBN).

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3.2.2 Climate types and PFTs

We found higher average model accuracy in arid climate zones (Fig. 4a), such as the Cold semi-arid (steppe) climate (BSk) and Cold desert climate (BWk). Most of these studies were located in northwest China and the western USA. It may be caused by the simpler relationship between water fluxes and biophysical covariates in arid regions. In arid zones, due to the high potential ET, the variability in the actual ET may be largely explained by water availability (moisture supply) and vegetation change with the effect of variability in thermal conditions reduced. As for the various PFTs, the average model accuracy was slightly lower for forest types than for cropland and grassland types (Fig. 4b). The lowest average accuracy was found for shrub sites, which may be related to the difficulty of the remote sensing-based vegetation index (e.g., NDVI) to quantify the physiological and ecological conditions of shrubs (Zeng et al., 2022), and the heterogeneity of the spatial distribution of shrubs within the EC observation area may also cause difficulties in capturing their relationships with biophysical variables. We also found high model accuracy for the wetland type, although records as evidence to support this finding may be limited. Compared to other PFTs, the more steady and adequate water availability in the wetland type may make the variations of water fluxes less explained by other biophysical covariates.

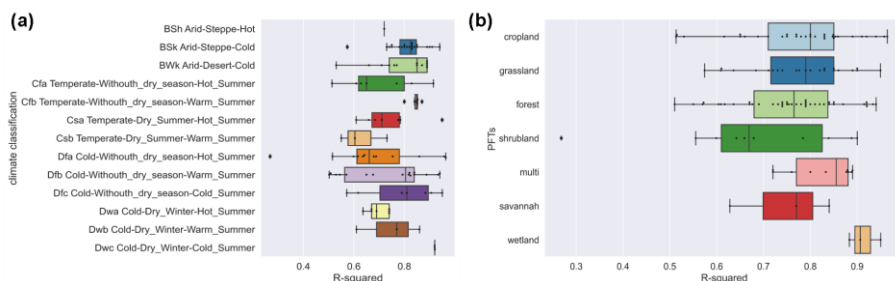



Figure 4. Differences in model accuracy (R-squared) of (a) various climate zones (classified by Köppen climate classification) across studies and (b) PFTs. BSh, Hot semi-arid (steppe) climate. BSk, Cold semi-arid (steppe) climate. BWk, Cold desert climate. Cfa, Humid subtropical climate. Cfb, Temperate oceanic climate. Csa, Hot-summer Mediterranean climate. Csb, Warm-summer Mediterranean climate. Dfa, Hot-summer humid continental climate. Dfb, Warm-summer humid continental climate. Dfc, Subarctic climate. Dwa, Monsoon-influenced hot-summer humid continental climate. Dwb, Monsoon-influenced warm-summer humid continental climate. Dwc, Monsoon-influenced subarctic climate.

3.3.3 Predictors and their combinations

On one hand, for the effects of individual predictors, the use of Rn/Rs, Prec, Ta, and FAPAR improved the accuracy of the model (Fig. S1). This pattern partially changed in the different PFTs. In the forest sites, the accuracy of the models with Rn/Rs and Ta used was higher than that of the models with Rn/Rs and Ta not used. For the grassland sites, the use of Ws, FAPAR, Prec, and Rn/Rs improved the model accuracy. For the cropland sites, Ta and FAPAR were more important for improving the model accuracy.

On the other hand, the evaluation of the effect of individual predictors on model accuracy is not necessarily reliable because some predictor variables are used together (e.g., the high model accuracy corresponding to a particular variable may be because it is often used together with another variable that plays the dominant role in

250 improving accuracy). Therefore, we tested for independence between the use of variables and assessed the effect

251 of the combination of variables on model accuracy. We calculated the correlation matrix (Fig. S2) between the

252 use of various predictors (not used is set as 0 and used is set as 1). We found there was a dependence between

253 the use of some predictors, the use of NDVI/EVI, LAI, and SM was significantly negatively correlated with the

254 use of Rn/Rs and Ta (Fig. S2). It indicated that many of the models that used Rn/Rs and Ta did not use

255 NDVI/EVI, LAI, and SM, and the models that used NDVI/EVI, LAI, and SM also happened to not use Rn/Rs

256 and Ta. Given this dependence, we evaluated the effect of the combination of variables on the model accuracy

257 (Fig. 5). In Fig. 5, the three variable combinations on the left side are mainly meteorological variables while the

258 three variable combinations on the right side are mainly vegetation-related variables based on remote sensing

259 (e.g., NDVI, EVI, LAI, LSWI). We found that, overall, the accuracy of the models using only meteorological

260 variable combinations was higher than that of the models using only remote sensing-based vegetation-related

261 variables. It demonstrated the importance of using meteorological variables in machine learning-based ET

262 prediction (probably especially for models with small time scales such as hourly scale, and daily scale). For

263 example, in the forest type, the combination of Ta and Rn/Rs is very effective compared to using only remote

264 sensing-based vegetation index variable combinations. The combination of Ta and Rn/Rs is also effective in the

265 grassland and cropland types. The combination of Ws and Rn/Rs played an important role in the grassland type

266 for improving model accuracy. Despite this, it does not negate the positive role of remote sensing-based

267 vegetation-related variables in ET prediction. This effectiveness can be dependent on the time scale of the model

268 as well as the PFTs. In models with large time scales (monthly scale, seasonal scale) and PFTs in which ET is

269 sensitive to vegetation dynamics, remote sensing-based vegetation-related variables may also be of high

270 importance.

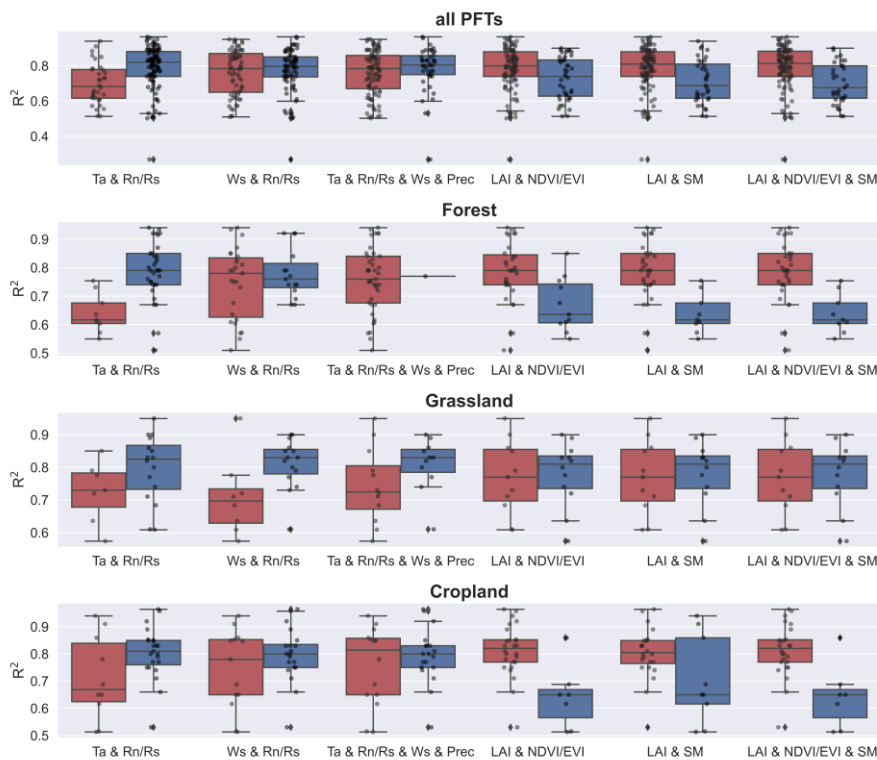
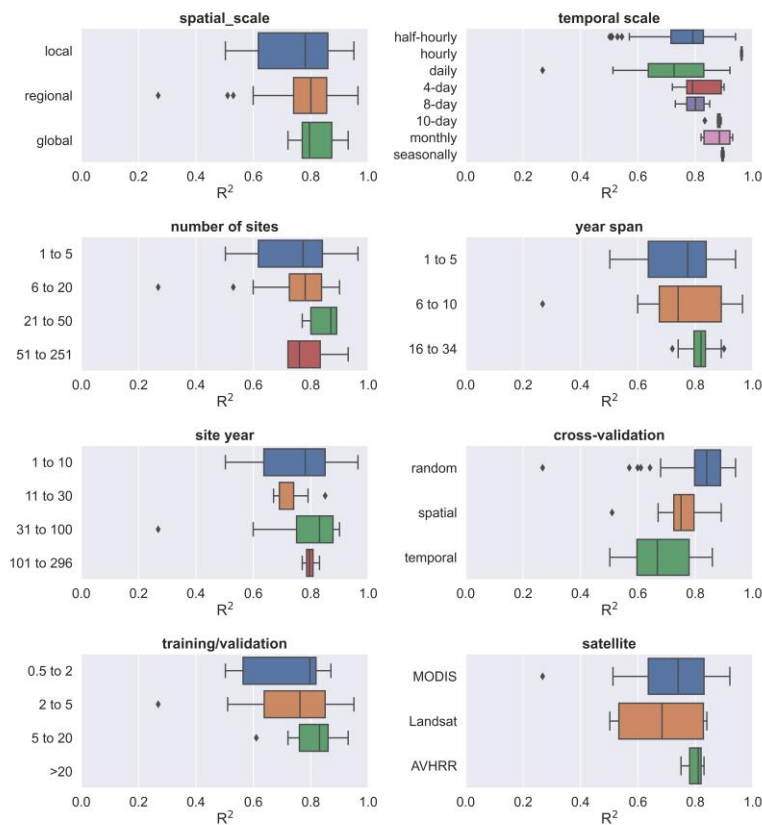



Figure 5. Effects of combinations of predictor variables on model accuracy in various PFTs (all data, forest, grassland, and cropland). Dark blue boxes indicate that the predictors were together used in the model (e.g., for 'Ta & Rn/Rs', the dark blue box represents Ta and Rn/Rs were together used in the model), while dark red boxes indicate the other conditions (i.e., the combination was not used). Predictors: precipitation (Prec), soil moisture/remote sensing-based land surface water index (SM), net radiation/solar radiation (Rn/Rs), enhanced vegetation index (EVI), air temperature (Ta), leaf area index (LAI), Normalized Difference Vegetation Index/Enhanced Vegetation Index (NDVI/EVI).

3.3.4 Other model features

We also evaluated the impact of some other features on accuracy. The differences in the accuracy of models with different spatial scales, year spans, number of sites, and volume of data (Fig. 6) appear to be insignificant. This seems to be related to the fact that in large-scale water flux simulations, the sites of similar PFTs are selected such as for modeling multiple forest sites across Europe (Van Wijk and Bouten, 1999) which focus on 'forest' and multiple grassland sites across arid northern China (Xie et al., 2021; Zhang et al., 2021) which focus on 'grassland', rather than mixing different PFT types to train models as the way in machine learning modeling of carbon fluxes (Zeng et al., 2020). In terms of the time scales of the models, the 4-day, 8-day, and monthly scales appear to correspond to higher accuracy compared to the half-hourly and daily scales. The higher the ratio of the volume of data in the training and validation sets, the higher the model accuracy. Compared to the models

289 using Landsat data, the models using MODIS data showed slightly higher accuracy probably due to the
290 advantage of MODIS data in capturing the temporal dynamics of biophysical covariates. There were significant
291 differences in the accuracy of the models using different cross-validation methods, with the models using
292 random cross-validation showing higher accuracy than those using temporal cross-validation. This suggests that
293 interannual variability may have a high impact on the models in water flux simulations. The driving mechanism
294 of ET may vary significantly across years, and the inclusion of some extreme climatic conditions in the training
295 set may be important for model accuracy and robustness.

296
297 Figure 6. The effects of other model features (i.e. spatial scale, number of sites, temporal scale, year span, site
298 year, validation method, training/validation ratio, and satellite imagery used) on the R-squared.

3.3.5 Linear correlation of quantitative features and R-squared

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300 We also analyzed the linear correlation (Fig. 7) between multiple quantitative features and the R-squared. We
301 found that the magnitude of the linear correlation coefficients between the use of predictor combinations and the
302 R-squared was higher than other features. The use of the predictor combination 'Ta and Rn/Rs' significantly
303 improved the model accuracy. 'Temporal scale', 'time span', 'training/validation ratio', and 'number of sites'

304 showed weak positive correlations with R-squared (not significant, p-value > 0.1). The positive correlation

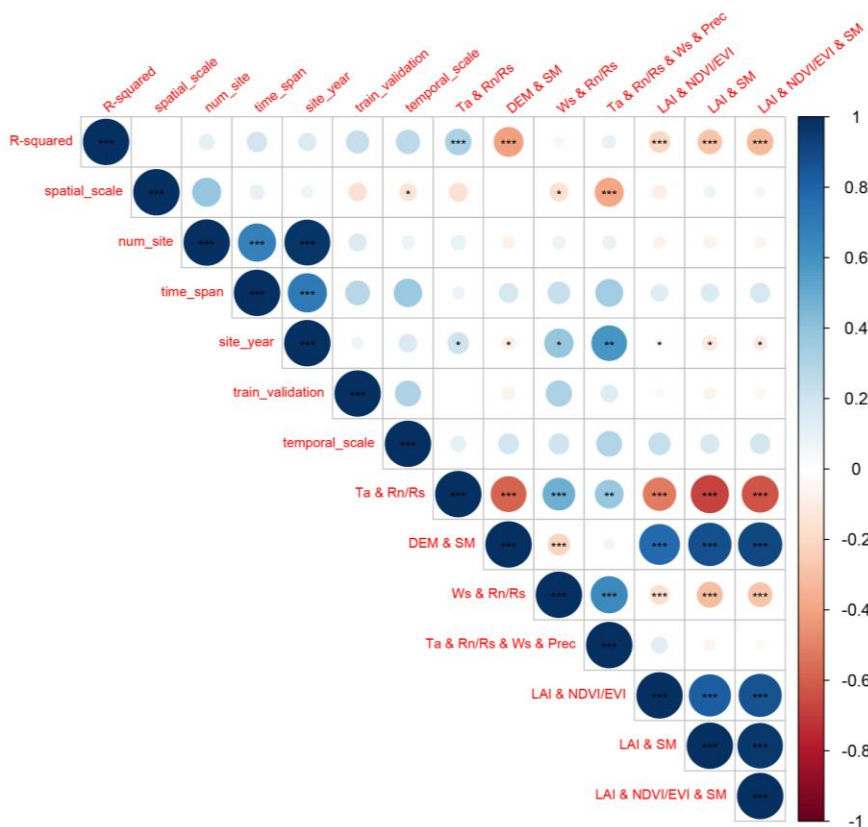
305 between 'temporal scale' and R-squared is higher among these features, although not significant. It should also

306 be paid more attention to in future studies. The feature 'training/validation ratio' and 'time span' are also

307 positively correlated (although not significantly) with the R-squared, suggesting the importance of the volume of

308 data in the training set in a data-driven machine learning model. Larger 'training/validation ratio' and 'time span'

309 may correspond to greater proportional coverage of the scenarios/conditions in the training set over the

310 validation set, and thus correspond to higher accuracy.

311

312 Figure 7. Evaluation of linear correlations between multiple features and the R-squared records with the

313 statistical significance test. For the feature 'spatial scale', the 'local' scale was set to 1, the 'regional' scale was

314 set to 2, and the 'global' scale was set to 3 in the analysis of linear correlation. For the use of various predictor

315 combinations with '&', the value for 'together used' is set as 1 and other conditions are set as 0 (e.g., for the

316 feature 'Ta & Rn/Rs & Ws & Prec', if Ta, Rn/Rs, Ws, and Prec were used together in the model, the value is set

317 as 1). Significance: the p-value < 0.01 (***), 0.05 (**), and 0.1 (*).

4 Discussions

With the accumulation of in situ EC observations around the world, the study of ET simulations based on data-driven approaches has received more attention from researchers in the last decade. Many studies have combined EC observations, various predictors, and machine learning algorithms to improve the prediction accuracy of water fluxes. To date, the results of these studies have not been comprehensively evaluated to provide clear guidance for feature selection in water flux prediction models. To better understand the approach and guide future research, we performed a meta-analysis of such studies. Machine learning-based water flux simulations and predictions still suffer from high uncertainty. By investigating the expected improvements that can be achieved by incorporating different features, we can avoid practices that may reduce model accuracy in future research.

4.1 Opportunities and challenges in the water flux simulation

In the above meta-analysis of the models, we found that water flux simulations based on EC observations can achieve high accuracy but also have high uncertainty through the modeling workflow. The R-squared of many water flux simulation models exceeds 0.8, possibly higher than some remote sensing-based and process-based models, and possibly higher than carbon flux simulations such as the net ecosystem exchange (NEE) in a similar modeling framework (Shi et al., 2022). This may be because many data on important variables affecting carbon flux such as soil and biomass pools, disturbances, ecosystem age, management activities, and land use history are not yet effectively and continuously measured (Jung et al., 2011) with the global spatially and temporally explicit information. While ET simulations rely on observations of moisture and energy conditions and vegetation conditions, much of the current available meteorological and remote sensing data have been effective to represent and capture the spatial and temporal dynamics of these predictors well.

4.1.1 Comprehensive insights on model features

Biophysical and meteorological variables are considered both important in ET simulations. This study found that models using a combination of meteorological variables had higher accuracy than models using only remotely sensed vegetation dynamic information. However, due to the high proportion of models with small temporal scales (e.g., half-hourly scale, hourly scale, and daily scale) in this study, this advantage of the combination of meteorological variables may be more suitable for small temporal scales. A possible explanation is that vegetation-related variables such as NDVI and LAI at the daily scale, 8-day scale, and 16-day scale have limited explanatory ability for hourly or daily-scale variability in ET, especially under cloudy conditions (e.g., tropical rainforest regions), the temporal continuity of the vegetation index data may be greatly limited (Zeng et al., 2022). This should be given more attention and some vegetation indices derived from hourly temporal resolution satellite remote sensing data such as GOES (Zeng et al., 2022) can be used for ET simulations to investigate the possible adding-values of vegetation indices at smaller time scales. In contrast, at a small temporal scale, the use of combinations of meteorological variables can capture moisture and energy conditions that control the rapid fluctuations of ET and thus has a dominant role in hourly or daily-scale ET prediction. This also corroborates the high accuracy of some physic-based ET estimation models (Rigden and Salvucci, 2015) that use only meteorological variables and not vegetation-related variables such NDVI (only an estimate

of vegetation height derived from land cover maps is used to represent vegetation conditions (Rigden and Salvucci, 2015)).

There are differences in model accuracy among different PFTs. For example, in forest sites, limitations in data accuracy of factors were possible because some remote sensing-based predictors such as NDVI, FAPAR, and LAI have limited accuracy when applied to forest types (Liu et al., 2018b; Zeng et al., 2022). In addition, factors such as crown density, which may significantly affect the proportion of soil evaporation, transpiration, and evaporation of canopy interception, were not considered in these models, which may also lead to low model accuracy. This suggests that in water flux simulation, the driving mechanisms of water fluxes in different PFTs do affect the accuracy of machine learning models, and we need to consider more the actual and specific influencing factors in specific PFTs. More variables that can quantify the ratio of evaporation and transpiration should be considered for inclusion, which also appears to improve the mechanistic interpretability of such machine learning models. A previous study (Zhao et al., 2019) combined the physics-based approach (e.g., Penman-Monteith equation) and machine learning to build hybrid models to improve interpretability. We should make full use of empirical knowledge and experiences from process-based models to improve the accuracy and interpretability of the machine learning approach.

Among the validation methods, random cross-validation has higher accuracy than spatial cross-validation and temporal cross-validation. However, spatial cross-validation and temporal cross-validation may be able to better help us recognize the robustness of the model when extrapolated (i.e., applied to new stations and new years). The lower accuracy in the temporal cross-validation approach implies that we need to focus on interannual hydrological and meteorological variability in the water flux simulations. In cropland sites, we may also need to pay more attention to the effects of interannual variability in anthropogenic cropping patterns. If some extreme weather years are not included, the robustness of the model when extrapolated to other years may be challenged, especially in the context of the various extreme weather events of recent years. This can also inform the siting of future flux stations. Regions where climate extremes may occur and biogeographic types not covered by existing flux observation networks should be given more attention to achieve global-scale, accurate and robust machine learning-based spatio-temporal prediction of water fluxes. Furthermore, although the R-squared and the training/validation ratio show a positive correlation (Fig. 7) (i.e., a higher training/validation ratio may correspond to a higher R-squared), we should still be cautious in reducing this ratio in our modeling. For a really small validation set, it would be very challenging to determine which model is better given the potential uncertainty caused by the considerable randomness.

4.1.2 Differences from NEE predictions in the similar model framework

In general, predictors related to meteorological, vegetation, and soil conditions were common to both ET and NEE simulations in a similar framework (Shi et al., 2022). However, in NEE predictions, explanatory variables such as soil organic content, photosynthetic photon flux density, and growing degree days (Shi et al., 2022) are not necessary for ET predictions. The selection of these variables requires our prior knowledge of the dominant drivers of ET and NEE anomalies of particular ecosystems and their differences.

The accuracy of NEE predictions (Shi et al., 2022) can be more limited by global variability across biomes and locations (Nemani et al., 2003) given the lack of locally measured data on soil and biomass pools, disturbances, ecosystem age, management activities and land use history (Jung et al., 2011). It can result in a higher heterogeneity of the training data in large-scale modeling with multiple flux sites (Shi et al., 2022) and the weak ability to capture the NEE anomalies. In contrast, in ET predictions, meteorological variables and vegetation conditions appear to be already sufficient to capture a considerably large fraction of the ET variations in most conditions.

In future ET prediction studies, given that few current ET products have time scales smaller than daily scale (Jung et al., 2019; Pan et al., 2020), improvements in the accuracy of daily and hourly models may be necessary to fill this gap. Besides, the partitioning of ET components (i.e., transpiration, interception evaporation, and soil evaporation) can be more focused to better decouple the contributions of vegetation and soil to ET with machine learning (Eichelmann et al., 2022). It can be further matched with the partitioning of NEE (i.e., to GPP and ecosystem respiration) to increase our knowledge of the global water cycle and ecosystem functioning and obtain further refined global carbon-water fluxes coupling relations (Eichelmann et al., 2022). Also, the above two promising improvements can be beneficial for research on topics related to the global terrestrial water cycle (Fisher et al., 2017).

4.2 Uncertainties and limitations of this meta-analysis

4.2.1 The limited number of available literature and model records

Despite many articles and model records collected through our efforts to perform this meta-analysis, there still appears to be a long way to go to finally and completely understand the various mechanisms involved in water flux simulation with machine learning. Some of the insights provided by this study can be not robust (due to the limited sample size available when the goal is to assess the effects of multiple features), but this does not negate the fact that this study does obtain some meaningful findings. Therefore, researchers should treat the results of this study with caution, as they were obtained only statistically. Overall, it is still positive to conduct a meta-analysis of such studies, considering their rapid growth in the number and lack of guiding directions.

4.2.2 Publication bias and weighting

Publication bias and weighting: ~~Due to the relatively limited number of articles that could be included in the~~ In a meta-analysis, ~~this study did not focus much on publication bias. Meta-analytic studies~~ in other fields ~~typically measure~~, weights for different studies can be assigned based on the quality of ~~journals~~the journal and the ~~public availability of~~ extent to which the research data are publicly available (Borenstein et al., 2011; Field and Gillett, 2010) ~~to determine the weighting of the literature in a comprehensive assessment.~~. However, most of the articles included in this study did not ~~publicly provide~~ fully publish the flux ~~observations or share~~data they used, the models they developed ~~models. Meta-analysis studies~~, and the predicted ET data. Given this limitation, we were unable to assign them small weights due to the relatively limited available sample size of this study. Besides, in meta-analyses in other fields ~~typically measure~~, the ~~impact of included studies based on~~ sample size and the variance of ~~experimental~~the results of the experiments can also be used to adjust the weights of the effects among studies (Adams et al., 1997; Don et al., 2011; Liu et al., 2018a). ~~In~~However, for this study, due to

432   the lack of a convincing ~~manner~~way to determine the weights ~~among articles~~, we briefly assigned ~~the same~~equal

433   weight values to ~~the results for~~ all the ~~literature~~included studies.

434   **4.2.3 Uncertainties in the information of the extracted features**

435   At the information extraction level, the following issues may also introduce uncertainties:

436   a)   Uncertainties caused by data quality control (e.g. gap-filling (Hui et al., 2004)) are difficult to assess

437   effectively. Gap-filling is a commonly used technique to fill in low-quality data in flux observations.

438   However, the impact of this practice on machine learning-based ET prediction models is unclear, due to the

439   difficulty of directly assessing how this technique is performed in various studies by this meta-analysis.

440   Typically, models with small time scales (e.g., hourly scale, daily scale) can exclude low-quality

441   observations and use only high-quality data. However, for models with large time scales (e.g., monthly

442   scales), gap-filling (e.g., based on meteorological data) may be unavoidable. This may lead to a decrease in

443   training data purity and introduce uncertainty in the subsequent prediction model development.

444   b)   Systematic uncertainties caused by the energy balance closure (EBC) issue in eddy-covariance flux

445   measurements are also difficult to assess by this meta-analysis. EBC is a common problem (Eshonkulov et

446   al., 2019) in eddy-covariance flux observations. For that reason, the latent heat flux measured potentially

447   underestimates ET. Some prediction models corrected EBC (e.g., using Bowen ratio preserving (Mauder et

448   al., 2013, 2018) and energy balance residuals (Charuchittipan et al., 2014; Mauder et al., 2018)) in the

449   processing of training data, but some did not. How this will affect the accuracy of the prediction model is

450   not clear due to multiple factors that need to be evaluated that influence EBC (Foken, 2008), including

451   measurement errors of the energy balance components, incorrect sensor configurations, influences of

452   heterogeneous canopy height, unconsidered energy storage terms in the soil-plant-atmosphere system,

453   inadequate time averaging intervals, and long-wave eddies (Jacobs et al., 2008; Foken, 2008; Eshonkulov

454   et al., 2019). To reduce this uncertainty, more attention to flux site characteristics (Eshonkulov et al., 2019)

455   related to PFT, topography, flux footprint area, etc., to select the appropriate correction method is

456   necessary for future studies.

457   c)   As most studies used far more water flux observation records than the number of covariates in their

458   regression models, we did not adjust the R-squared in this study to an adjusted R-squared.

459   d)   The various specific ways in which the parameters of the model are optimized are not differentiated. They

460   are broadly categorized into different families or kinds of algorithms, which may also introduce uncertainty

461   into the assessment.

462   e)   The assessment of some features is not detailed due to the limitations of the available model records. For

463   example, the classification of PFT could be more detailed. 'Forest' could be further classified as broadleaf

464   forest, coniferous forest, etc. while 'cropland' could be further classified as rainfed and irrigated cropland

465   based on differences in their response mechanisms of water fluxes to environmental factors.

466   **5 Conclusion**

467   We performed a meta-analysis of the water flux ~~simulations combining in situ flux~~simulation studies which

468   focus on using machine learning approaches to combine flux station observations from flux stations/networks,

469 meteorological, biophysical, and other ancillary predictors, ~~and machine learning~~. The main conclusions are as
470 follows:

471 1. SVM (average R-squared = 0.82) and RF (average R-squared = 0.81) outperformed over evaluated
472   algorithms with sufficient sample size in both cross-study and intra-study (with the same training dataset)
473   comparisons.

474 2. The average accuracy of the model applied to arid regions is higher than in other climate types.

475 3. The average accuracy of the model was slightly lower for forest sites (average R-squared = 0.76) than for
476   cropland and grassland sites (average R-squared = 0.8 and 0.79), but higher than for shrub sites (average R-
477   squared = 0.67).

478 4. Among various predictor variables, the use of Rn/Rs, Prec, Ta, and FAPAR improved the model accuracy.
479   The combination of Ta and Rn/Rs is very effective especially in the forest type, while in the grassland type
480   the combination of Ws and Rn/Rs is also effective.

481 5. Among the different validation methods, random cross-validation shows higher model accuracy than spatial
482   cross-validation and temporal cross-validation.

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Acknowledgements

We thank the editor and two anonymous reviewers for their insightful comments which contributed substantially to the improvement of this manuscript.

Financial support

This research ~~was~~has been supported by the National Natural Science Foundation of China (~~Grant No~~grant no. U1803243), the Key ~~projects~~Projects of the Natural Science Foundation of Xinjiang Autonomous Region (~~Grant No~~grant no. 2022D01D01), the Strategic Priority Research Program of the Chinese Academy of Sciences (~~Grant No~~grant no. XDA20060302), and the High-End Foreign Experts ~~Project~~project of China.

Author Contributions

HS and GL were responsible for the conceptualization, methodology, formal analysis, investigation, visualization, and writing. OH contributed to the investigation. XM, XY, YW, WZ, MX, CZ and YZ processed the data. AK, TVDV and PDM provided supervision.

Competing interests

The authors declare that they have no conflict of interest.

Code availability

The codes that were used for all analyses are available from the first author (shihaiyang16@mails.ucas.ac.cn) upon request.

Data availability

The data used in this study can be accessed by contacting the first author (shihaiyang16@mails.ucas.ac.cn) upon request.

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