PyEt v1.3.1: a Python package for the estimation of potential evapotranspiration

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Abstract.

Evapotranspiration (ET) is a crucial flux of the hydrological water balance, commonly estimated using (semi-)empirical formulas. The estimated flux may strongly depend on the formula used, adding uncertainty to the outcomes of environmental studies using ET. Climate change may cause additional uncertainty, as the ET estimated by each formula may respond differently to changes in meteorological input data. To include the effects of model uncertainty and climate change, and facilitate the use of these formulas in a consistent, tested, and reproducible workflow, we present *PyEt*. *PyEt* is an open-source Python package for the estimation of daily potential evapotranspiration (PET) using available meteorological data. It allows the application of twenty different PET methods on both time series and gridded datasets. The majority of the implemented methods are benchmarked against literature values and tested with continuous integration to ensure the correctness of the implementation. This article provides an overview of *PyEt*'s capabilities, including the estimation of PET with twenty PET methods for station, and gridded data, a simple procedure for calibrating the empirical coefficients in the alternative PET methods, and estimation of PET under warming and elevated atmospheric CO_2 concentration. Further discussion on the advantages of using *PyEt* estimates as input for hydrological models, sensitivity/uncertainty analyses, and hind/forecasting studies, especially in data-scarce regions, is provided.

1 Introduction

Evaporation — the process by which water is converted from its liquid to vapor phase — is a central component of the global hydrological cycle (Katul et al., 2012). Evaporation has far-reaching impacts on both human societies and ecosystems (Oki and Kanae, 2006; Fisher et al., 2011). In the remainder of this paper, the term evapotranspiration is used to refer to the total evaporation flux from soil and water bodies (evaporation) and vegetated surfaces (transpiration; Allen et al., 1998; Dingman, 2015). Information about the magnitude of the ET flux is important across different geoscience disciplines: it assists in predicting irrigation demands and crop water requirements in agriculture, supports efficient water resources management, guides operational strategies in hydropower and meteorological studies, and plays a crucial role in ecological research and climate-change impact assessments. Given that climate change - through warming and elevated CO_2 concentrations - is set to

alter evapotranspiration, the need for its accurate estimation is of paramount importance, as it affects our understanding and
25   assessment of past, present, and potential future impacts on ecosystem functioning (Milly and Dunne, 2016; Yang et al., 2019;
Caretta et al., 2022).

Evapotranspiration (ET) can hardly be measured directly (Wang and Dickinson, 2012; Jensen and Allen, 2016), and is
therefore commonly estimated using (semi-)empirical formulas from other, more easily obtained meteorological variables
such as temperature, wind speed, and radiation. Over time, dozens of methods have been proposed and applied. Each of these
30   methods generally results in slightly different estimates of evapotranspiration, depending on the methods and data used (Oudin
et al., 2005; McMahon et al., 2013; Xu and Singh, 2000, 2001; Lemaitre-Basset et al., 2022). Most of these formulas estimate
either the reference crop evapotranspiration (ET_0), which is ET from a reference surface or crop that is not short of water
(Allen et al., 1998), or the potential evapotranspiration (PET), which is the maximum rate of ET that would occur given a
sufficient water supply (Xiang et al., 2020). Potential evapotranspiration is determined by meteorological conditions, whereas
35   water availability determines if actual evapotranspiration occurs at its potential rate (Jensen and Allen, 2016). Differences in
the potential evapotranspiration estimate may cascade through a modeling chain and ultimately impact the results of a study.
For example, Prudhomme and Williamson (2013); Lemaitre-Basset et al. (2022); Bormann (2010) showed that the method used
affects the results from hydrological climate change impact studies. Similarly, the estimation of water demand for efficient crop
and irrigation management depends on potential evapotranspiration, and may thus be impacted by the methods used (Kumar
40   et al., 2012).

To account for the structural uncertainty of the different PET models, it has been recommended to use multiple methods
(Seiller and Anctil, 2016; Beven and Freer, 2001; Velázquez et al., 2013). Such an approach can help improve the understanding
of the effect of model uncertainty on PET estimates in, for example, historical climate studies (Zhou et al., 2020; Dakhlaoui
et al., 2020; Yang et al., 2019) and climate change impact studies (Bormann, 2010; Seiller and Anctil, 2016; Gharbia et al.,
45   2018; Shi et al., 2020). It may also be necessary to account for environmental variables that change over time and impact
the evapotranspiration, such as vegetation changes and increases in atmospheric CO_2 concentrations (Fatichi et al., 2016;
Ainsworth and Rogers, 2007; Vremec et al., 2022). To efficiently account for the structural uncertainty, the software used to
compute PET should ideally have multiple methods available, and be flexible enough to deal with such changing environmental
variables.

50   The FAIR principles of findability, accessibility, interoperability, and reusability are of crucial importance for the credibility
and reproducibility of scientific studies (Barker et al., 2022). Tools for calculating evapotranspiration, such as 'Evapotran-
spiration' in R (Guo et al., 2016), and "PyETo" (Richards, 2019) and 'pyfao56' in Python (Thorp, 2022), have significantly
advanced the field by offering valuable computational solutions. While these tools represent important advances in research
software development, there is an opportunity to enhance their compliance with the FAIR standards. This involves improv-
55   ing methodological testing through continuous integration, expanding compatibility with various data formats like NetCDF to
support regional and global ET estimation, inclusion of alternative PET methods, and enabling more flexibility in adjusting
internal empirical coefficients. Such enhancements not only adhere to best practices in software development but also broaden
the scope and applicability of these tools in diverse geoscientific contexts. The refinement and development of evapotranspi-

ration estimation tools that fully embrace the FAIR principles are therefore crucial steps toward advancing the field, ensuring
60 more reliable and comprehensive research outcomes in the face of evolving scientific needs (Wood et al., 1998; DeJonge and
Thorp, 2017).

In this paper we introduce *PyEt*, an open-source Python package for the estimation of potential evapotranspiration. The aim
of *PyEt* is to provide researchers and practitioners with a wide variety of tested, documented, and flexible Python functions
for the estimation of potential evapotranspiration. All methods have a common application programming interface, allowing
65 users to easily test different PET models for their application and, if desired, address structural uncertainty and changing
conditions. The majority of the implemented methods are benchmarked against literature values and tested with continuous
integration to ensure the correctness of the implementation. Allowing different types of input data, *PyEt* is also applicable in
regions with sparsely distributed measurement stations, where standard meteorological data (e.g., wind, relative humidity) are
often unavailable. The software is available under MIT-license from the Python Package Index (PyPI) (Vremec and Collenteur,
70 2022), and developed as a community project on GitHub (www.github.com/pyet-org/PyEt).

The remainder of this paper is structured as follows. In the next section, the software design, capabilities, and benchmarking
tests are described. The third section introduces the software through four examples, showing potential future users how to
apply *PyEt* in real-world applications. These examples concentrate on addressing practical problems commonly faced by
geoscientists in their daily work. The fourth section discusses future potential applications of *PyEt*, and how we think it can
75 help the scientific community improve the estimation of potential evapotranspiration. In the fifth and final section, conclusions
and future plans are outlined.

2 PyEt Python Package

2.1 Software design

The basic design principle for *PyEt* was to build a software that is intuitive and easy-to-use by novice users with little pro-
80 gramming experience, yet flexible enough to allow advanced users to perform more complex analyses. The software uses a
modular design, with formulas shared by different PET methods implemented as a single function. This reduces the amount
of code and makes it easier to maintain the software and implement new methods. All the PET methods are intended to work
with the minimum input data required by the PET models (e.g., radiation, temperature), but also allow more user input if such
data is available and allowed by the PET method (e.g., humidity, surface resistance in the Penman-Monteith model). Utility
85 functions are available to the user or are called internally to compute unavailable variables (e.g., solar radiation from latitude
value). Moreover, the constants in the empirical PET formulas (e.g., the Stefan Boltzmann constant) are function arguments
with default values from the literature, which may also be changed by the user to adapt the empirical relationship to another
region. Finally, the available methods should work for both station (1D) and gridded data (2D/3D).

PyEt is part of the wider Python ecosystem, and depends on three widely used and well-developed Python packages from
90 the scientific Python stack: Numpy (Harris et al., 2020), Pandas (McKinney, 201), and Xarray (Hoyer and Hamman, 2017).
The input and output data of *PyEt* are formatted as time series data in `Pandas.Series` or `Xarray.DataArrays`, which

allows using all the Pandas and/or Xarray functions on the data (Harris et al., 2020; McKinney, 201; Hoyer and Hamman, 2017). These functions include gap-filling and selection functions for interpolation, resampling, clustering, and many more. Being part of a wider ecosystem, users can leverage other Python packages for visualization (e.g., Matplotlib (Hunter, 2007),

95   MetPy (May et al., 2022)) and optimization and uncertainty analyses (Scipy (Virtanen et al., 2020), SpotPy (Houska et al., 2015)).

The software is hosted and developed on the GitHub platform, and distributed under MIT-license through the Python Packaging Index (PyPI). Documentation and example applications are available on a dedicated ReadTheDocs website (http://pyet.readthedocs.io). The documentation for individual methods is also directly available in Python from the documentation

100   strings. Each release of *PyEt* is automatically stored in the Zenodo repository and assigned a Digital Object Identifier (DOI). As such, *PyEt* complies with many of the recommendations for good research software development as given in, for example, Hutton et al. (2016) and the FAIR4RS (FAIR for Research Software) principles (Barker et al., 2022). The scripts or the Jupyter notebooks used to apply *PyEt* improve the reproducibility and provide a transparent report of the entire calculation process (Kluyver et al., 2016).
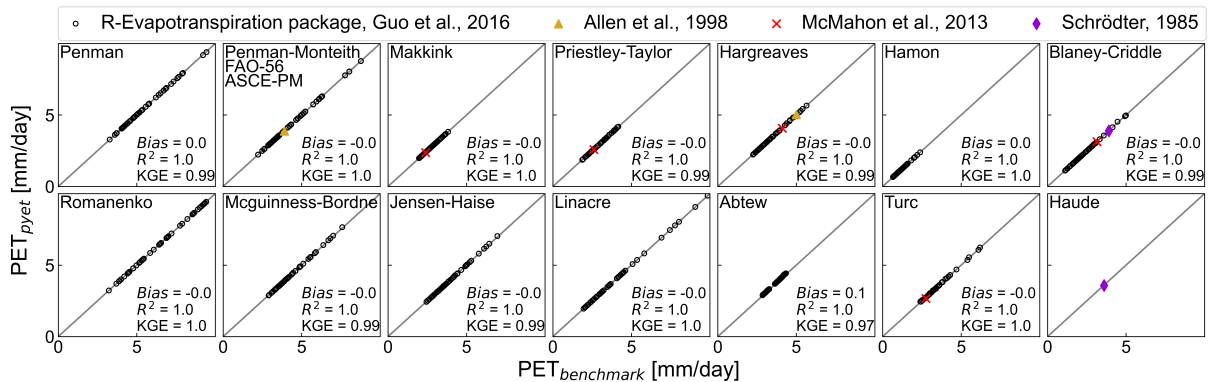
Figure 1. Scatter plots showing estimated PET with *PyEt* against PET values estimated with the R package $Evapotranspiration$ from Guo et al. (2016), and literature values from Allen et al. (1998), McMahon et al. (2013), and Schrödter (1985).

105   ## 2.2   Implemented methods and benchmarking

Twenty methods are currently implemented in *PyEt* for the estimation of daily potential evapotranspiration. In this paper, the Penman-Monteith method is considered the standard for estimating potential evapotranspiration due to its widespread use and acceptance. All other methods implemented in *PyEt* will be referred to as alternative methods. An overview of these methods and the required input data is provided in Table 1. Depending on the method, different (amounts of) input data are required

110   to compute the potential evapotranspiration. It is often also possible to provide different input data to the same method (e.g., the average or the minimum and maximum daily temperatures), or even that some input data is optional (as described in the footnotes of Table 1). In the case of optional input data, utility functions are used internally to estimate that data. In the example

Table 1. Data requirements for different PET or ET_0 models, the corresponding *PyEt* function, and if benchmarking of the method was performed. The literature references include both the original publications of the models and the manuscripts from which the equations were taken: [1] McMahon et al. (2013), [2] Oudin et al. (2005) [3] Xu and Singh (2001), [4] Ansorge and Beran (2019); Rosenberry et al. (2004), [5] Schrödter (1985), [6] Schiff (1975), [7] Jensen and Allen (2016), [8] Xu and Singh (2000)

Method name[0]	*PyEt* function	Climate data				Location		Bench.	Literature
		T	RH	R	u_2	Lat.	El.		
Penman	*penman*	$\checkmark^a$	$\checkmark^{b,c}$	$\checkmark^d$	$\checkmark$	$\checkmark^d$	$\checkmark^e$	$\checkmark$	Penman (1948)
Penman-Monteith	*pm*	$\checkmark^a$	$\checkmark^{b,c}$	$\checkmark^d$	$\checkmark$	$\checkmark^d$	$\checkmark^e$	$\checkmark$	Monteith (1965)
ET_0: ASCE-PM	*pm_asce*	$\checkmark^a$	$\checkmark^{b,c}$	$\checkmark^d$	$\checkmark$	$\checkmark^d$	$\checkmark^e$	$\checkmark$	Walter et al. (2000)
ET_0: FAO-56	*pm_fao56*	$\checkmark^a$	$\checkmark^{b,c}$	$\checkmark^d$	$\checkmark$	$\checkmark^d$	$\checkmark^e$	$\checkmark$	Allen et al. (1998)
Priestley-Taylor	*priestley_taylor*	$\checkmark$	$\checkmark^h$	$\checkmark^h$	-	$\checkmark^h$	$\checkmark^e$	$\checkmark$	Priestley and Taylor (1972)
Kimberly-Penman	*kimberly_penman*	$\checkmark^a$	$\checkmark^{b,c}$	$\checkmark^d$	$\checkmark$	$\checkmark^d$	$\checkmark^e$	-	Wright (1982)
Thom-Oliver	*thom_oliver*	$\checkmark^a$	$\checkmark^{b,c}$	$\checkmark^d$	$\checkmark$	$\checkmark^d$	$\checkmark^e$	-	Thom and Oliver (1977)
Blaney–Criddle	*blaney_criddle*	$\checkmark$	$-^i$	$-^i$	$-^i$	$\checkmark$	-	$\checkmark$	Blaney and others (1952), [1, 3, 5]
Hamon	*hamon*	$\checkmark$	-	-	-	$\checkmark$	-	$\checkmark$	Hamon (1963), [2, 4]
Romanenko	*romanenko*	$\checkmark$	$\checkmark$	-	-	-	-	$\checkmark$	Romanenko (1961), [3]
Linacre	*linacre*	$\checkmark^j$	-	-	-	$\checkmark$	-	$\checkmark$	Linacre (1977), [3]
Haude	*haude*	$\checkmark$	$\checkmark^k$	-	-	-	-	$\checkmark$	Haude (1955), [6]
Turc	*turc*	$\checkmark$	$\checkmark$	$\checkmark$	-	-	-	$\checkmark$	Turc (1961), [8]
Jensen–Haise	*jensen_haise*	$\checkmark$	-	$\checkmark^l$	-	$\checkmark^l$	-	$\checkmark$	Jensen and Haise (1963), [2, 7]
McGuinness–Bordne	*mcguinness_bordne*	$\checkmark$	-	-	-	$\checkmark$	-	$\checkmark$	McGuinness and Bordne (1972), [8]
Hargreaves	*hargreaves*	$\checkmark^m$	-	-	-	$\checkmark$	-	$\checkmark$	Hargreaves and Samani (1982), [1, 7]
ET_0: FAO-24	*fao_24*	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	-	$\checkmark^e$	-	Jensen et al. (1990)
ET_0: Abtew	*abtew*	$\checkmark$	-	$\checkmark$	-	-	-	$\checkmark$	Abtew (1996), [8]
Makkink	*makkink*	$\checkmark$	-	$\checkmark$	-	-	$\checkmark^e$	$\checkmark$	Makkink (1957), [1]
Oudin	*oudin*	$\checkmark$	-	-	-	$\checkmark$	-	-	Oudin et al. (2005)

[0] The corresponding literature to each method is provided in Table A1, in Appendix. [a] T_{max} and T_{min} can also be provided. [b] RH_{max} and RH_{min} can also be provided. [c] If actual vapor pressure is provided, RH is not needed. [d] Input for radiation can be (1) Net radiation, (2) solar radiation or (3) sunshine hours. If (1), then latitude is not needed. If (1, 3) latitude and elevation is needed. [e] One must provide either the atmospheric pressure or elevation. [f] The PM method can be used to estimate potential crop evapotranspiration, if leaf area index or crop height data is available. [g] The effect of CO_2 on stomatal resistance can be included using the formulation of Yang et al. 2019. (Yang et al., 2019). [h] If net radiation is provided, RH and Lat are not needed. [i] If method==2, u_2, RH_{min} and sunshine hours are required. [j] Additional input of T_{max} and T_{min}, or T_{dew}. [k] Input can be RH or actual vapor pressure. [l] If method==1, latitude is needed instead of R_s. [m] T_{max} and T_{min} also needed.

of the Penman-Monteith method, solar radiation does not necessarily need to be provided by the user and can be estimated from the latitude and actual duration of sunshine hours instead.

115   The *PyEt* project is intended to be used by a wide community, and any errors in the code may have consequences for other studies applying *PyEt* to obtain PET estimates. Special attention was therefore paid to benchmark the available methods to

published literature values and data from well-known research and meteorological institutes (Allen et al., 1998; McMahon et al., 2013; Schrödter, 1985; Walter et al., 2000). These benchmarks are also implemented in the continuous integration and tested using the *unittest* testing framework (unittest, 2022). This ensures that the benchmarks are satisfied each time the software

120   is updated in the future. New methods added to *PyEt* will be required to be accompanied by the appropriate benchmark data and tests. Figure 1 shows the results for each benchmarked method, indicating that the PET estimates from all these methods are equal to the benchmark values (i.e., all values are on the 1:1 line). Despite our best efforts, we acknowledge here that 4 methods have not (yet) been benchmarked due to a lack of appropriate data.

2.3   The Penman-Monteith equation

125   To illustrate how *PyEt* might be helpful in several applications, one of the most used and most versatile PET methods is discussed in more detail, the Penman-Monteith method (Monteith, 1965). In its different forms, the Penman-Monteith equation can be used to estimate reference crop evapotranspiration (Allen et al., 1998; Walter et al., 2000), potential evapotranspiration (Monteith, 1965), and potential crop evapotranspiration. The latter is defined as "the maximum value of ET from a specific crop type having specific properties under conditions of full soil water supply, but not necessarily having a saturated surface" by

130   Jensen and Allen (2016).Through the introduction of the Penman-Monteith equation by Monteith (1965), a broad applicability to different surfaces and vegetation types was achieved (Jensen and Allen, 2016). This was done by implementing the plant aerodynamic resistance (r_a) and the surface resistance (r_s) in the PET formula.

Users of *PyEt* can include leaf/canopy cover measurements (Leaf Area Index - LAI) to calculate surface resistance (r_s), thereby accounting for the effects of crop management and phenology on ET. A modified stomatal resistance model also

135   allows for the inclusion of the sensitivity of the stomatal resistance (r_l) to the atmospheric CO_2 concentration (as shown in, for example, Yang et al., 2019; Vremec et al., 2022):

$$r_s = \frac{r_l(\mathrm{CO_2})}{0.5\mathrm{LAI}} = \frac{r_{r_l-300} \times \left\{1 + S_{r_l-CO_2} \times (\mathrm{CO_2} - 300)\right\}}{0.5\mathrm{LAI}} \tag{1}$$

where $S_{r_l-[CO_2]}$ [ppm^{-1}] is the relative sensitivity of r_l to Δ [CO_2] and r_{r_l-300} [s m^{-1}] is the reference stomatal resistance when atmospheric CO_2 concentration is 300 ppm. The relative sensitivity of r_l to Δ [CO_2] represents the change in r_l per ppm

140   increase in CO_2 concentration.

If measurements of crop height exist, these data can be used to calculate the aerodynamic resistance to vapor and heat transfer (r_a) to represent the effects of crop phenology on PET:

$$r_a = \frac{\ln\left[\frac{z_m - d}{z_{om}}\right] \ln\left[\frac{z_h - d}{z_{oh}}\right]}{k^2 u_z} \tag{2}$$

where z_m is the reference level at which the wind speed is measured; z_h is the height of the temperature and humidity mea-

145   surements; k is the von Karman constant ($= 0.41$), u_z is the measured wind speed (Allen et al., 1998) and d is the zero plane

displacement height, taken as $0.67h_c$ [m]; z_{om} is the roughness parameter for momentum $(= 0.123h_c)$ [m] and z_{oh} is the roughness parameter for heat and water vapor $(= 0.1z_{om})$ [m] (Jensen and Allen, 2016).

2.4 Performance

The computational efficiency of various PET methods was assessed by examining the computation times in relation to the
150 time series length and the number of cells in an Xarray dataset. Computation time was evaluated by running all models on a benchmark configuration (with time series of varying lengths) using a 12th Gen Intel Core i7-1255U processor with 10 cores and 12 logical processors. All `Xarray.DataArrays` cover a period of 1 year, while the spatial resolution changes. This comparison highlights the trade-offs between computational complexity and data size, but also demonstrates the performance of the methods.

155 Figure 2 demonstrates that all *PyEt* methods maintain computational times below 1 second for time series data with lengths ranging from 10 to 10,000 days. For multi-dimensional data the computation time does not exceed 10 seconds for larger `Xarray.DataArrays` up to 100,000 cells. Moreover, the results in Figure 2 show that the problem scales well, and does not take proportionally more time for larger data sets. Notably, the Penman-Monteith and Priestley-Taylor methods exhibited the largest processing times, whereas methods like Jensen-Haise, Turc, Makkink, and Romanenko were faster. Future
160 improvements will aim to increase this efficiency, in particular to support faster calculations in large-scale global studies.
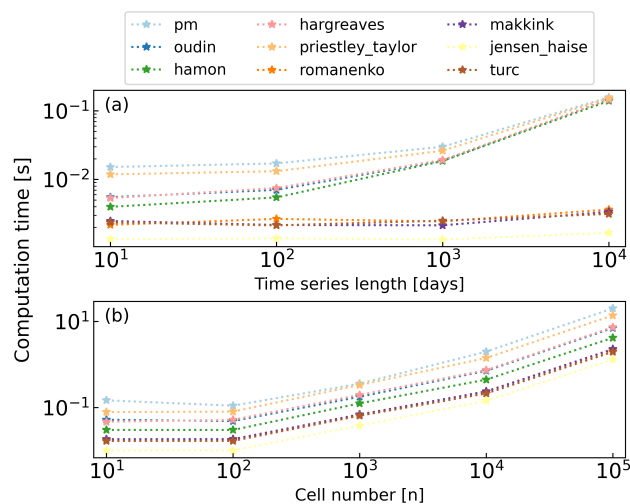
Figure 2. Computational efficiency of different PET methods:This figure shows the comparative processing times of different PET estimation methods with respect to the length of the time series (a) and the size of the Xarray data (b).

3 Example use cases

Below, four example use cases of *PyEt* are presented to illustrate how the software can be used. The first example shows how to efficiently compute different potential evapotranspiration estimates using 20 various methods for station data. This example also illustrates how to use *PyEt* in general. The second example illustrates how to provide 3D estimates of PET using 3 different

165 methods and gridded Xarray data. The third example shows how to calibrate different PET methods to local conditions and use the calibrated formula for hindcasting. The fourth and final example illustrates a workflow to account for the effects of warming and elevated CO_2 in climate change impact studies. The source code for these and other examples can be found in a Zenodo repository related to this paper (Matevz Vremec and Raoul Collenteur, 2024).

3.1 Example 1: Estimation of PET from station data

170 In this example, potential evapotranspiration is estimated for the town of De Bilt in The Netherlands using data provided by the Royal Netherlands Meteorological Institute (KNMI). The reference method used by the KNMI for the estimation of potential evapotranspiration is the Makkink method, also implemented in *PyEt*. The PET computed with the Makkink method is compared to the PET values from all other methods in *PyEt*. A number of steps are taken in a Python script to estimate PET. The code implementing these steps is shown in the code example below. *PyEt* provides a convenient way to compute the PET

175 with all available methods, *pyet.calculate_all()*:

1. Import the necessary Python packages.

```
import pandas as pd
import pyet
```

2. Load the meteorological data.

180
```
meteo = pd.read_csv("meteo.csv",
    index_col=0, parse_dates=True)
```

3. Determine the necessary input data for the PET model.

```
tmean, tmax, tmin, rh, rs, wind, \
pet_knmi = (meteo[col] for col in
            meteo.columns)
lat = 0.91  # latitude
elev = 4  # elevation
```

4. Estimate the potential evapotranspiration with all methods or the method of choice.
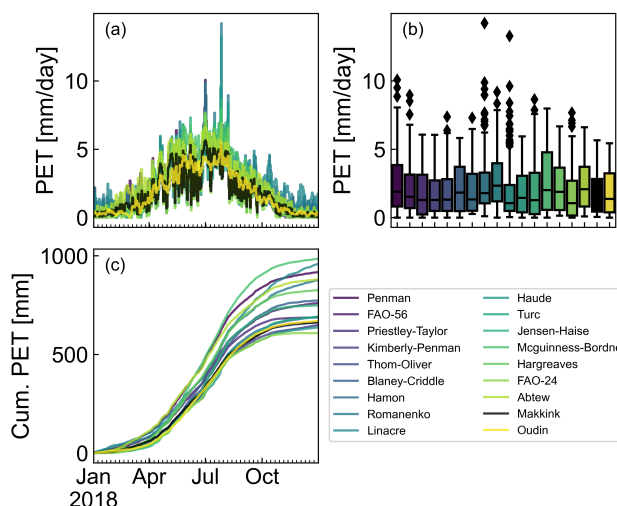
Figure 3. Potential evapotranspiration estimates for the year 2018 computed with all available PET methods, plotted as (a) time series, (b) box plots (b), (c) cumulative PET.

```
pet_df = pyet.calculate_all(tmean,
    wind, rs, elev, lat, tmax, tmin, rh)
pet_mak = pyet.makkink(tmean, rs,
    elevation=elev)
```

5. Visualize and analyze the results.

```
pet_df.plot()
pet_df.boxplot()
pet_df.cumsum().plot()
```

The results from this analysis are shown in Figure 3. From these visualizations, it is clear that the potential evapotranspiration depends on the chosen method. This can accumulate up to a 35% deviation of the estimated annual flux from the mean in this example. Such substantial differences between the estimated fluxes motivate the use of multiple methods (ensemble modelling) (Beven and Freer, 2001; Krueger et al., 2010; Shi et al., 2020; Oudin et al., 2005). This example showed how *PyEt* can be used efficiently for this task.

3.2 Example 2: Estimate PET for gridded data

Gridded 3-dimensional data (x, y, t) obtained from satellites, radar imagery, or post-processed products is rapidly becoming widely available. More and more public data sets exist with global PET estimates at 0.1 degree resolution (e.g., Martens et al., 2017; Xie et al., 2022). *PyEt* also supports such gridded data, as illustrated here for the E-OBS gridded data set (Cornes et al.,
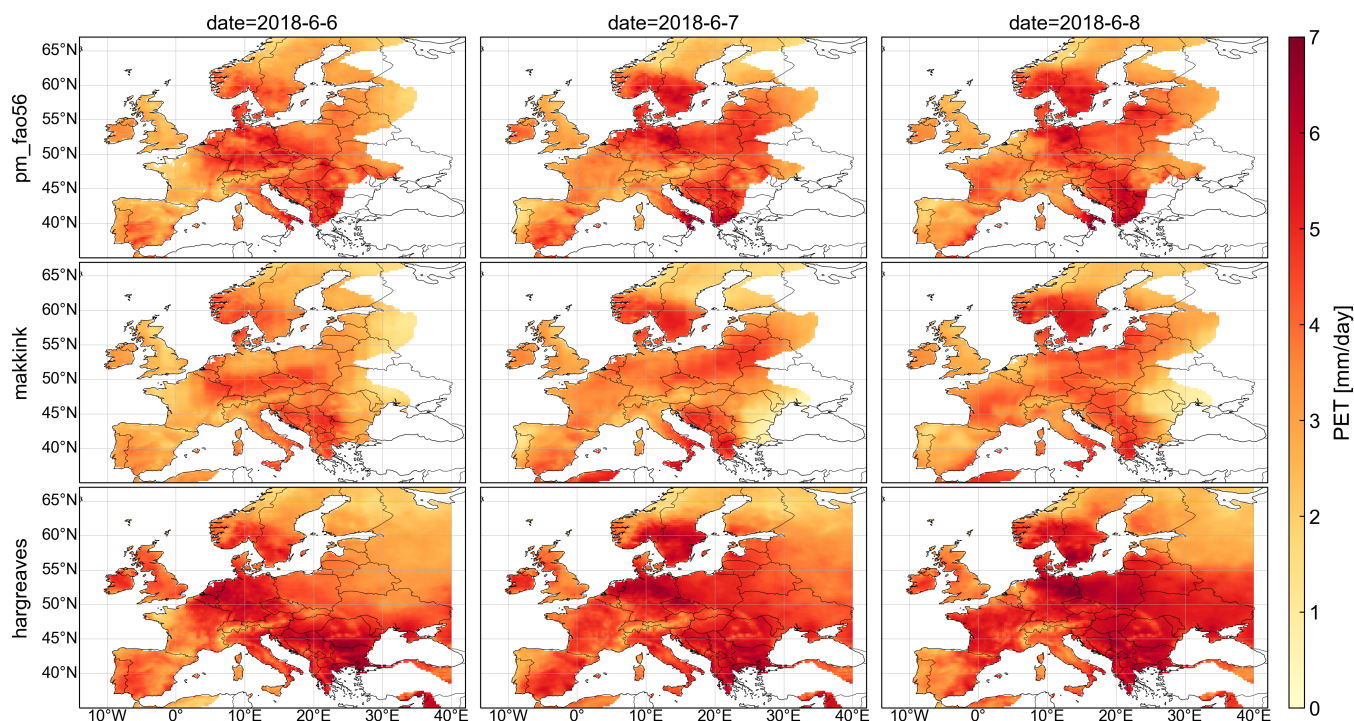
Figure 4. Daily PET estimates for Europe from 2018-6-6 to 2018-6-8 using meteorological data obtained from the E-OBS dataset (Cornes et al., 2018).

2018) for Europe. The application of *PyEt* on gridded datasets is illustrated for the FAO-56, Makkink, and Hargreaves method. `Xarray.DataArrays` are used as input data instead of `Pandas.Series`. *PyEt* methods will return the same data type, a `Xarray.DataArray`. The workflow is comparable to that in the first example, except that now the individual PET methods were used.

210   The results for the three methods and three time steps are shown in Figure 4. These again show that, depending on the PET method, results may differ, also spatially. Looking more closely at Figure 4, we can observe that the FAO-56 and Makkink method do not compute PET in eastern parts of Europe. The data do not include relative humidity and solar radiation for these areas, and thus PET cannot be computed using the FAO-56 or Makkink method. If NaN (not-a-number) values are present in the required input data for a *PyEt* method, the method also returns a NaN value. The Hargreaves method, on the other hand,
215   does not require solar radiation or relative humidity data. It can therefore be used to compute PET in the eastern parts of Europe. This example showed how *PyEt* can be applied to estimate PET using gridded data and demonstrated the benefits of using alternative PET methods when data such as radiation or relative humidity are missing.

3.3 Example 3: Calibration of PET models

The available input data often does not suffice to compute potential evapotranspiration with the Penman-Monteith equation.
220 This can be the case in data-scarce regions or time periods, or when using historical data or data from climate models. In such cases, alternative PET methods can be calibrated to the estimates obtained from the Penman-Monteith equation for a period when sufficient data is available. The calibrated method can then be used to estimate PET in periods of data scarcity. As concluded by several authors (Jensen and Allen, 2016; Valipour, 2015; Yang et al., 2021; Dlouhá et al., 2021), calibration of alternative models is often crucial to ensure that the model fits the regional climate. In this example, it is shown how the
225 calibration of temperature-based PET models affects the model uncertainty for studies focusing on current and past climates.

The approach is illustrated for the town of Graz, Austria, where the input data required for Penman-Monteith are only available from 2000 to 2021. Imagine, however, that for our study we also need potential evapotranspiration data for the period 1961 to 2021, but only temperature data is available (e.g., from the Spartacus temperature dataset (Hiebl and Frei, 2016)). Several steps are taken to calibrate the following five temperature-based methods: Oudin, Hargreaves, McGuiness-Bordne,
230 Hamon, and Blaney-Criddle. First, the PET for the period 2000-2021 is computed using the Penman-Monteith equation. In the second step, the coefficients of the temperature-based PET equations are estimated by calibrating the estimated PET from temperature-based methods to the Penman-Monteith PET. Calibration is done by minimizing the sum of the squared residuals between these two PET estimates, using SciPy's (Virtanen et al., 2020) *least_squares* method. In the third and final step, these calibrated coefficients are used to estimate the PET for the period 1961-2021.

235 Figure 5 shows the computed PET with default (row 1) and the calibrated coefficients (row 2). The model bias (mm/day) and the coefficient of determination (R^2) between simulated and observed (Penman-Monteith) PET show an improved model fit for all methods after calibration. The use of calibrated methods reduces the model bias, which is visually illustrated by the annual PET flux (composed of daily values) in the last column of Figure 5. Using the Spartacus temperature dataset (Hiebl and Frei, 2016), PET can now be estimated back to 1961 using the calibrated alternative PET methods.

240 3.4 Example 4: The effect of CO_2 on future PET estimates

In this example, it is shown how to account for changing environmental conditions affecting the PET flux when modelling the effects of climate change. Under a warmer and CO_2 richer future (Caretta et al., 2022), potential evapotranspiration tends to increase with increasing temperature (and vapor pressure deficit). A reduction in PET is expected under elevated CO_2 due to an increased stomatal resistance (Field et al., 1995; Ainsworth and Rogers, 2007). The increase in CO_2 is still commonly ignored
245 in PET models employed for climate change studies, although excluding its stomatal effect may lead to an overestimation of PET (Kingston et al., 2009; Milly and Dunne, 2016; Vremec et al., 2022; Riedel et al., 2023). The effect of temperature increases on PET can be easily modelled with all available PET methods, as temperature is an input for all methods. The CO_2 stomatal effect, however, can only be directly accounted for with the Penman-Monteith method (Liu et al., 2022). Using a CO_2-dependent stomatal resistance model implemented in *PyEt* (Yang et al., 2019), the effect of elevated CO_2 on stomatal
250 resistance can be considered (see Eq. 1). When calculating PET with alternative methods, Kruijt et al. (2008) and Trnka et al.
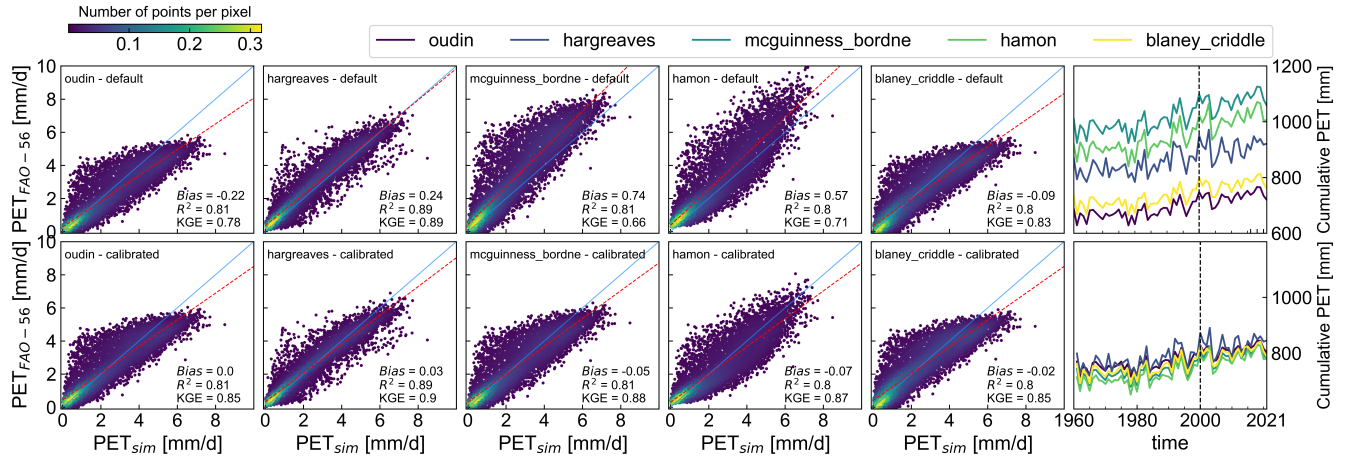
Figure 5. Density scatter plots comparing simulated and observed (FAO-56) PET for uncalibrated (row 1) and calibrated models (row 2). The last column shows the annual PET sums for the period 1961-2021 using uncalibrated (row 1) and calibrated models (row 2).

(2014) argued that an adjustment factor for the atmospheric CO_2 concentration (f_{CO_2}) can be used to account for the effect of elevated CO_2 concentrations on PET. The scaling factor can be obtained from literature values (Kruijt et al., 2008; Trnka et al., 2014). Alternatively, the factor can be calibrated using the Penman-Monteith equation together with the CO_2-dependent stomatal resistance model (Eq. 1) to match the local climate and vegetation:

$$\text{PET}_{CO_2} = f_{CO_2}\text{PET}_{300}$$

255
$$= (1 + S_{\text{PET}_{CO_2}}(CO_2 - 300))\text{PET}_{300} \tag{3}$$

where $S_{PET_{CO_2}}$ is the relative sensitivity of PET to CO_2, PET_{300} is the computed Penman-Monteith estimate at 300ppm [CO_2] (preindustrial concentration), while PET_{CO_2} is the computed Penman-Monteith estimate under elevated CO_2 concentration (Yang et al., 2019). Such relationships can be easily implemented in *PyEt*, and f_{CO_2} can be obtained by calculating PET_{300} and PET_{CO_2} with the Penman-Monteith equation (Eq. 1) at ambient and elevated CO_2 concentration, respectively.

260   Building on the previous example, the Graz study area served as a practical example to demonstrate the application of the calibrated models in assessing the impact of warming and elevated CO_2 concentration on PET based on the projected increase in temperature and CO_2 concentration from the representative concentration pathways (RCPs) (Van Vuuren et al., 2011). Daily PET was calculated for each RCP scenario (2.6, 4.5, 6.0, and 8.5) by adding the projected increase in temperature and CO_2 concentration to the existing data for 2020-2021. Figure 6 shows the increase in the average annual PET (aggregated from daily

265   values) under warming and elevated CO_2 concentrations according to the RCP scenarios. In figure 6c, the effects of elevated CO_2 concentration on PET were neglected, and only increases in temperature were considered. Similar to Milly and Dunne (2016), Yang et al. (2019), and Vremec et al. (2022), this example shows that neglecting the effect of elevated CO_2 on PET (Fig, 6-c) can lead to overestimation of PET under future conditions.
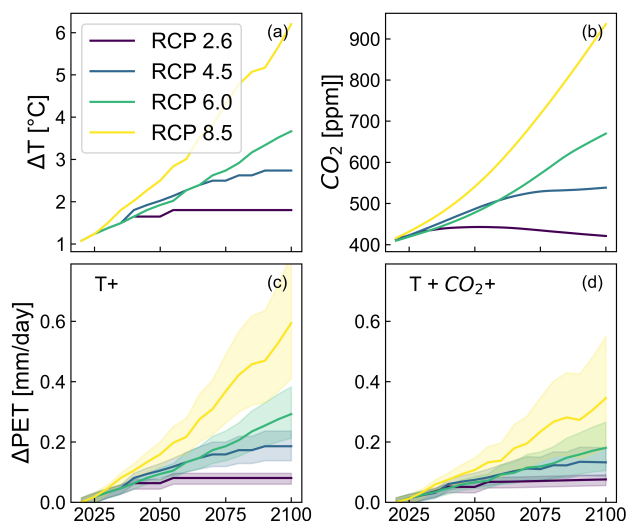
Figure 6. Projected increase in temperature (6-a) and atmospheric CO_2 concentration (6-b) under the RCP scenarios, and calculated increase in the average annual PET with warming (6-c), and PET with warming and elevated CO_2 concentration (6-d). The uncertainty bounds represent the 5th-95th percentile of the PET model ensemble.

4 Discussion

4.1 Improved handling of PET in scientific studies

Evapotranspiration data from lysimeter or eddy correlation measurements (Pastorello et al., 2020) are rare and, if available at all, only locally available for relatively short time periods. Thus, there is a widespread need to estimate evapotranspiration from more readily available meteorological data using (semi-)empirical approaches. In general, these approaches follow three steps, as outlined for example by Allen et al. (1998). Firstly, the potential evapotranspiration of a reference surface (hence reference evapotranspiration) is estimated using meteorological data. Secondly, a crop coefficient may be applied to transform the reference evapotranspiration into the potential crop evapotranspiration. Thirdly, a soil-water balance approach is used to account for reduced actual evapotranspiration if the soil-water storage is depleted. *PyEt* is designed to perform the first two steps. It can be easily complemented by soil-water balance approaches to calculate actual evapotranspiration. Hydrological models, however, often use PET directly as input.

Rainfall-runoff models represent one type of hydrological model where PET is commonly used as an input, either as gridded data in distributive models, or as a spatially aggregated values in lumped-parameter models. Some studies (e.g., Andréassian et al., 2004; Oudin et al., 2005; Sperna Weiland et al., 2012) found that PET had little impact on the performance of such models, and thus advocated the use of simplistic PET models. However, Jayathilake and Smith (2021) found that model performance was clearly sensitive to PET at sites where evapotranspiration was water limited. More importantly, the choice of the PET model has been shown to affect the results of hydrological projections in climate change impact assessments (Kay and

influential in the assessment of groundwater recharge (e.g., Bakundukize et al., 2011) and crop water demands (e.g., Webber
et al., 2016)), which – compared to runoff – are more directly linked to evapotranspiration. Thus, the selection of appropriate
PET models needs to account for the research context and variable of interest.

290   Bormann (2010) found that PET models that are based on the same or similar climate variables exhibit different sensitivity
to observed climate change. This finding suggests that appropriate PET models need to be specifically selected for the given
region of interest. Guo et al. (2017) provides pointers to examining which variables are likely to be the most important for a
particular location. For more detailed insights into the application of individual PET methods across various climates, refer to
Table A1 and the studies by Allen et al. (1998); McMahon et al. (2013); Jensen and Allen (2016); Yang et al. (2021); Pimentel

295   et al. (2023). The comparison of PET estimates for Europe shown in Figure 4 illustrates the spatial variability of differences
in PET estimates obtained from different methods; as can be seen, the magnitude and pattern of PET estimates are similar in
some regions (e.g., Scandinavia) but differ more strongly in others (e.g., Southeast Europe).

    As indicated above, the performance of PET models may vary depending on the region considered. Approaches that were
found applicable in one region may perform less well in other regions. In this case, PET models can be calibrated to a reference

300   data set by adjustment of the coefficients in the model equation, as shown in the third example. The reference data set can
either be observed evapotranspiration (e.g., from lysimeters) or PET obtained from a model considered to be reliable. This
has been illustrated by Example 3, where the coefficients of temperature-based models were adjusted to achieve the best fit
to the Penman-Monteith model. This approach can also be used to obtain consistent spatial distributions of PET. As shown in
Example 2 (Figure 4), the limited data availability for Eastern Europe did not allow the application of the FAO-56 or Makkink

305   method, while sufficient data was available for the Hargreaves method. Thus, one may consider calibrating the latter to one
of the former methods where these are applicable, and only then apply it to obtain estimates for the entire region. For a more
advanced calibration procedure, see for example Haslinger and Bartsch (2016).

    In many cases, the range of PET models that can potentially be employed is pre-determined by data availability. This may
be the case if historical records of climate data are to be used for the PET estimation, for example, as many weather stations

310   do not measure all climate variables included in the Penman-Monteith equation. Yet, this is also often the case in assessments
of hydrological impacts of climate change if projected climate variables have high uncertainty. Lai et al. (2022), for example,
concluded that the high uncertainty of wind speed projected in complex terrain may increase the uncertainty in PET, whereas
air temperature and solar radiation have low uncertainty and thus should be the parameters preferred in the PET model. Given
the climate variables for which data is available, Table 1 can be used to identify the PET models that come into consideration.

315   However, it is advised to evaluate the assumptions and limitations of the individual methods regarding their applicability
in the given case. Please refer to the comments in Table A1 and the references in Table 1 for this purpose. We generally
recommend applying all models that have been identified as suitable (PET model ensemble), but the purpose and specific
implementation of such a multi-model approach will depend on the research context. Example 4 (section 3.4) illustrated how
PET model ensembles can be used to include model uncertainties in PET projections under warming and elevated atmospheric

320   CO_2 concentration. Since the latter effect is frequently excluded in hydrological projections, Milly and Dunne (2016) and Yang

et al. (2019) advocate the inclusion of the effect of elevated CO_2 on stomatal resistance when estimating PET under warming and elevated atmospheric CO_2 concentrations.

To improve reliability and efficiency in estimating PET, it is crucial to use a reproducible workflow. Scripts provide an efficient way to document the modelling process and are an important step towards full reproducibility. As shown in the
325 examples, Jupyter Notebooks (Kluyver et al., 2016) provide a solution for publishing code, results, and explanations in a single document. As such, the presented package and its application in this paper are in line with the steps suggested by Hutton et al. (2016) to improve reproducibility in hydrological studies. To speed up adaptation of the methods and allow a faster transfer between research teams, formal procedures such as benchmarking (e.g., Maxwell et al., 2014) can help to ensure confidence in key complex codes.

330 ## 4.2 Building the PyEt community and outlook

As a community project, the success of *PyEt* depends on the uptake from and interaction with the community. This, in turn, depends on the ease of use and the trust in the project. Emphasis was put on designing a user-friendly, well-documented software, including various user examples, and extensive benchmark testing using continuous integration. Since the initial launch of *PyEt*, the package has already seen a good community uptake. Apart from applications of the software in projects
335 related to the Authors, which include estimating PET under conditions of warming and elevated CO_2 concentrations, assessing potential crop evapotranspiration, and providing inputs for hydrological models (e.g., Vremec et al., 2022; Forstner et al., 2022; Collenteur et al., 2023; Jemeljanova et al., 2023), *PyEt* has also been independently used by other researchers. These studies have utilized *PyEt* for a variety of purposes: integrating PET estimates with machine learning models for enhanced analytical capabilities (Vaz et al., 2022), and combining them with software for computing groundwater recharge and the water balance
340 (Hassanzadeh et al., 2023). The software has also played a role in evaluating hydroclimatic changes and generating regional PET estimates (e.g., Tercini and Mello Júnior, 2023; Aguayo et al., 2024). The quick uptake of the software by the community shows the need for this software.

The primary channel for communication with the *PyEt* community is GitHub, which provides several options for discussions, tracking code issues, and code development. Users are encouraged to ask questions in GitHub discussions and to report
345 potential issues, suggest improvements, and feature requests via the GitHub issue tracker. As a community project, we plan to continue to improve the existing code and develop new capabilities based on feedback and with help from the community. An example of developments that are currently underway is the adaptation of the current methods to also work for hourly data, allowing the estimation of hourly PET. Other future work will focus on improvements in usability and the inclusion of other alternative methods.

5 Conclusions

This paper introduced *PyEt*, a Python package for the estimation of daily potential evapotranspiration (PET). The package enables the inclusion of model uncertainty and climate change in the PET estimation in a consistent, tested, and reproducible environment. With *PyEt*, PET can be estimated using 20 different methods with just a few lines of Python code not only for (1D) time series but also for (3D) gridded data sets, which goes beyond existing tools for PET calculation. The examples described in this paper illustrate how *PyEt* can be used in geoscientific studies to (1) facilitate the characterization of model uncertainty using a multi-model approach (model ensembles); (2) calibrate PET models and apply them in data-scarce regions and time periods; (3) include the effects of warming and elevated atmospheric CO_2 concentrations. The use of Python scripts and Jupyter Notebooks ensure reproducibility and provides a transparent report of the PET computation process. We believe that *PyEt* will help improve the handling of PET and allow a more sophisticated and comprehensive consideration of PET in environmental studies, particularly those related to climate change.

Code and data availability. The Jupyter Notebook and data used in this study are available in the "examples" folder of the GitHub repository and also available on Zenodo (version v.1.3.1, DOI: 10.5281/zenodo.5896799). The authors welcome code contributions, bug reports, and feedback from the community to further improve the software. *PyEt* is free and open-source software available under the MIT license. Source code is available at the project's home page on GitHub. Full documentation is available on ReadTheDocs. *PyEt* is meant as a community project, and the Authors welcome contributions and feedback to continue to improve and develop the project are welcome.

Appendix: PET Methods - Climate suitability and applications

Table A1. Overview of PET methods: climate suitability, applications, and limitations. ET_0 - reference crop/surface ET, PET_C - potential crop/surface ET, PET_{OW} - potential ET for open water, PET_{SL} - potential ET for shallow lakes, PET_{RR} - potential ET for rainfall-runoff modelling. Based on Allen et al. (1998); McMahon et al. (2013); Jensen and Allen (2016); Yang et al. (2021); Pimentel et al. (2023)

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Method name	Application	Climate	Limitations/Comments
Penman	PET_{OW}, PET_{SL}, PET_{RR}	All climates	High input data requirement
Penman-Monteith	ET_0, PET_C, PET_{RR}	All climates	High input data requirement
FAO-56	ET_0	All climates	High input data requirement
Priestley-Taylor	PET_C, PET_{RR}	Temperate/polar	Calibration recommended for semi-arid and arid regions; often underestimates in high vapor pressure deficit areas.
Kimberly-Penman	ET_0-alfalfa	Temperate/continental	High input data requirement
Thom-Oliver	ET_0	Temperate/continental	High input data requirement
Blaney–Criddle	ET_0, PET_{RR}	Temperate	Overestimates in calm, moist, shaded areas; underestimates in windy, dry, sunny ones.
Hamon	PET_C	All climates	Recommended regional calibration.
Romanenko	PET_C, PET_{RR}	All climates	Best recommended model for PET in China.
Linacre	PET_C	All climates	Recommended regional calibration.
Haude	PET_C	All climates	Recommended regional calibration.
Turc	ET_0, PET_C	Humid	Underestimates in areas with large daily vapor pressure deficits.
Jensen–Haise	PET_0, PET_{RR}	Continental	Recommended regional calibration.
McGuinness–Bordne	PET_C, PET_{RR}	All climates	Recommended regional calibration.
Hargreaves	ET_0, PET_{RR}	Tropical/dry	Not recommended in windy and/or low RH_{min} regions. May overestimate in humid climates.
FAO-24	ET_0	All climates	-
Abtew	PET_C	Humid	Poor performance in arid climates.
Makkink	PET_C, PET_{RR}	All climates	Originally designed for Western Europe, this method may underestimate higher PET.
Oudin	PET_{RR}	All climates	Mainly used for hydrological modelling.

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370 *Competing interests.* The authors declare no conflict of interest.

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